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# **FUNDAMENTAL ASPECTS OF DISLOCATION THEORY**

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UNITED STATES DEPARTMENT OF COMMERCE

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# FUNDAMENTAL ASPECTS OF DISLOCATION THEORY

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# VI FIELD THEORIES I

*Chairman:*

**E. KRÖNER**



# THE PROBLEM OF NON-LOCALITY IN THE MECHANICS OF SOLIDS: REVIEW ON PRESENT STATUS

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The concept of non-locality, in particular with reference to the mechanics of solids, is discussed. A brief report is given on the derivation of the non-local theory of elasticity from atomic lattice theory. In addition some simple solutions of this theory, concerning the interaction of dilatation centers and wave propagation, are quoted. A generalization of the theory which would include dislocations is indicated.

Key words: Dilatation centers; lattice statics; non-local theories; solid mechanics; wave propagation.

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## I. Introduction

Except for relativistic and nuclear fission effects, quantum electrodynamics and quantum mechanics are the correct theories for handling the problems of solid state physics, including those of dislocations. Since they have small masses, electrons in a solid move so much faster than the nuclei that in a rather good approximation—the so-called adiabatic approximation—the electrons can be considered to be in dynamic equilibrium with respect to the configuration of the nuclei at any time. In that case, a potential energy  $U$  exists which depends on the coordinates of the nuclei alone and which can be obtained in principle from the solution of the corresponding many-electron 'problem'. The dependence of the potential energy on the nuclei alone is the indispensable basis, for instance, for the lattice theories presently in use. Since the calculation of  $U$  is extremely involved, one is often content to work with  $U$  assumed on the ground of experimental observation.

With this potential energy, it is quite simple to establish the quantum mechanical equations of motion for the nuclei. Quantum mechanics rather than classical mechanics is necessary to describe the motion of the nuclei in certain situations, for instance in the cases of interactions among phonons and of those between phonons and lattice defects. On the other hand, classical equations of motion should be good enough to describe

more macroscopic effects at temperatures that are not too low. The interaction problem of lattice defects which are some distance apart would belong to this class of problems.

The above remarks are not novel. They just remind us of the restrictions involved from the very beginning in the classical theory of atomic lattices.

In recent time several workers—Krumhansl, Mindlin, Toupin, Kunin, myself, and others—have reconsidered the old problem of deriving continuum mechanics, in particular elasticity theory, from the atomic lattice theory. A fundamental insight has been gained in these attempts: The conventional elasticity theory is a very special case of a more general continuum elasticity theory. The two effects which are included in this general elasticity theory, but not in the conventional theory, are:

(1) the non-primitivity (or polar) effect, which is found in non-primitive crystal lattices. The deformation of such bodies can be described by  $n$  displacement fields if  $n$  is the number of atoms in the elementary cell [1]. In addition to the acoustical branches, one finds the optical branches of the vibration spectrum which are already known from the calculations of the lattice theory.

(2) the non-locality effect. This effect takes into account the finite range of the atomic cohesive forces. It is incorporated in the form of a non-local constitutive law which gives the response at point  $\mathbf{r}$  in the body in dependence on the strain at the points  $\mathbf{r}'$  all over the body.

Since this paper has been prepared specifically for the session on the non-local theory, the complications implied by the effect of type (1) above are omitted. Section II brings some general considerations on non-locality. Section III contains comments on the derivation of the non-local continuum theory from the lattice theory. In section IV are reported results on the solution of “non-local” problems. Some remarks in section V on possible implications for dislocation theory conclude the report.

## II. General Remarks on Non-Locality

Non-local field theories have been used by physicists for about 30 years. The concept of non-locality was introduced in the hope of removing some of the divergencies which appear in the fundamental physical theories such as quantum electro-dynamics, meson theories, etc. Such theories can be based on a Lagrange density, a function of  $\mathbf{r}$ , which is an integral over all positions  $\mathbf{r}'$  of the region. The Lagrange function itself, and hence also the energy, is then a double volume integral over  $\mathbf{r}$  and  $\mathbf{r}'$ , which means that interactions of a certain range play a role in the behaviour of the fields.

Let us now consider the response of a body subjected to a deformation. The cohesive forces are of electrical nature. They act on the nuclei and

electrons which constitute the body. Assume that one nucleus at point  $\mathbf{r}$  suffers a small displacement  $u_i$ . According to elasticity theory, another nucleus at point  $\mathbf{r}'$  will notice the displacement at  $\mathbf{r}$  in the moment when the sound wave emitted by the displacement at  $\mathbf{r}$  has reached  $\mathbf{r}'$ . However, in reality the movement of the nucleus at  $\mathbf{r}$  will change the electric fields<sup>1</sup> and this change spreads out with the velocity of light. In this way the nucleus at  $\mathbf{r}'$  feels the displacement of the nucleus at  $\mathbf{r}$  after a time interval which is extremely short compared to those time intervals which could possibly be of interest in applications of elasticity theory. This means that the displacement of a nucleus at  $\mathbf{r}$  leads to a practically instantaneous response at all points  $\mathbf{r}'$  in the body.

If the foregoing considerations are correct, one is compelled to question the validity of the conventional elasticity theory. The important point is that the change in the electric field due to a small displacement of a particle has a certain range which depends on the particular material. In some materials this range is of the order of an atomic distance; in others it is of larger order. To the latter materials belongs the group of the metals, for instance. One finds that the conventional elasticity theory is good as long as the true solution of a problem, when given in terms of Fourier integrals or sums, involves, with essential amplitudes, only such wavelengths which are large compared to the range of the cohesive forces. This is the wavelength interval in which dispersion is negligible.

On the other hand, it is clear that in order to describe phenomena on an atomic scale no theory can be used which overlooks the discreteness of the matter. In other words: the non-local continuum theory which extends the conventional elasticity theory towards shorter wavelengths ceases to apply where the wavelengths become comparable with the lattice parameter. Here a lattice type theory must be applied. Since classical theories usually fail on an atomic scale, it seems that classical lattice theories do not possess a much larger range of applicability than classical (non-local) continuum theories.

Another feature of the non-local theory deserves to be mentioned. By assuming that the response to a displacement of a nucleus is spread out instantaneously over the range of interaction, one practically eliminates the electric part from the theory.<sup>2</sup> The electric parameters are then comprised into the material tensors by which the various materials are distinguished.

More exact would be a theory which includes the finiteness of the velocity of light. In this way electric fields and polarizations would come in. In addition to stress and strain they describe the state of the body. To

<sup>1</sup> We think here of the fields on a microscopic scale.

<sup>2</sup> Hence this theory is not suitable to treat piezo-electric materials in which macroscopic electric fields are essential state variables.

some extent the complication of having more state variables is only ostensible. In fact, the response of the body is no longer non-local in the sense that other parts of the body feel instantaneously what happens at one point in the body. So the combined elasto-electric theory is local;<sup>3</sup> hence one has differential equations instead of the (fewer) integrodifferential equations of the non-local theory. An advantage of the non-local formulation seems to be that the approximation of infinite light velocity brings a considerable simplification into the problem.

### III. Non-Local Elasticity: Derivation From Atomic Lattice Theory

The non-local theory can be formulated without reference to the atomic lattice. The derivation from lattice theory leads to the same result, however with an added advantage: The material tensors appear expressed in terms of the atomic potentials, which are accessible for quantum mechanical calculation or experimental observation. Hence quantitative predictions can be made about the importance of the nonlocal effects.

The derivation from lattice theory has been treated by several authors (see, e.g., refs. [2 and 3]). Here I refer to a paper of Dr. Datta and myself which was prepared for this conference (see p. 737 of these Proceedings). The theory is developed in linear approximation and for the finite body. Hence we have not assumed a homogeneous lattice. The crucial point in such considerations is the application of rigorous mathematical formulas for converting lattice sums into integrals. Pursuing a suggestion of J. Kestin,<sup>4</sup> we have worked out a three-dimensional version of the Euler-MacLaurin formula and applied this to the potential energy of the crystal lattice. The continuized form of the potential energy reads, in cartesian coordinates,

$$U = \frac{1}{2} \int \int c_{ijkl}(\mathbf{r}, \mathbf{r}') \beta_{ij}(\mathbf{r}) \beta_{kl}(\mathbf{r}') dV dV' \quad (1)$$

where  $\beta_{ij} = \partial_i u_j$  is the displacement gradient (or distortion) and  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  is the material tensor function which is determined by a set of differential equations and boundary conditions in which the atomic coupling parameters appear as the sources. It is shown that the symmetry relations (observe the dashes)

$$c_{ijkl}(\mathbf{r}, \mathbf{r}') = c_{jikl}(\mathbf{r}, \mathbf{r}') = c_{ijlk}(\mathbf{r}, \mathbf{r}') = c_{klij}(\mathbf{r}', \mathbf{r}) \quad (2)$$

<sup>3</sup> This is true for ionic and van der Waals crystals but not for metals because in metals already the electric theory alone is non-local. The reason is that here the electrons travel long distances.

<sup>4</sup> Oral comment on a lecture given by the author at Brown University in 1966.

can (but need not) be superimposed on the tensor function  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$ . In this case the distortions can be replaced by the strains in eq (1). If one defines a stress tensor function by  $\sigma_{ij} = \delta U / \delta \epsilon_{ij}$ , where  $\epsilon_{ij}$  is the strain tensor, one obtains a non-local stress-strain relation in the form

$$\sigma_{ij}(\mathbf{r}) = \int c_{ijkl}(\mathbf{r}, \mathbf{r}') \epsilon_{kl}(\mathbf{r}') dV'. \quad (3)$$

Since real materials have strong short-range repulsive forces between neighbour ions, it seems not only mathematically but also physically sensible to split the tensor function  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  into a short-range and a long-range part by setting

$$c_{ijkl}(\mathbf{r}, \mathbf{r}') = C_{ijkl}(\mathbf{r}) \delta(\mathbf{r}, \mathbf{r}') + c_{ijkl}^*(\mathbf{r}, \mathbf{r}') \quad (4)$$

where  $\delta$  is the Dirac's delta function. In this way the stress-strain law obtains the form of a Fredholm integral equation for the strains  $\epsilon_{kl}$ , given the stresses  $\sigma_{ij}$ :

$$\sigma_{ij}(\mathbf{r}) = C_{ijkl}(\mathbf{r}) \epsilon_{kl}(\mathbf{r}) + \int c_{ijkl}^*(\mathbf{r}, \mathbf{r}') \epsilon_{kl}(\mathbf{r}') dV'. \quad (5)$$

This equation has a solution for quite general kernels  $c_{ijkl}^*(\mathbf{r}, \mathbf{r}')$ . The solution can be written in the form of the inverse constitutive law

$$\epsilon_{ij}(\mathbf{r}) = S_{ijkl}(\mathbf{r}) \sigma_{kl}(\mathbf{r}) + \int s_{ijkl}^*(\mathbf{r}, \mathbf{r}') \sigma_{kl}(\mathbf{r}') dV'. \quad (6)$$

The existence of this solution seems to be an indispensable requirement for the physical consistency of the present theory (see the contribution of Dr. Barnett at this conference).

#### IV. Solutions of the Non-Local Elasticity Theory

In some generality it can be stated: The determination of the stress for given stress sources exhibits increasing difficulty in the sequence: conventional elasticity theory  $\rightarrow$  non-local elasticity theory  $\rightarrow$  lattice theory. This observation justifies the application of conventional elasticity theory in many situations. It justifies the use of non-local elasticity theory at other occasions.

To give an example: The interaction energy of two dilatation centers of strength  $P$  and  $Q$  at distance  $r = |\mathbf{r}_P - \mathbf{r}_Q|$  in an infinite isotropic and homogeneous continuum with non-local response of the form (6) where

$$S_{ijkl}^*(\mathbf{r}, \mathbf{r}') = S_{ijkl} g^*(| \mathbf{r} - \mathbf{r}' |) \quad (7)$$

has been calculated to be

$$\frac{-1}{\lambda + 2\mu} PQg^*(r) \quad (8)$$

where  $\lambda, \mu$  are the Lamé's constants. In the case of van der Waals interaction between the particles of the body, one finds  $g^*(r) \sim r^{-5}$ . In this case, the interaction of the two dilatation centers is the same as the van der Waals interaction of two atoms or molecules in a gas.

Transition to local response implies  $g^* = 0$ . So we recover the well-known result: No interaction of two dilatation centers in an infinite, isotropic, homogeneous continuum with local response.

It is a quite different question as to what extent such a dilatation center can be representative for a point defect in a crystal lattice.

The above solution was obtained in a very simple way. Use of computers was not necessary. The existence of simple solutions can enable one to find phenomena of a new type which are not observed in continua with local response.

As an example, I mention the problem of wave propagation in medias with non-local response. This problem is the subject of the paper of Kunin and Waisman prepared for this conference. Using Green's function techniques, the authors find new types of damped and undamped surface waves. They also obtain dispersion and maximum frequencies for undamped waves. Since all these phenomena also occur in the lattice theory, we see that the non-local continuum theory has incorporated essential parts of the information of the lattice theory.

## V. Reference to Dislocations

In the linearized lattice theory, the potential energy is expressed in terms of small displacements from an equilibrium state, usually the perfect crystal state. The potential energy of a dislocated crystal cannot be given in such a form, since large displacements are necessary to produce a dislocated state or even a small change of a dislocated state. Besides this, the displacements during plastic deformation are in a way less continuous than they are in the situations governed by conventional lattice theory. In fact, the relative displacement of two lattice planes adjacent to a glide plane of a dislocation is of higher order of magnitude than the relative displacement of other neighbouring lattice planes. This leads to difficulties in the application of the Euler-Maclaurin continuization: Neither by this nor by any other procedure one can derive a macroscopically continuous displacement field from the displacements of the nuclei.

It has been well known for a long time that, in the presence of continuous distributions of dislocations, the notion of displacement field does not exist. It is possible to define elastic strains  $\epsilon_{ij}$  and distortions  $\beta_{ij}$ , however. Since the curl of  $\beta_{ij}$  is equal to the dislocation density, one finds that only in the absence of dislocations  $\beta_{ij}$  has the simple form  $\partial_i u_j$  in which it had appeared in the potential energy eq (1)

$$U = 1/2 \int \int c_{ijkl}(\mathbf{r}, \mathbf{r}') \beta_{ij}(\mathbf{r}) \beta_{kl}(\mathbf{r}') dV dV'. \quad (9)$$

In the cited paper of Dr. Datta and myself, an explicit expression was given for the material tensor function  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  in terms of the atomic potentials (eqs (20, 32-34)). It was argued that this  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  can be complemented by an additional  $c'_{ijkl}(\mathbf{r}, \mathbf{r}')$ , say, which does not contribute to the energy in eq (9) as long as  $\beta_{ij}$  is a displacement gradient. It would contribute, however, if the curl of  $\beta_{ij}$  would not vanish. The potential energy then would contain a part which can be put into the form

$$\int \int a_{inkq}(\mathbf{r}, \mathbf{r}') \alpha_{iu}(\mathbf{r}) \alpha_{kq}(\mathbf{r}') dV dV' \quad (10)$$

where  $e_{jmn} \partial_m \beta_{ij}$  was replaced by the dislocation density tensor  $\alpha_{in}$ . The tensor function  $a_{inkq}(\mathbf{r}, \mathbf{r}')$  follows from

$$c_{ijkl}(\mathbf{r}, \mathbf{r}') = e_{juun} e_{lpq} \partial_{ju} \partial_{lp} a_{inkq}(\mathbf{r}, \mathbf{r}') \quad (11)$$

where  $e_{jmn}$  is the alternating tensor. Hence, apart from surface terms, the additional potential energy is the mutual interaction energy of the dislocations. However, in this interpretation, some precaution is necessary. The point is, that a dislocation element at  $\mathbf{r}'$ , say, feels a small displacement of a dislocation element at  $\mathbf{r}$  firstly by the change of the electric field and secondly by the change of the elastic field. Light and sound velocity are here important as explained in other connection in section 2. Further investigation on this seems necessary.

If we use the decomposition formula

$$\beta_{ij} = \partial_i u_j + e_{ikl} \partial_k \zeta_{lj} \quad (12)$$

in the potential energy (9) and write down a kinetic energy in terms of the potentials  $u_j$  and  $\zeta_{lj}$ , then we can obtain equations of motion by application of the Lagrange formalism. Because the motion of dislocations is always accompanied by irreversible processes, I do not believe in the Lagrange method when it is applied to dislocations. Notwithstanding, I think that one point comes out clearly from this consideration: There are dynamical equations for the potentials  $u_j$  and  $\zeta_{lj}$ . This result shows

that *two* types of motions are essential in a dislocated body: The motion of the matter and the motion of the defects. Both motions possess a specific inertia. For this reason all the so-called dynamical theories of dislocations which work with three equations of motion, are, if not wrong, at least incomplete.

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# NON-LOCAL THEORY OF ELASTICITY FOR A FINITE INHOMOGENEOUS MEDIUM—A DERIVATION FROM LATTICE THEORY

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In the linear theory of non-local elasticity the strain energy can be written as a double volume integral summing up the interactions of pairs of mass elements. The properties of the material, in this case, are described by a two-point-tensor function  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$ . It is found that for finite bodies  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  does not have the symmetries of the (Hooke's) elasticity tensor  $C_{ijkl}$  of the local theory. However, the symmetries of this tensor function are sufficient to exclude the rotations from the strain energy expression. It is shown that with the help of the elastic Green's function one can express  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  in terms of force constants of the lattice. It is also shown that an infinite homogeneous body is not a suitable model either for the non-local or for the local theory, because in this case  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  as well as  $C_{ijkl}$  obey the Cauchy relations.

Key words: Green's tensor; Hooke's elasticity, non-local elasticity; solid mechanics.

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## I. Introduction

The study of the mechanical behaviour of crystals has from the very beginning been approached from two different viewpoints, which have resulted respectively in the phenomenological theory and the atomic theory. The former is based on the concept that the internal forces of the body are contact forces and, therefore, the total energy of the solid is obtainable as the sum of the energies of the individual volume elements into which it can be subdivided. It is obvious that these conditions can be incorporated for a crystal with lattice structure only if the volume elements under consideration are sufficiently large in comparison to the range of interatomic forces in the solid. The range of applicability of this theory is, therefore, limited and its results can be expected to be sustainable only in relation to phenomena involving large volume elements, such as the propagation of waves of wavelengths large enough compared to the range of interatomic forces.

A more faithful description of bodies requires more elaborate continuum theories, which enable us to explain certain facts which elude the classical theory altogether. For instance, in the lattice theory of elasticity one usually deals with frequency versus wavelength curves, dispersion of waves, surface effects, defect interaction, and so on. To justify a generalized continuum theory of elasticity, then, we must be able to provide simpler methods for some of the problems that are important in the lattice theory.

We have shown earlier [1] how a simple and straightforward generalization of the classical theory of elasticity is obtained by converting the lattice theory of Bravais crystals into a continuum theory. The resulting theory is of non-local character because the lattice theory takes into account a finite range of interatomic forces from the very beginning. The procedure used in our first work (and in that of Kunin [2]) to convert the discrete lattice theoretical expressions into an integral form used the idealization of infinite homogeneous crystals. In real problems, however, the crystals are finite and therefore inhomogeneous, at least always in the boundary layer. We shall see in section III that the idealization of the infinite homogeneous crystal leads to particular difficulties in the here applied Born-Huang formalism. Hence it should be avoided.

It is the purpose of this paper to investigate the relationship between the lattice theory and the continuum theory of the elastic behaviour of finite Bravais crystals.<sup>1</sup> In particular we establish the symmetry correspondence between the elastic parameters of the continuum theory and those obtained from the lattice theory. This is achieved by the same method which was used by Kröner [3] in the case of infinite homogeneous crystals.

## II. The Potential Energy in Lattice and Continuum Theory

As is usual in the (harmonic) lattice theory,<sup>2</sup> we write the potential energy  $U$  of the deformed lattice as a bilinear form in the displacements

$$U = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} \Phi_{ik}^{\mathbf{r}\mathbf{r}'} u_i u_k'. \quad (1)$$

Here  $u_i$  and  $u_k'$  are Cartesian components of the displacements of the particles at points  $\mathbf{r}$  and  $\mathbf{r}'$  respectively, and the  $\Phi_{ik}^{\mathbf{r}\mathbf{r}'}$  are the coupling

<sup>1</sup>The complications implied by non-primitiveness of the lattice have recently been discussed by Baumgarte and Kröner [4].

<sup>2</sup>See, e.g., Leisfried [5].

parameters. Observe the obvious symmetry of the parameters:

$$\Phi_{ik}^{rr'} = \Phi_{ki}^{r'r} . \quad (2)$$

In order to convert the sum in (1) into an integral, we apply the (rigourous) Euler-Maclaurin formula, which in the three-dimensional form reads

$$\sum_r f^r = \int_V \frac{f(\mathbf{r})}{V_0(\mathbf{r})} dV + \frac{1}{2} \int_S \frac{f(\mathbf{r})}{S_0(\mathbf{r})} dS + \dots . \quad (3)$$

Here  $f(\mathbf{r})$  is a continuous function which coincides with the discrete values  $f^r$  to be summed at the lattice points  $\mathbf{r}$ ;  $V_0(\mathbf{r})$  is the volume of the elementary cell, which depends on the position if the lattice is inhomogeneous; and  $S_0(\mathbf{r})$  is the contribution to the surface of the cell at point  $\mathbf{r}$  on the surface.<sup>3</sup> Among the terms omitted in eq (3) the line integral and the summation over corner points become effective only if the number of atoms is very small. The other terms containing the derivatives can be omitted only if  $f(\mathbf{r})$  varies sufficiently slowly. This can be made more precise as follows. Using Taylor's expansion we have

$$f(\bar{\mathbf{r}}) = f(\mathbf{r} + \mathbf{a}) = f(\mathbf{r}) + a_i \partial_i \bar{f} + \dots$$

where  $\mathbf{a}$  is the primitive lattice vector and

$$\partial_i \bar{f} = \frac{\partial f(\bar{\mathbf{r}})}{\partial \bar{x}_i} \Big|_{\bar{\mathbf{r}} = \mathbf{r}}.$$

The terms containing the derivatives can be neglected if the condition

$$|a_i \partial_i \bar{f} / f(\mathbf{r})| \ll 1 \quad (4)$$

is satisfied. Thus the formula given by (3) can be considered as a generalization of trapezoidal rule of integration.

In our application then two assumptions must be valid:

1. The variation of displacement  $u_i(\mathbf{r})$  is small, which is the same thing as saying that the difference in displacements  $|\Delta \mathbf{u}|$  of two neighbouring atoms should be small when compared with the nearest neighbour distances. Of course, this is the case in any linear theory.

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<sup>3</sup> A detailed derivation of eq (3) was worked out by B. K. Datta and is given in D. Kessel [6].

2. We must assume weak inhomogeneity, so that the variation of  $\Phi_{ik}(\mathbf{r}, \mathbf{r}')$ , the continuous counterpart of  $\Phi_{ik}^{rr'}$ , is small enough to satisfy the condition (4).

Applying eq (3) to eq (1) we obtain

$$\begin{aligned} U = & \frac{1}{2} \int \int \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{V_0(\mathbf{r})V_0(\mathbf{r}')} u_i(\mathbf{r}) u_k(\mathbf{r}') dV dV' \\ & + \frac{1}{4} \int \int \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{V_0(\mathbf{r})S_0(\mathbf{r}')} u_i(\mathbf{r}) u_k(\mathbf{r}') dV dS' \\ & + \frac{1}{4} \int \int \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{S_0(\mathbf{r})V_0(\mathbf{r}')} u_i(\mathbf{r}) u_k(\mathbf{r}') dS dV' \\ & + \frac{1}{8} \int \int \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{S_0(\mathbf{r})S_0(\mathbf{r}')} u_i(\mathbf{r}) u_k(\mathbf{r}') dS dS' \end{aligned} \quad (5)$$

Now let us introduce a two-point tensor function  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  defined by the following set of equations

$$\partial_j \partial'_l c_{ijkl}(\mathbf{r}, \mathbf{r}') = \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{V_0(\mathbf{r}) V_0(\mathbf{r}')} \quad (6)$$

$$n_j \partial'_l c_{ijkl}(\mathbf{r}, \mathbf{r}') = -\frac{1}{2} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{S_0(\mathbf{r}) V_0(\mathbf{r}')} \quad (7)$$

$$n'_l \partial_j c_{ijkl}(\mathbf{r}, \mathbf{r}') = -\frac{1}{2} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{V_0(\mathbf{r}) S_0(\mathbf{r}')} \quad (8)$$

$$n_j n'_l c_{ijkl}(\mathbf{r}, \mathbf{r}') = -\frac{1}{4} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{S_0(\mathbf{r}) S_0(\mathbf{r}')} \quad (9)$$

Where  $n_j$  is the external unit vector normal to the surface  $S$  and  $\partial_j = \partial/\partial x_j$ . Substitution of eqs (6) to (9) in (5) leads to the result

$$U = \frac{1}{2} \int \int c_{ijkl}(\mathbf{r}, \mathbf{r}') (\partial_j u_i) (\partial'_l u'_k) dV dV'. \quad (10)$$

As is clear from our derivation and from the form (10) of the potential energy, the two-point tensor function  $c_{ijkl}(\mathbf{r}', \mathbf{r})$  contains the whole information about the material properties. The dependence on the two points  $\mathbf{r}$  and  $\mathbf{r}'$  expresses the non-local character of the atomic cohesive forces of the body. Observe the obvious symmetry

$$c_{ijkl}(\mathbf{r}, \mathbf{r}') = c_{klji}(\mathbf{r}, \mathbf{r}'). \quad (11)$$

### III. Symmetry of the Material Tensor $c_{ijkl}(\mathbf{r}, \mathbf{r}')$

It can easily be shown that the tensor functions  $c_{ijkl}$  are not defined uniquely by eqs (6) to (9). However, it is clear from our derivation that it suffices to have any solution of eqs (6) to (9) in order to obtain a workable theory. A particularly useful choice would be one which satisfies the additional symmetry relations

$$c_{ijkl}(\mathbf{r}, \mathbf{r}') = c_{jikl}(\mathbf{r}, \mathbf{r}') = c_{ijlk}(\mathbf{r}, \mathbf{r}') \quad (12)$$

because in that case the strains

$$\epsilon_{ij} = 1/2 (\partial_j u_i + \partial_i u_j) \equiv (\text{Def})_{ijk} u_k \quad (13)$$

can replace the displacement gradients in eq (10).  $(\text{Def})_{ijk}$  in eq (13) is the deformation operator defined by

$$(\text{Def})_{ijk} \equiv 1/2 (\delta_{ik} \partial_j + \delta_{jk} \partial_i). \quad (14)$$

In order to obtain a unique solution, the further restrictions

$$(\text{Ink})_{ikmn} c_{ijkl}(\mathbf{r}, \mathbf{r}') = 0, (\text{Ink}')_{jlmn} c_{ijkl}(\mathbf{r}, \mathbf{r}') = 0 \quad (15)$$

will be imposed on  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$ . Here  $(\text{Ink})_{ikmn}$  is the incompatibility operator defined as

$$(\text{Ink})_{ikmn} \equiv \epsilon_{ipm} \epsilon_{kqn} \partial_p \partial_q. \quad (16)$$

The restrictions (15) are physically sensible. In fact, any other solution of eqs (6) to (9), (11), and (12) will differ from the solution which satisfies eqs (15) by a part which does not contribute to the energy in eq (10).<sup>4</sup>

Using the identity

$$(\text{Ink})_{ikmn} (\text{Def})_{mnp} \equiv 0 \quad (17)$$

it can easily be shown (ref. [7]) that eq (15) has the general solution

$$c_{ijkl}(\mathbf{r}, \mathbf{r}') = (\text{Def})_{ikm} (\text{Def}')_{jln} a_{mn}(\mathbf{r}, \mathbf{r}') \quad (18)$$

<sup>4</sup> It would contribute if the displacement gradients would be replaced by more general second rank tensors (sometimes called distortions), as it is done in the theory of self stresses, for instance in the theory of dislocations.

where due to eq (11) the auxiliary potential  $a_{mn}(\mathbf{r}, \mathbf{r}')$  should possess the symmetry

$$a_{mn}(\mathbf{r}, \mathbf{r}') = a_{nm}(\mathbf{r}', \mathbf{r}). \quad (19)$$

In a different notation, eq (18) is rewritten as

$$\begin{aligned} c_{ijkl}(\mathbf{r}, \mathbf{r}') &= \partial_j \partial_l' a_{ik}(\mathbf{r}, \mathbf{r}') + \partial_i \partial_l' a_{jk}(\mathbf{r}, \mathbf{r}') \\ &\quad + \partial_j \partial_k' a_{il}(\mathbf{r}, \mathbf{r}') + \partial_i \partial_k' a_{jl}(\mathbf{r}, \mathbf{r}') \end{aligned} \quad (20)$$

In the following we shall derive a unique solution for the auxiliary potential  $a_{ik}(\mathbf{r}, \mathbf{r}')$ .

First we substitute eq (20) in the set of eqs (6) to (9) and obtain

$$D_{ij} D'_{kl} a_{jl}(\mathbf{r}, \mathbf{r}') = \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{V_0(\mathbf{r}) V_0(\mathbf{r}')} \quad (21)$$

$$D_{ij} N'_{kl} a_{jl}(\mathbf{r}, \mathbf{r}') = -\frac{1}{2} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{V_0(\mathbf{r}) S_0(\mathbf{r}')} \quad (22)$$

$$N_{ij} D'_{kl} a_{jl}(\mathbf{r}, \mathbf{r}') = -\frac{1}{2} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{S_0(\mathbf{r}) V_0(\mathbf{r}')} \quad (23)$$

$$N_{ij} N'_{kl} a_{jl}(\mathbf{r}, \mathbf{r}') = \frac{1}{4} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{S_0(\mathbf{r}) S_0(\mathbf{r}')} \quad (24)$$

where

$$D_{ij} \equiv \delta_{ij} \partial_m \partial_m + \partial_i \partial_j, \quad N_{ij} \equiv \delta_{ij} n_m \partial_m + n_j \partial_i \quad (25)$$

and the primed  $D$  and  $N$  are the corresponding quantities taken with respect to the primed operators. Observe that  $D$  and  $N$  are special cases of the operators

$$D_{ik} = C_{ijkl} \partial_j \partial_l, \quad N_{ik} = C_{ijkl} n_j \partial_l \quad (26)$$

which play an important role in the general theory of elasticity, in particular in the application of Green's method to elastic problems.<sup>5</sup> In fact, the expressions (25) are obtained from (26) if one assumes  $C_{ijkl}$  to be an isotropic elasticity tensor with Lamé's constants  $\lambda = 0$ ,  $\mu = 1$ .

<sup>5</sup> See, e.g., the article of A. Seeger in ref. [8], especially pp. 516 and 517.

The equations (21) to (24) can be simplified by making the substitution

$$\begin{aligned} D'_{kl} a_{jl}(\mathbf{r}, \mathbf{r}') &= b_{jk}(\mathbf{r}, \mathbf{r}') \\ N'_{kl} a_{jl}(\mathbf{r}, \mathbf{r}') &= c_{jk}(\mathbf{r}, \mathbf{r}'). \end{aligned} \quad (27)$$

Thus we get

$$D_{ij} b_{jk}(\mathbf{r}, \mathbf{r}') = \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{V_0(\mathbf{r})V_0(\mathbf{r}')} \quad (28)$$

$$N_{ij} b_{jk}(\mathbf{r}, \mathbf{r}') = -\frac{1}{2} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{S_0(\mathbf{r})V_0(\mathbf{r}')}$$

and

$$\begin{aligned} D_{ij} c_{jk}(\mathbf{r}, \mathbf{r}') &= -\frac{1}{2} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{V_0(\mathbf{r})S_0(\mathbf{r}')} \\ N_{ij} c_{jk}(\mathbf{r}, \mathbf{r}') &= \frac{1}{4} \frac{\Phi_{ik}(\mathbf{r}, \mathbf{r}')}{S_0(\mathbf{r})S_0(\mathbf{r}')}. \end{aligned} \quad (29)$$

Equations (28) (and just as well eq (29)) can be solved by introducing the Green's function tensor  $G_{jk}(\mathbf{r}, \mathbf{r}'')$  of an elastic body with  $\lambda=0$ ,  $\mu=1$  which gives the displacement field due to a point force of unit strength acting at point  $\mathbf{r}''$  under load free surface condition.  $G$  is defined by

$$\begin{aligned} D_{ij} G_{jk}(\mathbf{r}, \mathbf{r}'') &= -\delta_{ik} \delta(\mathbf{r}, \mathbf{r}'') \\ N_{ij} G_{jk}(\mathbf{r}, \mathbf{r}'') &= 0 \end{aligned} \quad (30)$$

For infinite bodies

$$G_{jk}(\mathbf{r}, \mathbf{r}'') = \frac{1}{16\pi |\mathbf{r} - \mathbf{r}''|} \left[ \frac{(x_j - x'_{j''})(x_k - x'_{k''})}{|\mathbf{r} - \mathbf{r}''|^2} + 3\delta_{jk} \right]. \quad (31)$$

For finite bodies a term has to be added which takes care of the correct boundary values of  $G_{jk}$ . Since the procedures of obtaining  $G_{jk}$  are well-known in elasticity theory, we need not pursue this further. We rather consider  $G_{jk}$  as given.

In terms of the Green's function tensor  $G_{jk}$ , the solution of eqs (27), (28), and (29) can be written down immediately

$$a_{jl}(\mathbf{r}, \mathbf{r}') = \int c_{jk}(\mathbf{r}, \mathbf{r}''') G_{kl}(\mathbf{r}', \mathbf{r}''') dS''' - \int b_{jk}(\mathbf{r}, \mathbf{r}''') G_{kl}(\mathbf{r}', \mathbf{r}''') dV''' \quad (32)$$

where

$$b_{jk}(\mathbf{r}, \mathbf{r}') = -\frac{1}{2} \int \frac{\Phi_{lk}(\mathbf{r}'', \mathbf{r}')}{S_0(\mathbf{r}'') V_0(\mathbf{r}')} G_{jl}(\mathbf{r}, \mathbf{r}'') dS'' - \int \frac{\Phi_{lk}(\mathbf{r}'', \mathbf{r}')}{V_0(\mathbf{r}'') S_0(\mathbf{r}')} G_{jl}(\mathbf{r}, \mathbf{r}'') dV'' \quad (33)$$

and

$$c_{jk}(\mathbf{r}, \mathbf{r}') = \frac{1}{4} \int \frac{\Phi_{lk}(\mathbf{r}'', \mathbf{r}')}{S_0(\mathbf{r}'') S_0(\mathbf{r}')} G_{jl}(\mathbf{r}, \mathbf{r}'') dS'' + \frac{1}{2} \int \frac{\Phi_{lk}(\mathbf{r}'', \mathbf{r}')}{V_0(\mathbf{r}'') S_0(\mathbf{r}')} G_{jl}(\mathbf{r}, \mathbf{r}'') dV'' \quad (34)$$

These equations inserted into eq (20) provide the unique solution of the problem stated earlier, namely, to find a solution of eqs (6) to (9) with the symmetries of  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  given by eqs (11) and (12). Using this particular  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  we can rewrite the potential energy (10) in the form

$$U = \frac{1}{2} \int \int c_{ijkl}(\mathbf{r}, \mathbf{r}') \epsilon_{ij} \epsilon'_{kl} dV dV' \quad (35)$$

which has been the aim of this investigation.

For the infinite homogeneous medium,  $\Phi_{ik}$  depends on  $\mathbf{r} - \mathbf{r}'$  alone; hence  $\Phi_{ik} = \Phi_{ki}$ , as can be seen from eqs (1) and (2). Then  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  as obtained in eqs (20) and (32) to (34) has, in addition to (12), the symmetry

$$c_{ijkl}(\mathbf{r}, \mathbf{r}') = c_{kjl}(\mathbf{r}, \mathbf{r}'), \quad (36)$$

which means that  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  is totally symmetric in all subscripts. In other words: The infinite homogeneous Bravais crystal should obey the Cauchy relations. This result is physically incorrect. It shows that the infinite homogeneous crystal is an inadmissible idealization within the Born-Huang formalism. A similar situation can arise also within the framework of the local theory, as has been pointed out by Lax [9].

#### IV. Conclusion

The local theory is obtained from eq (34) by putting

$$c_{ijkl}(\mathbf{r}, \mathbf{r}') = C_{ijkl}\delta(\mathbf{r}, \mathbf{r}'),$$

where  $C_{ijkl}$  are the components of the local elasticity tensor. Since  $\delta(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}', \mathbf{r})$ , the tensor  $C_{ijkl}$  has in addition to the symmetries

$$C_{ijkl} = C_{jikl} = C_{ijlk}$$

also the symmetry

$$C_{ijkl} = C_{klij}.$$

Hence it has the correct symmetries known from the conventional elasticity theory.

In Born and Huang's derivation from atomic lattice theory of the conventional elasticity theory, the correct symmetries of  $C_{ijkl}$  did not come out primarily. Rather, extra considerations were needed in order to establish the correct symmetries. The first proposal was due to Huang [10]. Later it was shown by Leibfried and Ludwig [11]—and in a somewhat different way by Kunin [2]—that the condition of rotational invariance of the potential energy enforces the correct symmetries.

In our derivation, rotational invariance did not occur. Obviously, the condition of rotational invariance does not suffice to eliminate the rotations from the potential energy in the non-local theory. The reason is clear: In this theory a relative rotation of two volume elements does contribute to the mutual potential energy of these elements. Notwithstanding, it is possible to eliminate the rotations since the rotation field is functionally dependent on the strain field. Hence the potential energy is determined by the strains alone, from which consideration the form (35) of the energy can be predicted.

Hereafter it is clear that one could work with tensor functions  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$  which do not possess the symmetries (12). Then rotations occur in the energy. The functional form of these  $c_{ijkl}(\mathbf{r}, \mathbf{r}')$ , which are correct too, would be different from the form obtained in our present calculation (eqs (20, 32–34)).

#### V. Acknowledgement

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# ON PROBLEMS OF THE NON-LOCAL THEORY OF ELASTICITY

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The paper contains new results concerning the linear theory of an elastic medium with non-local interactions:

**I. The structure of the general solution of the equations of motion.** The dependence of the general solution on the distribution of energy operator zeroes. Specific effects of the non-locality: new types of damped and undamped waves, the existence of a maximum frequency for the latter ones, the space dispersion. The Green's function.

**I. Approximate models.** Two types of approximate models: the long-wave approximations and the first zeroes approximations. Domains of their applicability.

**III. Boundary value problems.** The replacing of the boundary by a boundary layer of width of the interaction radius. Generalized Green's formula. Fundamental boundary value problems, their correct formulation for first zeroes approximations. The comparison with couple-stress theories. Examples of exact and approximate solutions. The existence of new types of surface waves different from Rayleigh waves.

Key words: Green's tensor; non-local elasticity; solid mechanics; surface waves.

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Non-local theories of solids closely connected with the crystal lattice theory have been developed by Krumhansl [1], Kröner and Datta [2], Kröner [3], Kunin [4, 5], Vdovin and Kunin [6] (see also the survey [7]). This paper contains new results obtained by the authors in this field.

## I. The Structure of the General Solution of the Equations of Motions

In this section we shall consider a linear elastic medium with non-local interactions between particles. The non-locality is due to the discreteness of the medium and to long range forces. When the radius of the interaction is much greater than the distance between particles one can

neglect the discreteness and consider the non-local theory of the elastic continuum.

We shall restrict ourselves to the case of a medium with simple structure [4], i.e., it is assumed that particles have no internal degrees of freedom.

For the sake of simplicity we shall begin with one-dimensional case. The corresponding equation of motion has the form [4]

$$\rho(x)\ddot{u}(x, t) + \int \Phi(x, x')u(x', t)dx' = q(x, t) \quad (1.1)$$

Here  $u$  and  $q$  are displacements and external forces respectively considered as function of the coordinate  $x$  and the time  $t$ ,  $\rho$  is the mass density,  $\Phi(x, x')$  is the kernel of the elastic energy operator  $\Phi$  satisfying the conditions

$$\Phi(x, x') = \Phi(x', x), \quad \int \Phi(x, x')dx' = 0 \quad (1.2)$$

It follows from this that  $\Phi(x, x')$  is represented in the form

$$\Phi(x, x') = \psi(x)\delta(x - x') - \Psi(x, x'), \quad \psi(x) = \int \Psi(x, x')dx' \quad (1.3)$$

where  $\Psi(x, x')$  can be interpreted as the rigidity of the elastic coupling between points  $x$  and  $x'$ . It is more convenient to use in some cases  $\Psi(x, x')$  than  $\Phi(x, x')$  especially when boundary value problems are considered. We shall assume that the radius of the interaction is limited, i.e.,

$$\Psi(x, x') = 0 \text{ if } |x - x'| > l.$$

In addition to functions of  $x, t$  we shall consider their Fourier-representations, for which we shall preserve the same notations but with the arguments  $k, w$ , for instance

$$u(k, w) = \iint u(x, t)e^{i(kx - wt)}dxdt$$

Then (1.1) can be expressed in the form [4]

$$-w^2 \int \rho(k - k')u(k', w)dk' + \int \Phi(k, k')u(k', w)dk' = q(k, w) \quad (1.4)$$

This equation of motion can describe the elastic continuum with non-local interactions as well as the discrete medium. In the latter case Fourier-representations of the field variables must be concentrated in  $k$ -space on the segment  $|k| \leq \pi/a$  where  $a$  is the distance between particles.

In this section we shall consider the case of homogeneous media. Then  $\rho(x) = \rho_0$ ,  $\Phi(x, x') = \Phi(x - x')$ ,  $\Psi(x, x') = \Psi(x - x')$  and

$$\Phi(k) = 2 \int_0^l \Psi(x) (1 - \cos kx) dx \quad (1.5)$$

Consider properties of the function  $\Phi(k)$  and its zeroes. It can be shown that  $\Phi(k)$  can be expanded in the complex  $k$ -plane as the entire analytic function of the exponential type. For the absolutely integrable function,  $\Psi(x)$ , function  $\Phi(k)$  is bounded on the real axis. If  $k_1$  is a zero ( $\Phi(k_1) = 0$ ) then  $\bar{k}_1$ ,  $-k_1$  and  $-\bar{k}_1$  are also zeroes.

Let us assume that all elastic couplings are stable, i.e.,  $\Psi(x) \geq 0$ . Then it is easy to show that  $\Phi(k)$  has no zeroes on the real and imaginary axes except the double zero  $k=0$ . The following representation is valid

$$\Phi(k) = c_0 k^2 \prod_{n=1}^{\infty} \left( 1 - \frac{k^2}{k_n^2} \right) \quad (1.6)$$

where  $k_n$  are the zeroes in the upper half-plane numbered in the order of increasing modulus. The constant

$$c_0 = \int_0^l x^2 \Psi(x) dx \quad (1.7)$$

has the meaning of the elastic modulus in the long wave approximation.

Note, that for the discrete model the permissible domain of  $k$  is the complex cylinder  $|\operatorname{Re} k| \leq \pi/a$ . The number of the zeroes is equal to  $2N$  where  $N$  is the number of the interacting neighbours.

The equation of motion (1.4) now takes the form

$$[-w^2 \rho_0 + \Phi(k)] u(k, w) = q(k, w). \quad (1.8)$$

A solution of this equation can be obtained by using of the waves  $\exp[ik(w)x]$ , where  $k(w)$  are the zeroes of the function

$$\Phi_w(k) = -w^2 \rho_0 + \Phi(k). \quad (1.9)$$

The characteristic feature of the non-local theory is the existence of the counting number of the usually complex zeroes  $k_n(w)$  for a given  $w$  (as it was mentioned above the number of the zeros is finite for the discrete model). In the case of unbounded media the real  $k_n(w)$ , corresponding to undamped waves, are of main interest. They are defined completely by the dispersive curve  $w=w(k)$  ( $\operatorname{Im} k=0$ ) and their group velocity  $w'(k)$  depends on  $k$  (the space dispersion).

It is important to note that the boundedness of the  $\Phi(k)$  leads to the existence of the maximum frequency  $w_{\max}$  of the undamped waves. Thus, in spite of wide-spread opinion, this effect exists not only in the discrete media.

When the dispersion of waves, due to inhomogeneities, and boundary value problems are considered one must take into account not only real but also complex  $k_n(w)$  corresponding to damped waves.

For a fixed  $w \neq 0$ , similar to (1.6), we have

$$\Phi_w(k) = -w^2 \rho_0 \prod_{n=0}^{\infty} \left(1 - \frac{k^2}{k_n^2(w)}\right), \quad \operatorname{Im} k_n(w) \geq 0 \quad (1.10)$$

where  $k_0^2(w) \rightarrow c_0^{-1} \rho_0 w^2$  when  $w \rightarrow 0$ .

The general solution of eq (1.8), in  $(x, w)$  — representation, has the form

$$u(x) = \int G_w(x - x') q(x') dx' + \sum_{n=0}^{\infty} [\alpha_n e^{ik_n(w)x} + \beta_n e^{-ik_n(w)x}] \quad (1.11)$$

where the first term is the partial solution constructed with the help of Green's function  $G_w(x)$  and  $\alpha_n, \beta_n$  are arbitrary constants.

It follows from (1.10) that  $G_w(k) = \Phi_w^{-1}(k)$  is a meromorphic function. Under some fairly unrestricted conditions we can write ( $w \neq 0$ )

$$G_w(k) = 2 \sum_{n=0}^{\infty} \frac{k_n(w)}{\Phi'(k_n(w)) [k^2 - k_n^2(w)]} \quad (1.12)$$

the following estimate for the coefficients being valid

$$|k_n(w) \Phi'(k_n(w))|^{-1} \leq A(w) e^{-l \operatorname{Im} k_n(w)}. \quad (1.13)$$

In  $(x, w)$  — representation

$$G_w(x) = \sum_{n=0}^{\infty} \frac{i e^{ik_n(w)|x|}}{\Phi'(k_n(w))} \quad (1.14)$$

When  $w \ll w_{\max}$  the expression (1.12) takes the form

$$G_w(k) = \frac{1}{c_0 k^2 - w^2 \rho_0} + 2 \sum_{n=1}^{\infty} \frac{k_n}{\Phi'(k_n) (k^2 - k_n^2)} + O(w^2), \quad (1.15)$$

and for the static case we have

$$G(x) = -\frac{|x|}{2C_0} + \sum_{n=1}^{\infty} \frac{ie^{ik_n|x|}}{\Phi'(k_n)} \quad (1.16)$$

where the first term is the usual Green's function.

Note, that multiple zeroes can exist for some frequencies (corresponding, for example, to extreme points of the dispersive curve). Then the solutions of type  $x^m \exp[ik_n(w)x]$  must be added to (1.11).

Let us consider now the simplest three-dimensional generalization on the case of a medium with central interactions. By definition in such a medium the interaction force between two particles is proportional to the change of distance and has a direction along a line connecting these particles.

It can be shown that the kernel of the elastic energy operator has the form

$$\Phi^{\alpha\beta}(\mathbf{r}, \mathbf{r}') = \psi^{\alpha\beta}(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') - \Psi^{\alpha\beta}(\mathbf{r}, \mathbf{r}'), \quad (1.17)$$

$$\psi^{\alpha\beta}(\mathbf{r}) = \int \Psi^{\alpha\beta}(\mathbf{r}, \mathbf{r}') d\mathbf{r}'$$

where

$$\Psi^{\alpha\beta}(\mathbf{r}, \mathbf{r}') = \frac{(x^\alpha - x'^\alpha)(x^\beta - x'^\beta)}{|\mathbf{r} - \mathbf{r}'|^2} \Psi(\mathbf{r}, \mathbf{r}') \quad (1.18)$$

and  $\Psi(\mathbf{r}, \mathbf{r}') = \Psi(\mathbf{r}', \mathbf{r})$  is the rigidity of the elastic coupling between points  $\mathbf{r}$  and  $\mathbf{r}'$ . We shall assume that  $\Psi(\mathbf{r}, \mathbf{r}') = 0$  when  $|\mathbf{r} - \mathbf{r}'| > l$ .

For a homogeneous isotropic medium

$$\Psi(\mathbf{r}, \mathbf{r}') = \Psi(\mathbf{r} - \mathbf{r}'), \quad \Psi(\mathbf{r}) = \Psi(r) \quad (1.19)$$

where  $r = |\mathbf{r}|$ .

The general solution of the equation of motion

$$[-w^2\rho_0\delta^{\alpha\beta} + \Phi^{\alpha\beta}(\mathbf{k})]u_\beta(\mathbf{k}, w) = q^\alpha(\mathbf{k}, w) \quad (1.20)$$

can be constructed in a way analogous to the one-dimensional case if the Green's function is known. Below we shall give an expression for the static Green's function.

Resolving the energy operator  $\Phi^{\alpha\beta}$  in longitudinal,  $\Phi_{(l)}^{\alpha\beta}$ , and transverse,  $\Phi_{(t)}^{\alpha\beta}$ , components we have ( $k = |\mathbf{k}|$ )

$$\Phi_{(l)}^{\alpha\beta}(\mathbf{k}) = \frac{k^\alpha k^\beta}{k^2} \Phi_{(l)}(k), \quad \Phi_{(t)}^{\alpha\beta}(\mathbf{k}) = \left( \delta^{\alpha\beta} - \frac{k^\alpha k^\beta}{k^2} \right) \Phi_{(t)}(k), \quad (1.21)$$

$$\Phi_{(l,t)}(k) = 4\pi \int_0^l r^2 \Psi_{(l,t)}(r) \left( 1 - \frac{\sin kr}{kr} \right) dr$$

where  $\Psi_{(l)}$ ,  $\Psi_{(t)}$ , and  $\Psi$  are connected by relations

$$\Psi(r) = \Psi_{(l)}(r) + 2\Psi_{(t)}(r), \quad \Psi_{(t)}(r) = \int_r^l r^{-1}\Psi(r)dr \quad (1.22)$$

In accordance with (1.20) we have on resolving the Green's function

$$G_{\alpha\beta}(\mathbf{k}) = \frac{k_\alpha k_\beta}{k^2} G_{(l)}(k) + \left( \delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2} \right) G_{(t)}(k) \quad (1.23)$$

where

$$G_{(l,t)}(k) = \Phi_{(l,t)}^{-1}(k) \quad (1.24)$$

If the stability condition  $\Psi(r) \geq 0$  is fulfilled the properties of the entire analytic functions  $\Phi_{(l,t)}(k)$ , and in particular the distribution of their zeroes, are completely analogous to the properties of  $\Phi(k)$  in the one-dimensional case. It permits one to resolve  $G_{(l,t)}(k)$  into simple fractions.

For example

$$G_{(l)}(k) = \frac{1}{c_{(l)}k^2} + g_{(l)} + 2 \sum_{n=1}^{\infty} \frac{k_n}{\Phi'_{(l)}(k_n)(k^2 - k_n^2)} \quad , \quad \text{Im } k_n > 0, \quad (1.25)$$

$$c_{(l)} = \frac{2\pi}{3} \int_0^l r^4 \Psi_{(l)}(r) dr,$$

In  $\mathbf{r}$ -representation we have

$$G_{(l)}(r) = \frac{1}{4\pi r} \left[ c_{(l)}^{-1} + \sum_{n=1}^{\infty} \frac{k_n e^{ik_n r}}{\Phi'_{(l)}(k_n)} \right]. \quad (1.26)$$

## II. Approximate Models

In this section we shall discuss various types of models taking into account approximately the main features of the non-local theory.

The simplest models can be obtained if we assume that

$$\Phi(k) \approx c_0 k^2 P_m(k^2) \quad (2.1)$$

where  $P_m(k^2)$  is the polynomial of  $2m$ th degree. It is equivalent to replacing the integral operator by a differential one.

The equation of motion takes the form

$$w^2 \rho_0 u(x, w) + c_0 D_x^2 P_m(-D_x^2) u(x, w) = -q(x, w) \quad (2.2)$$

All phenomenological theories with high order derivatives (couple-stress theory, multi-polar theory and so on) have equations of motion of such a type.

These approximate models can be interpreted from two different points of view. The usual approach is that the polynomial  $c_0 k^2 P_m(k^2)$  coincides

with first members of the expansion  $\Phi(k)$  in the vicinity of  $k=0$ . If  $\Phi(k)$  is given, or the behavior of the dispersive curve at small  $k$  (long waves) is known, one can obtain the first approximation assuming  $P_1(k^2)=1+l^2A_1k^2$ , where  $A_1$  is a suitable non-dimensional constant. It permits one to describe correctly the dispersion of long waves (the dispersion must be considered as small).

This approach is known as long-wave approximation and corresponding models are called media with weak space dispersion. The scale parameter  $l$  must be considered as small and the theory can not be applied at distances of the order of  $l$  and especially for distances smaller than  $l$ .<sup>1</sup>

If we extrapolate  $P_1(k^2)$  in the domain of large  $k$  (short waves) we can formally obtain additional eigenfunctions corresponding to zeroes of  $P_1(k^2)$ . However, these functions in general have nothing to do with the exact ones. Hence this approximation is not suitable for describing the dispersion of waves on inhomogeneities and formulating the boundary value problems. Note that  $w_{\max}$  does not exist for any polynomial approximation.

A different possible approach is based on the idea replacing  $\Phi(k)$  by a polynomial having the same first zeroes. If the condition  $\Psi(x) \geq 0$  is fulfilled then the first order approximation has the form

$$\Phi_1(k) = c_0 k^2 \left(1 - \frac{k^2}{k_1^2}\right) \left(1 - \frac{k^2}{k_2^2}\right) \quad (2.3)$$

to which corresponds the differential operator of the sixth order.

Evidently the first zeroes approximation when compared with the long-wave one has a little less exactness at small  $k$  but its advantages are as follows. Firstly a qualitatively correct description of the effects, for which the waves with length of order  $l$  are essential, becomes possible. Secondly the main terms of the asymptotic solution are preserved. Thirdly the correct formulation of the approximate boundary value problems (it will be discussed below) becomes possible.

Assuming  $w < w_{\max}$  we have

$$\Phi_w(k) \approx -w^2 \rho_0 + \Phi_1(k) = -w^2 \rho_0 \prod_{n=0}^2 \left(1 - \frac{k^2}{k_n^2(w)}\right) \quad (2.4)$$

and the corresponding Green's function is

$$G_w(x) \approx \sum_{n=0}^2 \frac{ie^{ik_n(w)|x|}}{\Phi'_1(k_n(w))} \quad (2.5)$$

<sup>1</sup> Unfortunately this misunderstanding is widespread.

For the static Green's function we have

$$G(x) \approx \frac{1}{2} c_0^{-1} |x| - 2 \operatorname{Im} \frac{e^{ik_1|x|}}{\Phi'_1(k_1)}. \quad (2.6)$$

If the condition  $\Psi(x) \geq 0$  is omitted the first zeroes of  $\Phi(k)$  can be situated on the imaginary axis. In this case the differential operator of the first approximation will be of the fourth order. The equation of motion is the one-dimensional analogue of the couple-stress theory.

Let us now mention some other possible approximations different from polynomial ones. Sometimes the approximation of the dispersive curve by a suitable function of  $k$  is of interest (for example, when interpolating between experimental points). This model is valid for undamped waves but it can not be extended in the complex  $k$ -plane and hence has nothing to do with boundary value problems. For the latter purpose models based on the approximations of the type

$$\Psi(x) = \begin{cases} 3c_0 l^{-3} & \text{when } |x| \leq l \\ 0 & \text{when } |x| > l, \end{cases} \quad \Psi(x) = \sqrt{\frac{2}{\pi}} c_0 l^{-3} e^{-x^2/2l^2}$$

are valid. We have respectively

$$\Phi(k) = 6c_0 l^{-2} \left( 1 - \frac{\sin lk}{lk} \right), \quad \Phi(k) = 2c_0 l^{-2} (1 - e^{-l^2 k^2/2})$$

Such models describe correctly all specific effects of non-locality.

### III. Boundary Value Problems

Let us assume that the equation of motion (1.4), which we can rewrite in an operator form as

$$\Phi_w u \equiv (-w^2 \rho + \Phi) u = q \quad (3.1)$$

describes two distinct media connected with elastic couplings and occupying the regions  $V$  and  $V^*$ . We can pick out in each medium boundary layers  $S$  and  $S^*$  (of width  $l$  and  $l^*$  respectively) in which parameters of the medium are disturbed owing to the interaction. Non-disturbed regions are denoted by  $D$  and  $D^*$  so that  $V = D + S$  and  $V^* = D^* + S^*$ .

The equations of motion of the transition region  $S + S^*$  have the form

$$-w^2 \rho_s u_S + S \Phi u = q_S, \quad -w^2 \rho_{S^*} u_{S^*} + S^* \Phi u = q_{S^*} \quad (3.2)$$

where  $u_S = S u$  and so on. Owing to non-locality the terms  $S \Phi u$  and  $S^* \Phi u$  cause the connection of these equations both between themselves and with the equations for the undisturbed regions. Below, the boundary conditions will be derived using eq (3.2).

To formulate fundamental boundary value problems we resolve the elastic coupling operator  $\Psi$  into the sum

$$\Psi = \Psi_V + \Psi_{V*} + \Psi_{VV*}. \quad (3.3)$$

Where

$$\Psi_V = V\Psi V, \quad \Psi_{VV*} = V\Psi V^* + V^*\Psi V.$$

The operators  $\Psi_V$ ,  $\Psi_{V*}$  and  $\Psi_{VV*}$  characterize the interaction of the points inside each medium and between them, respectively.

Correspondingly

$$\Phi = \Phi_V + \Phi_{V*} + \Phi_{VV*} \quad (3.4)$$

where, for example,

$$\Phi_V = \psi_V I - \Psi_V, \quad \psi_V(x) = \int \Psi_V(x, x') dx' \quad (3.5)$$

and  $I$  is the identical operator.

When the media do not interact then  $\Psi_{VV*} = 0$  and hence  $\Phi_{VV*} = 0$ . In this case eq (3.1) resolves into two independent equations. For the medium in the region  $V$  we have

$$-w^2 \rho u_V + \Phi_V u_V = q_V. \quad (3.6)$$

Taking into account that

$$\Phi_V = D\Phi + \Gamma, \quad \Gamma = S\Phi_V \quad (3.7)$$

we can replace (3.6) by the equivalent system of equations

$$D\Phi_w u \equiv -w^2 \rho u_D + D\Phi u = q_D, \quad (3.8)$$

$$\Gamma_w u \equiv -w^2 \rho u_S + \Gamma u = q_S. \quad (3.9)$$

The first equation connects displacements with given forces in the  $D$ -region. When  $l \rightarrow 0$  it turns into the usual equation of motion of local theory of elasticity. The second equation connects displacements with given forces in the boundary layer  $S$ . When  $l \rightarrow 0$  it turns into the usual boundary force conditions. These considerations permit one to interpret eqs (3.8) and (3.9) as the first fundamental boundary value problem of the non-local theory of elasticity.

For the second fundamental boundary problem we have

$$D\Phi_w u = q_D, \quad u_S = h, \quad (3.10)$$

where  $h(x)$  is given in  $S$ .

It can be shown that in the static case both the first and second boundary value problems can be reduced to the Fredholm's equation with symmetric kernel.

It is important to emphasize the distinction between the first and the second problems. The latter can be reduced to the integral equation with difference-type kernel in the case of the homogeneous medium. But it is not so for the first problem because of the inhomogeneity of couplings in the boundary layer. Hence in the non-local theory the solution of the first boundary value problem is more difficult than that of the second one.

In a manner analogous to that used in the local theory we can introduce potentials of the simple and double layers and derive the Green's formula

$$u_D = G_w q_D + G_w q_S - G_w \Gamma_w^+ u_S, \quad (3.11)$$

where  $G_w$  is the fundamental solution of eq (3.1) and  $\Gamma_w^+$  is conjugate to  $\Gamma_w$ . This formula permits one to formulate mixed boundary value problems.

As an illustration we shall construct the solution of fundamental static boundary value problems for the homogeneous half-restricted medium assuming that  $D(0 \leq x < \infty)$  and  $S(-l \leq x < 0)$ . We shall start with the second problem which is the simplest one.

$$\int \Phi(x-x') u(x') dx' = q(x), \quad x \in D, \quad (3.12)$$

$$u_S(x) = h(x), \Phi \quad x \in S. \quad (3.13)$$

We shall represent the solution as the sum

$$u = \tilde{u} + v \quad (3.14)$$

where  $\tilde{u}(x)$  is the particular solution of eq (3.12) vanishing at  $x \rightarrow \infty$  and  $v(x)$  is the solution of the homogeneous equation satisfying the boundary condition  $v_S = h - \tilde{u}_S$ .

Let  $\tilde{G}(x) = G(x) - x/2c_0$ , where  $G(x)$  is the static Green's function defined by eq (1.16), then

$$\tilde{u}(x) = \int_D \tilde{G}(x-x') q_D(x') dx'. \quad (3.15)$$

The function  $v(x)$  can be written in the form

$$v(x) = \sum_{n=0}^{\infty} v^n e_n(x), \quad (3.16)$$

where  $e_n(x) = \exp(ik_n x)$  and  $k_n$  are zeroes of  $\Phi(k)$  for which  $\text{Im } k_n > 0$ ,

( $k_0=0$ ). To find the coefficients  $v_n$  we shall construct the reciprocal functional basis  $e^m(x)$  satisfying the conditions

$$(e^m, e_n) \equiv \int e^m(x) e^{ik_n x} dx = e^m(k_n) = \delta_n^m. \quad (3.17)$$

For this purpose one will use the representation

$$\Phi(k) = \Phi_+(k) \Phi_-(k), \quad (3.18)$$

where  $\Phi_+(\Phi_-)$  are entire analytic functions having no zeroes in the upper (lower) half-planes. Their Fourier-preimages  $\Phi_+(x)$  and  $\Phi_-(x)$  are concentrated on intervals  $(0, l)$  and  $(-l, 0)$  respectively. It can be shown that

$$\Phi_-(k) = \exp \left[ \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{\ln \Phi(k')}{k' - k} dk' \right] \quad (\text{Im } k < 0) \quad (3.19)$$

and  $e^m(k)$  are given by the formula

$$e^m(k) = \frac{\Phi_-(k)}{\Phi'_-(k_m)(k - k_m)}. \quad (3.20)$$

Their Fourier-preimages are concentrated on  $S$  and have the form

$$e^m(x) = \frac{i}{\Phi'_-(k_m)} \int_{-\infty}^0 \Phi_-(x - x') e^{-ik_m x'} dx'. \quad (3.21)$$

Finally, for the coefficients  $v^n$  we have

$$v^n = (v_S, e^n) = \int_S v_S(x) e^n(x) dx, \quad (3.22)$$

and that completes the solution of the problem.

In the case of the first zeroes approximation the solution can be obtained in a similar way. The approximate Green's function is given by eq (2.6) and

$$e^0(k) \approx \left( 1 - \frac{k}{k_1} \right) \left( 1 + \frac{k}{\bar{k}_1} \right), \quad e^1(k) \approx \frac{k(k + \bar{k}_1)}{k_1(k_1 + \bar{k}_1)}. \quad (3.23)$$

Thus one can obtain the solution in an explicit form.

Note that approximate boundary conditions can be expressed in the form

$$\left( 1 - \frac{iD_x}{k_1} \right) \left( 1 + \frac{iD_x}{\bar{k}_1} \right) u(0) = u^0 \equiv (e^0, h), \quad (3.24)$$

$$\frac{iD_x(iD_x + \bar{k}_1)}{k_1(k_1 + \bar{k}_1)} u(0) = u^1 \equiv (e^1, h),$$

the second condition being equivalent to two real ones.

Consider the force boundary value problem taking now the form

$$\int \Phi(x-x')u(x')dx' = q_D(x), \quad x \in D, \quad (3.25)$$

$$\int \Gamma(x, x')u(x')dx' = q_S(x), \quad x \in S \quad (3.26)$$

The displacements appearing in the boundary conditions are determined in the region  $(-l \leq x \leq l)$ . The following decomposition is valid in this region

$$u(x) = \sum_{n=0}^{\infty} \tilde{u}^n \tilde{e}_n(x), \quad (3.27)$$

$$\tilde{e}_0(x) = 1, \quad \tilde{e}_1(x) = \frac{x}{l}, \quad \tilde{e}_n(x) = e^{ik_n x} \quad (n = 2, 3, \dots), \quad (3.28)$$

where  $k_n$ —all the zeroes of  $\Phi(l)$ . The coefficients are found by using the reciprocal basis  $\tilde{e}^m$

$$\tilde{u}^m = (u, \tilde{e}^m), \quad (\tilde{e}^m, \tilde{e}_n) = \delta_n^m. \quad (3.29)$$

The construction of  $\tilde{e}^m$  is performed by the formula analogous to (3.20) where  $\Phi(k)$  is used as the generating function.

The forces  $q_s$  like  $u_s$  can also be decomposed in the basis  $e_n$  so that the boundary condition (3.26) can be rewritten as

$$\Gamma_n u = \sum_{m=1}^{\infty} \Gamma_{nm} (\tilde{e}^m, u) = q_n \quad (n = 0, 1, \dots), \quad (3.30)$$

$$\Gamma_{nm} = (e_n, \Gamma \tilde{e}_m), \quad q_n = (e_n, q_s). \quad (3.31)$$

The exact solution of the formulated problem as it has been mentioned is much more difficult than the previous one. But in the first zeroes approximation the problem is essentially simplified. In this case the eq (2.3) is valid in the  $D$ -region. Corresponding boundary conditions can be easily obtained from (3.30) containing displacement derivatives up to the fifth order.

*Note 1.* In contrast to the couple-stress theories the connection between the approximate boundary conditions and exact ones is given above and, in particular, the method of calculating moments  $q_m$  through given forces  $q_s$  is indicated.

Note 2. Boundary effects can induce an additional disturbance of elastic couplings  $\Psi$  in the boundary layer  $S$ . This leads to corresponding changes in the coefficients  $\Gamma_{mn}$ .

For example

$$\Gamma_{01} = \int_{-l}^0 dx \int_{-l}^{l+x} dx' \Psi(x, x') (x - x'). \quad (3.32)$$

The boundary value problems considered above can be generalized for the three-dimensional case. For instance, the Green's formula becomes

$$u_\alpha = G_{\alpha\beta}^{(w)} q_B^\beta + G_{\alpha\beta}^{(w)} q_S^\beta - G_{\alpha\beta}^{(w)} \Gamma_{(w)}^+ \cdot_\lambda^\beta u_S^\lambda \quad (3.33)$$

where the notion will be obvious.

The existence of new types of surface waves can be shown to be a specific non-local three-dimensional boundary effect. The long surface waves fade into the boundary layer of order  $l$  in contrast to Rayleigh waves.

#### IV. Conclusion

We have the following specific distinctions of the non-local theory of elasticity from the local one:

- (a) There exists a scale parameter.
- (b) There are new types of undamped and damped waves (damped eigenfunctions in statics).
- (c) There is a maximum frequency for undamped waves.
- (d) The wave velocity depends on their length.
- (e) The boundary is replaced by a boundary layer.
- (f) There are new types of surface waves different from classical ones.

The approximate models can take into account some of these effects. The choice of the approximate model must depend on what effects we want to preserve. The simplest models are of the polynomial differential type to which all couple-stress theories belong. The usual approach is to consider them as long-wave approximations. The alternative approach is based on the first zeroes approximations. The latter is more adequate in the cases where boundary value problems and inhomogeneities are considered.

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# A NON-RIEMANNIAN CONSTRUCTION OF VARIATIONAL CRITERIA FOR PLASTIC MANIFOLDS WITH SPECIAL REFERENCE TO THE THEORY OF YIELDING

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The variational formalism is viewed not as an independent assumption but as a natural consequence following from a more fundamental penetration into the recognition of nature and this is shown in regard to the static aspects of plasticity. The energy is defined as the necessary quantity for the geometrical construction. With the Riemannian and non-Riemannian picture, a bridge is sought between the theory of yielding and the theory of dislocations, as also between the theory of dual yielding and theory of couple stresses. The standpoint of the theory of yielding and dual yielding is explained constitutively with a statistical construction to reconfirm the formulae which have been proposed. The meaning of the plastic constants involved in the theory is clarified by the construction.

Key words: Continuum mechanics; non-Riemannian theories; plasticity; yielding.

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## Introduction

A connecting link will be sought in this paper between the continuum theory of dislocations and the theory of yielding in Riemannian and non-Riemannian terminology. In order to carry this into effect, the variational criterion for the mechanical material manifold will be viewed from the standpoint of the dislocational and dual dislocational picture of the plastic disturbances. We shall treat the variational energy criterion not as an independent assumption but construct it as a natural consequence from an equivalence of two adjacent non-Riemannian configurations.

The important generalizations derived therefrom of the concepts of the mechanics of plastically deformable continua and a reconfirmation of some of them are as follows.

1. The Riemannian space of stress and stress function is introduced as the dual of the Riemannian space of strain and incompatibility, the possibility of the asymmetric stress and of the couple stress following spontaneously.

2. The strain-incompatibility Riemannian metric is modified to an asymmetric feature by the Lagrangian multiplier method.<sup>1</sup>

3. A constitutional derivation will be made of the fundamental equation of the theory of yielding and dual yielding including a constructive definition of the plastic material constants standing in the formula.

Another exposition of the same material but different in minor features from the present one will also be published elsewhere.

## I. Construction of a Variational Criterion

### I.1. Tearing of the strain space

The concepts which we call *incompatible deformations* need to be considered in order to release all the material elements from the strains. This is the process which we call the *naturalization*.

The material in the naturalized state has the Riemannian metric

$$ds^2 = a_{\lambda\kappa} dx^\kappa dx^\lambda \quad (\kappa, \lambda = 1, 2, 3) \quad (1.1)$$

where  $x^\kappa$ 's are the coordinates fixed to the material element and can be made to agree with the rectangular Cartesian coordinates of the point in space occupied by the material point before the naturalization. The unnaturalized state has then a Euclidean metric

$$dz^2 = \delta_{\lambda\kappa} dx^\kappa dx^\lambda \quad (\kappa, \lambda = 1, 2, 3).$$

The strain is represented by the difference of the two metrics  $ds^2 - dz^2$  so that the difference of the two metric tensors referred to the same coordinate system is an appropriate quantity to express it.

As an invariant expression of the strain, one can adopt

$$\epsilon_{\lambda\kappa} = -\theta_{\lambda\kappa} \stackrel{\text{def}}{=} \frac{1}{2}(\delta_{\lambda\kappa} - a_{\lambda\kappa}), \quad (1.2)$$

which reduces to the ordinary concept of strain tensor in the special case in which compatible deformations alone are considered, i.e., when the metric  $ds^2$  is also Euclidean.

Obviously, the metric tensor  $a_{\lambda\kappa}$  has the same dimensionality as the strain tensor  $\epsilon_{\lambda\kappa}$ .

The incompatible characters of the strain is represented by the Riemann-Christoffel curvature tensor

$$K_{\nu\mu\lambda}^{\kappa} = 2(\partial_{[\nu}\{\kappa\}_{\lambda]} + \{\kappa_{\nu|\rho|}\}\{\rho\}_{\lambda}\}) \quad (1.3)$$

<sup>1</sup> cf. footnote 5, p. 772.

where

$$\{\kappa_{\mu\lambda}\} = 1/2a^{\kappa\rho}(\partial_{\lambda}a_{\rho\mu} + \partial_{\mu}a_{\rho\lambda} - \partial_{\rho}a_{\mu\lambda}).$$

This is to assume a Levi-Civita parallelism.

Another metric connection can also be introduced. Its parameters of connection have the structure

$$\Gamma_{\mu\lambda}^{\kappa} = \{\kappa_{\mu\lambda}\} + S_{\mu\lambda}^{\kappa} - 2S_{(\mu}^{\kappa}{}_{\lambda)} \quad (1.4)$$

where  $S_{\mu\lambda}^{\kappa}$  is the torsion tensor. The process of introducing such a connection into the metric space will be called a *tearing of the given Riemannian manifold* (see e.g., [1], [2] etc.). It has been studied elsewhere that the torsion tensor thus introduced is the analytical representation of the density of *distributed dislocations*.

A Riemann-Christoffel curvature tensor of a more general kind than the foregoing one is also defined and associated with the new connection. It is given by

$$R_{\nu\mu\lambda}^{\kappa} = 2(\partial_{[\nu}\Gamma_{\mu]\lambda}^{\kappa} + \Gamma_{[\nu|\rho}^{\kappa}\Gamma_{\mu]\lambda}^{\rho}). \quad (1.5)$$

There is a specific kind of tearing which will be called the *perfect tearing*. This is the one, of which the curvature tensor  $R_{\nu\mu\lambda}^{\kappa}$  is annulled, or which constitutes a space of *teleparallelism* in the mathematician's terminology. It is related to a specific anholonomic reference frame ( $\kappa'$ ) in which the foregoing Riemannian metric of the naturalization assumes the form

$$ds^2 = \delta_{\lambda'\kappa'}(dx)^{\kappa'}(dx)^{\lambda'} \quad (\kappa', \lambda' = 1, 2, 3)$$

and the components of the torsion tensor agrees with the anholonomic object of the anholonomic transformation from

$$dx^{\kappa} = A_{\kappa'}^{\kappa}(dx)^{\kappa'} \text{ to } (dx)^{\kappa'} = A_{\kappa'}^{\kappa}dx^{\kappa}$$

so that

$$S_{\mu'\lambda'}^{\kappa'*} = A_{[\mu'}^{\mu} A_{\lambda']^{\lambda}} \partial_{\mu} A_{\lambda}^{\kappa'}.$$

Whether the tearing is perfect or imperfect, we shall distinguish the tearing dependent feature

$$M_{\nu\mu\lambda\kappa} \stackrel{\text{def}}{=} R_{\nu\mu\lambda\kappa} - K_{\nu\mu\lambda\kappa},$$

from  $K_{\nu\mu\lambda\kappa}$  and also write

$$\begin{aligned} M_{\mu\lambda} &= R_{\mu\lambda} - K_{\mu\lambda}, \quad K_{\mu\lambda} = K_{\nu\mu\lambda\kappa}a^{\kappa\nu}, \quad R_{\mu\lambda} = R_{\nu\mu\lambda\kappa}a^{\kappa\nu}, \\ I_{\mu\lambda} &= K_{\mu\lambda} - 1/2Ka_{\mu\lambda}, \quad N_{\mu\lambda} = M_{\mu\lambda} - 1/2Ma_{\mu\lambda}, \\ K &= K_{\mu\lambda}a^{\lambda\mu}, \quad M = M_{\mu\lambda}a^{\lambda\mu}. \end{aligned}$$

The tensor  $I_{\mu\lambda}$  is called the Einstein-tensor. In the three-dimensional problem of incompatible strain,  $I_{\mu\lambda}$  ( $\lambda, \mu=1, 2, 3$ ) is often called the *incompatibility tensor*.

For three dimensional problems we also have

$$K_{\mu\lambda} = I_{\mu\lambda} - Ia_{\mu\lambda}, \quad M_{\mu\lambda} = N_{\mu\lambda} - Na_{\mu\lambda},$$

where

$$N \stackrel{\text{def}}{=} N_{\mu\lambda}a^{\lambda\mu} = -1/2M.$$

## 1.2. Variation of connection

We shall consider two torn configurations, one real and one virtual, and we shall require the condition of their macroscopic equivalence.

Let one of the two connection configurations have the parameters such as (1.4). Let this be referred to rectangular coordinates, denoted by Roman indices, of the unnaturalized state, where

$$\bar{T}_{\mu\lambda}^{\cdot\cdot\kappa} = S_{\mu\lambda}^{\cdot\cdot\kappa} - 2S_{(\lambda\cdot\mu)}^{\cdot\cdot\kappa}$$

is a tensor. Then the other in small deviation therefrom, but equivalent thereto, is defined by

$$\delta\Gamma_{\mu\lambda}^{\kappa} = \delta\{\mu_{\lambda}^{\kappa}\} + \delta T_{\mu\lambda}^{\cdot\cdot\kappa} = 0. \quad (1.6)$$

Here the deviation, indicated by  $\delta\Gamma_{\mu\lambda}^{\kappa}$  is a tensor because  $\delta\{\mu_{\lambda}^{\kappa}\}$  is a difference of two affine connections.

At any rate, the variation ought to be expressed in terms of tensor quantities connected with the configurations of connection. The simplest tensor obtained from  $\Gamma_{\mu\lambda}^{\kappa}$  is the torsion tensor. However, this is not sufficient to represent the space characteristics.

The next simplest one is given as the Reimann-Christoffel curvature tensor or its equivalent in three dimensions the Ricci-tensor. It seems, to be appropriate to investigate whether or not the condition (1.6) is but in terms of these quantities.

The question is answered in the affirmative as far as the disturbances represented by  $\Gamma_{kj}^i$  are sufficiently small so that we have the following:

**EQUIVALENCE THEOREM:** *As far as the disturbances represented by the affine connection  $\Gamma_{kj}^i$  are small, the variational criterion,*

$$\delta\Gamma_{kj}^i = 0,$$

*is approximately equivalent to*

$$\delta W = 0 \quad (1.7)$$

where

$$W = \frac{1}{2} \int c^{\times mn} R_{nm} dX, \quad (1.8)$$

$dX$  is the volume element,  $R_{nm}$  is the Ricci-tensor and  $c^{\times mn}$ 's are arbitrary coefficients which are not varied.

Henceforth we shall use Roman indices referred to the rectangular coordinates of the location in space of the point in the unnaturalized state.

The proof of the Equivalence Theorem is given by considering

$$(\nabla_l h_{i.m}^{ij}) \delta \Gamma_{kj} = 0$$

where  $\nabla_l$  signifies a covariant differentiation. This is a general formula which needs to hold without any restriction and is equivalent to (1.6) as far as  $h_{i.m}^{ij}$  is an arbitrary tensor. Let this be multiplied by the volume element

$$dX = a^{1/2} 3! dx^{[k} dx^l dx^{m]},$$

where

$$a = \det (a_{ij}),$$

and be summed in regard to the indices  $k, l, m$ . Then we have

$$3! \int \nabla_l h_{i.m}^{ij} \delta \Gamma_{kj} dx^{[k} dx^l dx^{m]} = 0 \quad (1.9)$$

which also needs to hold without any restriction and is equivalent to (1.6).

Since small disturbances have been assumed, (1.9) is simplified to, by putting  $a^{1/2} = 1$  etc.,

$$\int \partial_{[l} h_{i.m}^{ij} \delta \Gamma_{k]i} dX = 0 \quad (i, j, k, l, m = 1, 2, 3), \quad (1.9.1)$$

where

$$dX = dx^1 dx^2 dx^3.$$

By integration by parts, we have

$$\oint h_{i.m}^{ij} \delta \Gamma_{k]i} dX_l - \int h_{i.m}^{ij} \partial_l \delta \Gamma_{k]i} dX = 0$$

where  $\oint \dots dX$  is the surface integral which is defined on the boundary, whose element is denoted by  $dX_l$ , and the volume integral covers the entire disturbed domain. Since the condition (1.6) holds also on the boundary, the surface integral is annulled a priori so that in terms of the Eddington quantity, we have

$$\int \epsilon^{klm} h^{ij} \partial_{[l} \delta \Gamma_{k]}{}^{ji} dX = 0$$

which means, as far as the disturbances are small,

$$\int k^{ijkl} \delta R_{lkji} dX = 0,$$

where  $R_{lkji}$  is the Riemann-Christoffel curvature tensor and

$$k^{ijkl} = \epsilon^{klm} h^{ij}{}_m.$$

Owing to the equivalence of  $R_{lkji}$  and  $R_{kj}$  in three dimensions, we have

$$\delta R_{lkji} = \delta(b_{lkji}{}^{mn} R_{nm})$$

where  $b_{lkji}{}^{mn}$  may depend on the coordinates, therefore,

$$k^{ijkl} \delta R_{lkji} = k^{ijkl} \delta(b_{lkji}{}^{mn} R_{nm}) = 1/2 \delta(c^{\times mn} R_{nm})$$

where

$$c^{\times mn} = 2k^{ijkl} b_{lkji}{}^{mn} = k^{lp} h^{ij}{}_{p} b_{lkji}{}^{mn}$$

and

$$\delta c^{\times mn} = k^{ijkl} \delta b_{lkji}{}^{mn},$$

viz.,  $c^{\times mn}$  is varied through, and only through, the factor  $b_{lkji}{}^{mn}$ . Anyhow,  $c^{\times mn}$  is varied and the manner of its variation is arbitrary since the coefficients  $h^{ij}{}_p$ 's and hence also  $k^{ijkl}$ 's are arbitrary.

Thus (1.9) is simplified to

$$\delta W = \frac{1}{2} \int \delta(c^{\times mn} R_{nm}) dX = 0, \quad (1.10)$$

so that we have defined the quantity

$$W = \frac{1}{2} \int k^{lmnk} R_{knml} dX \quad (1.8.1)$$

in terms of the tearing and we have

$$k^{lmnk} = c^{\times mn} a^{lk}. \quad (1.11)$$

Thus the proof is complete.

Moreover, we have

$$c^{\times mn} R_{nm} = a'^{\times mn} (I_{nm} + N_{nm})$$

where  $I_{nm}$  is the Einstein-tensor of the Riemannian feature representing the incompatibility and

$$a'^{\times mn} = c^{\times mn} - c^{\times} a^{mn}, \quad c^{\times mn} = a'^{\times mn} - \frac{1}{2} a^{\times} a^{mn}, \quad c^{\times} = c^{\times mn} a_{nm},$$

$$K_{nm} c^{\times mn} = I_{nm} a'^{\times mn}, \quad M_{nm} c^{\times mn} = N_{nm} a'^{\times mn} \quad (1.12)$$

as can easily be calculated.<sup>2</sup> Hence  $\delta W$  splits into <sup>3</sup>

$$\delta U = \frac{1}{2} \delta \int a'^{\times mn} I_{nm} dX \quad (1.13)$$

and

$$\delta V = \frac{1}{2} \delta \int a'^{\times mn} N_{nm} dX.$$

### I.3 Non-periphractic condition

Owing to the restriction to small disturbances involved in the construction of the Equivalence Theorem, the incompatibility tensor can be expressed by

$$I^{mn} = 1/2 \epsilon^{ikm} \epsilon^{jln} \partial_l \partial_k a_{ji}. \quad (1.15)$$

Substituting this expression for  $I^{mn}$  in the foregoing relations, and by integrating by parts, from formula (1.13), we have

$$\delta U = \frac{1}{2} \delta \int I'^{\times ij} a_{ji} dX - \frac{1}{2} \delta \oint L'^{\times kij} a_{ji} dX_k + \frac{1}{2} \delta \oint a'^{\times nm} L^{lmn} dX \quad (1.16)$$

where

$$I'^{\times ij} = 1/2 \epsilon^{ikm} \epsilon^{jln} \partial_l \partial_k a'^{\times nm},$$

$$L'^{\times kij} = 1/2 \epsilon^{ikm} \epsilon^{jln} \partial_l a'^{\times nm}, \quad L^{lmn} = 1/2 \epsilon^{ikm} \epsilon^{jln} \partial_k a_{ji}. \quad (1.17)$$

The asymmetric tensor  $I'^{\times ij}$  can be replaced, as far as it stands in (1.16), by its symmetric part

$$I^{\times ij} = 1/2 \epsilon^{ikm} \epsilon^{jln} \partial_l \partial_k a^{\times nm} \quad (1.17.1)$$

where

$$a^{\times nm} = a'^{\times nm}.$$

<sup>2</sup>  $K_{nm} c^{\times mn} = I_{nm} c^{\times mn} - I a_{nm} c^{\times mn} = I_{nm} c^{\times mn} - I_{kj} a^{jk} c^{\times} = I_{nm} (c^{\times mn} - c^{\times} a^{mn}) = I_{nm} a'^{\times mn};$   
 $M_{nm} c^{\times mn} = N_{nm} c^{\times mn} - N a_{nm} c^{\times mn} = N_{nm} c^{\times mn} - N_{kj} a^{jk} c^{\times} = N_{nm} a'^{\times mn}.$

<sup>3</sup> See (2.2) below.

Similarly  $L'^{\times kij}$  can be replaced, as far as it stands in (1.16), by

$$L'^{\times k(ij)} = 1/2 \epsilon^{(i|km|} \epsilon^{l)n} \partial_l a'_{nm}.$$

On the other hand, the quantity  $L'^{lmn}$  need not be symmetric with respect to  $m$  and  $n$ .

If the material manifold is continuous and simply connected and extends itself to remote regions where no plastic changes are going on, the surface integrals in (1.16) are annulled since the variation of the connection is excluded on the boundary located in such a region. Then  $\delta U$  equals

$$\delta U^\times = \frac{1}{2} \delta \int I'^{ij} a_{ji} dX. \quad (1.16.1)$$

The variational formula of the Equivalence Theorem is then simplified to

$$\delta W = \frac{1}{2} \delta \int (I'^{ij} + J^{ij}) a_{ji} dX = 0$$

(1.18)

where  $J^{ij}$  is defined by

$$J^{ij} a_{ji} = a'^{\times mn} N_{nm}.$$

Henceforth, we shall restrict ourselves to this *non-periphractic condition*. Obviously, then from (1.16) and (1.16.1), we have

$$\delta(U - U^\times) = 0 \quad (1.18.1)$$

and this should be equivalent to (1.18).

## II. Dual Riemannian Space

### II.1. A dual metric

Under the assumption of *non-periphracticity*, the roles of  $a_{ji}$  (or  $a^{ij}$ ) and  $a'_{nm}$  (or  $a'^{\times mn}$ ) can be exchanged mutually in entirely the dual manner between (1.15) and (1.17.1), as they stand in the integrands of the dual expressions  $U$  and  $U^\times$  of one and the same quantity.

Therefore, in order to preserve perfect duality, a new Riemannian space needs to be defined where  $a_{ji}^\times$  and  $I'^{ij}$  play the roles of the metric tensor and of the Einstein-tensor dually to  $a_{ji}$  and  $I^{ij}$ . This new three-dimensional Riemannian space having the fundamental metric form

$$ds^{\times 2} = a_{ji}^\times dx^i dx^j \quad (2.1)$$

can be called the *dual Riemannian space*, which can more realistically be called a *stress-space* or *stress-function space* from the point of view of section II.2.

Once  $ds^{*2}$  has been introduced, the derivation in section I.2 can now be repeated for the dual Riemannian manifold in the dual manner. Furthermore, we may preserve only the symmetric part of the tensor  $a'_{ji}^{\times}$  or  $a'^{\times ij}$  because it only enters into the dual metric form defined by (2.1), we obtain a perfect dual correspondence of:

$$\begin{aligned}\delta W = \delta(U + V) &= \frac{1}{2} \delta \int a^{\times mn} (I_{nm} + N_{nm}) dX \\ &= \frac{1}{2} \delta \int (a^{\times mn} I_{nm} + J_{ji} a^{\circ j}) dX\end{aligned}\quad (2.2)$$

and

$$\begin{aligned}\delta W^{\times} = \delta(U^{\times} + V^{\times}) &= \frac{1}{2} \delta \int a^{\circ j} (I_{ji}^{\times} + N_{ji}^{\times}) dX \\ &= \frac{1}{2} \delta \int (a^{\circ j} I_{ji}^{\times} + J_{nm}^{\times} a^{\times mn}) dX\end{aligned}\quad (2.2.1)$$

where

$$J_{ji} = a^{\times mn} (M_{jmni} - \frac{1}{2} M_{ji} a_{nm}), \quad J_{nm}^{\times} = a^{\circ j} (M_{njim}^{\times} - \frac{1}{2} M_{nm}^{\times} a_{ji}^{\times}).$$

Now that the two variational criteria,

$$\delta W = 0 \quad \text{and} \quad \delta W^{\times} = 0, \quad (2.3)$$

need to be mutually compatible, where the tensors  $a_{ji}$  and  $a_{nm}^{\times}$  alone are varied, producing one and the same configuration, it is necessary that

$$\alpha I_{nm} = J_{(nm)}^{\times} \quad \text{and} \quad I_{ji}^{\times} = \alpha J_{(ji)}, \quad (2.4)$$

and hence

$$\alpha U = V^{\times} \quad \text{and} \quad U^{\times} = \alpha V.$$

Hence the two formulae of (2.3) are unified into

$$\begin{aligned}\delta W = \delta(U + V) &= \delta(\alpha U + U^{\times})/\alpha = \delta(V + \alpha V)/\alpha \\ &= \delta(V^{\times} + U^{\times})/\alpha = \delta W/\alpha = 0.\end{aligned}\quad (2.4.1)$$

However, owing to the assumption of the non-periphractic condition (2.4.1) needs to be in conformance with (1.18.1). Hence

$$\alpha = -1 \quad (2.5)$$

is required.

## II.2. Concepts of stress, stress function and energy

The quantities such as  $U$ ,  $V$ , and  $W$  can be given the dimensions of what we call *energy* if the quantities, such as  $I^{\times ij}$  and for  $J^{ij}$  standing as the coefficient of  $a_{ji}$  in the integrand of the energy  $U$  and/or  $V$  need to have the dimensions of *stress* since  $a_{ji}$  has the dimensions of strain. With such a specialization, we can assume that the variational criterion (2.3) or (1.18.1) agrees with the *principle of conservation of energy at plastic changes*.

The stress  $I^{\times ij}$  is symmetric and its field is non-divergent as is easily proved, so that it has especially the character of the stress tensor applicable to problems of statical equilibrium. The stress field having its structure has been studied by E. Beltrami [3], H. Schaefer [4], etc. We shall call it the *Beltrami feature*. The restriction (2.4) under (2.5) i.e.,  $J^{ij} = I^{\times ij}$  may be called a *Beltramization*.

The Riemannian deviation of the dual metric tensor,

$$\chi_{ji} = -\theta_{ji}^{\times} = 1/2(\delta_{ji} - a_{ji}^{\times}),$$

turns out to be the *Beltrami stress function*. We have

$$I^{\times ij} = -\epsilon^{ikm}\epsilon^{jln}\partial_l\partial_k\chi_{nm}$$

as the expression of the Beltrami stress in terms of the stress functions. Its extension to  $I'_{ji}^{\times}$  will be called the *asymmetric Beltrami feature*.

## III. Energy Criterion for Full Asymmetry

So far only the stress-function metric has been susceptible of a modification to asymmetry whereas the strain metric has been treated as symmetric. Full duality could not be claimed until both have been extended to asymmetry. This will be done next.

### III.1. Extension of the strain-incompatibility from symmetry to asymmetry by an isoperimetric criterion

The antisymmetric part of  $I'^{\times ij} + J^{ij}$  did not contribute at all to the varied energy  $\delta W$  in the formula (1.18) where no finite boundaries come about. Such a situation is entailed where the isoperimetric condition

$$Q = 1/2(I'^{\times[ij]} + J^{ij})\lambda_{[ji]}dX = \text{const.} \quad (3.1)$$

is imposed with Lagrangian multipliers  $\lambda_{ji}$ . Under this restriction, without affecting the fundamental implication, one can substitute for the  $W$ , in the original formula (1.18) the modified energy

$$W' = W + Q = U' + V',$$

where

$$U' = U + 1/2 \int I'^{\times(ij)} \lambda_{ji} dX \quad (3.2)$$

and

$$V' = V + 1/2 \int J^{\{ij\}} \lambda_{ji} dX. \quad (3.3)$$

Therefore, without affecting the fundamental implication, the variational formula is modified to:

$$\delta W' = \frac{1}{2} \delta \int (I'^{\times ij} + J'^{ij}) a'_{ji} dX = 0. \quad (3.4)$$

where

$$a'_{ji} = a_{ji} + \lambda_{[ji]}. \quad (3.5)$$

As is well known, the subsidiary condition such as (3.1) can be neglected so long as the multipliers such as  $\lambda_{[ji]}$  are restricted to certain characteristic cases which are fixed by the problem itself.<sup>4</sup>

Once the asymmetric tensor  $a'_{ji}$  is so substituted for  $a_{ji}$ , the entire formalism included in the proof of the Equivalence Theorem can also be repeated, though approximately, as follows, to confirm (3.4). Especially, formula (1.16) is generalized to:

$$\delta U' = \frac{1}{2} \delta \int a'_{ji} I'^{\times ij} dX - \frac{1}{2} \delta \oint a'_{ji} L'^{\times kij} dX_k + \frac{1}{2} \delta \oint a'_{nm} L'^{lmn} dX_l \quad (3.6)$$

where  $a_{ji}$ ,  $I^{mn}$ ,  $L^{lmn}$  and  $U$  have been replaced by  $a'_{ji}$ ,

$$I'^{mn} = 1/2 \epsilon^{ikm} \epsilon^{jln} \partial_l \partial_k a'_{ji}, \quad L'^{lmn} = 1/2 \epsilon^{lkm} \epsilon^{jln} \partial_k a'_{ji} \quad (3.7)$$

and

$$U' = \frac{1}{2} \int I'^{mn} a'_{nm} dX. \quad (3.7.1)$$

Dually we have, by simple rearrangement of (3.6),

$$\delta U'^{\times} = \frac{1}{2} \delta \int a'_{nm} I'^{mn} dX - \frac{1}{2} \delta \oint a'_{nm} L'^{lmn} dX_l + \frac{1}{2} \delta \oint L'^{\times kij} a'_{ji} dX_k$$

where

$$U'^{\times} = \frac{1}{2} \int a'_{ji} I'^{\times ij} dX. \quad (3.8)$$

Or

$$\delta(U' - U'^{\times}) - \delta(\omega' - \omega'^{\times}) = 0 \quad (3.6.2)$$

where

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<sup>4</sup> See e.g., reference [5].

$$\begin{aligned}\omega' &= \frac{1}{2} \oint a'_{nm} L'^{lmn} dX_l, \\ \omega'^{\times} &= \frac{1}{2} \oint a'_{ji} L'^{\times kij} dX_k.\end{aligned}\tag{3.9}$$

If the periphractic effect represented by the surface integrals  $\delta\omega'$  and  $\delta\omega'^{\times}$  are neglected, (3.9) is reduced to

$$\delta(U' - U'^{\times}) = 0\tag{3.10}$$

which is the obvious generalization of the symmetric non-periphractic formula (1.18.1). In that case, it follows that  $U'$  and  $U'^{\times}$ , as well as  $U$  and  $U^{\times}$ , are mutually transformed.

In this extension the concept of stress is generalized to include:

- (i) not only the symmetric Beltrami feature which gives the non-divergent symmetric energy tensor  $J^{ij} = -I^{\times ij}$ ,
- (ii) but also an antisymmetric Beltrami feature which gives the non-divergent antisymmetric tensor  $J^{[ij]} = -I^{\times [ij]}$ .
- (iii) The quantities  $I^{mn}$  (incompatibility) and  $L^{lmn}$  are also extended to the asymmetric features,  $I'^{mn}$  and  $L'^{lmn}$ .

### III.2. Variation of an approximate affine connection

The affine connection is transformed from the  $\Gamma_{kji}$  of the foregoing to:

$$\Gamma'_{kji} = 1/2 (\partial_j a'_{ki} + \partial_k a'_{ji} - \partial_i a'_{kj}) + T_{kji},$$

where  $a'_{ji}$  is an asymmetric tensor whose symmetric part agrees with the metric tensor<sup>5</sup> and  $T_{kji}$  is a tensor as before. Then, when referred to the Cartesian rectangular coordinates of the unnaturalized state, the difference

$$\Gamma'_{kji} - \Gamma_{kji} = 1/2 (\partial_j \hat{a}'_{ki} + \partial_k \hat{a}'_{ji} - \partial_i \hat{a}'_{kj}),$$

which depends solely on the antisymmetric feature

$$\hat{a}'_{ji} \stackrel{\text{def}}{=} \lambda_{[ji]},$$

is not distinguished from

$$1/2 (\nabla_j \hat{a}'_{ki} + \nabla_k \hat{a}'_{ji} - \nabla_i \hat{a}'_{kj})$$

which is a tensor, so long as the disturbances are small. Hence

<sup>5</sup> We would refrain from calling it an asymmetric metric tensor. In strict sense, more geometrical constructions are needed for doing so.

$$\Gamma'_{kj}^i = \begin{Bmatrix} i \\ kj \end{Bmatrix} + T'_{kj}^i$$

is also *approximately* an affine connection since

$$T'_{kji} = T_{kji} + 1/2(\partial_j \hat{a}'_{ki} + \partial_k \hat{a}'_{ji} - \partial_i \hat{a}'_{kj})$$

is approximately a tensor.

Therefore, one can proceed in a way similar to the construction in section I.1 to obtain the variational function

$$W' = \frac{1}{2} \int k'^{ijkl} R'_{lkji} dX,$$

where

$$R'_{lkji} = 2\partial_{[l} \Gamma'_{kj]i},$$

small insignificant terms being neglected, and

$$k'^{ijkl} = c^{\times jk} c^{il}$$

where  $c^{il}$  is the dual of  $c^{\times jk}$ , i.e.,

$$c^{il} = a'^{il} - 1/2aa^{\times il}.$$

### III.3. Couple stress of the Beltramic feature

We have

$$S_{kji} \stackrel{*}{=} \partial_{[k} \theta_{j]i}, S_{lmn}^{\times} \stackrel{*}{=} \partial_{[l} \theta_{n]m}^{\times}, I^{mn} = \partial_l L^{lmn} = \partial_l (\epsilon^{mli} \epsilon^{nkj} S_{kji})$$

and

$$I^{\times ij} = \partial_k L^{\times kij} = \partial_k (\epsilon^{ikm} \epsilon^{jln} S_{lmn}^{\times}).$$

The quantity  $S_{kji}$  so defined is a torsion tensor introduced into the space of strain and incompatibility by what we have called in section I.1 a *perfect tearing* of the metric  $ds^2$ ; and the quantity  $S_{lmn}^{\times}$  is its dual. The latter is a torsion tensor introduced into the space of stress and stress function by a perfect tearing of the metric which will be called a *dual perfect tearing*.

Since  $-J^{(ij)} = I^{\times ij}$  is a stress of the Beltrami feature,  $L^{\times kij}$  is a kind of stress function. We shall call it a *derived stress function*. Its antisymmetric extension  $L'^{\times k[ij]}$  is related to the antisymmetric Beltrami stress by

$$-J^{[ij]} = \partial_k L'^{\times k[ij]}.$$

Hence it is a *couple stress*, as is well known.

The derived stress-function tensor  $L'^{kij}$  is given as a homogeneous linear function of the torsion tensor of a dual perfect tearing without dual rotations and the couple stress tensor  $L'^{\times k[ij]}$  is given as a homogeneous linear function of the torsion tensor of dual incompatible rotation.

The significant part of the couple stress in yielding the antisymmetric stress is

$$\hat{L}'^{kij} = \epsilon^{ikm} \epsilon^{jln} \hat{S}^{\times}_{lmn},$$

where

$$\hat{S}^{\times}_{lmn} = \partial_{[l} a'^{\times}_{n]m}$$

is a torsion tensor, given as the difference of two dual perfect tearings or two *dual incompatible rotation distributions*, dual to

$$\hat{S}_{kji} = \partial_{[k} a'^{\times}_{j]i}$$

which is the torsion tensor associated with an *incompatible rotation distribution*.

## IV. A Constitutional Construction of the Theory of Yielding and Dual Yielding

### IV.1. Multidimensional enveloping spaces of the asymmetric Beltramic features

We have obtained the extended variational formula (3.6.2). Its reduction to (3.10) can be effected even if the geometrical structure of the material is not perfectly non-periphractic, as follows.

If the disturbances are sufficiently small, we can set

$$\delta(\omega' - \omega'^{\times}) = \frac{1}{2} \oint (\delta_{nm} \delta L'^{lmn} dX_l - \delta_{ji} \delta L'^{\times kij} dX)$$

where  $L'^{lmn}$  and  $L'^{\times kij}$  are linear and homogeneous in

$$S'_{kji} = S_{kji} + \hat{S}_{kji} \text{ and } S'_{lmn} = S^{\times}_{lmn} + \hat{S}^{\times}_{lmn}$$

respectively. Hence, so long as the varied dislocational and dual dislocational fields are compensated by the incompatible rotations and dual rotations to satisfy respectively

$$L'^{(\nu)mn} = L'^{\times(\nu)ij} = 0 \quad (4.1)$$

on the boundary, where  $(\nu)$  indicates the direction of the surface normal,

(3.10) can be assumed. We shall restrict ourselves to such a case, so that we have

$$\delta W' = \frac{1}{2} \int (a'^{ij} \delta I'_{ji} - \delta a'_{ji} I'^{ij}) dX + \frac{1}{2} \int (\delta a'^{ij} I'_{ji} - a'_{ji} \delta I'^{ij}) dX = 0 \quad (4.2)$$

where we can put

$$a'_{ji} = \delta_{ji} + \sum_{\Lambda} \partial_j w^{\Lambda} \partial_i v^{\Lambda} \quad (4.3)$$

and

$$a'^{\times}_{ji} = \delta_{ji} + \sum_N \partial_j w^{\times M} \partial_i v^{\times M} \quad (4.4)$$

both  $\Lambda$  and  $M$  running from 1 to sufficiently large integers.

A more general treatment without assuming (4.1) is also feasible. Its analysis will be reported elsewhere.

By inserting (4.3) and (4.4) respectively into (3.7) and (1.17), we have

$$I'^{ij} = 1/2 \epsilon^{ikm} \epsilon^{jln} \sum \partial_k \partial_n w \partial_l \partial_m v \quad (4.5)$$

and

$$I'^{\times ij} = 1/2 \epsilon^{ikm} \epsilon^{jln} \sum \partial_k \partial_n w^{\times} \partial_l \partial_m v^{\times}, \quad (4.5.1)$$

where the indices  $\Lambda$  and  $M$  are suppressed.

## IV.2. Fundamental equations of yielding and dual yielding

The general variational criterion (4.2) is reduced to

$$\frac{1}{2} \int (a'^{ij} \delta I'_{ji} - \delta a'_{ji} I'^{ij}) dX = 0 \quad (4.2.1)$$

if the stress-function-stress configuration is unvaried, i.e., if

$$\delta a'^{\times}_{ji} = 0, \delta I'^{\times ij} = 0$$

and to

$$\frac{1}{2} \int (\delta a'^{\times}_{ji} I'^{ij} - a'^{ij} \delta I'^{\times}_{ji}) dX = 0 \quad (4.2.2)$$

if the strain-incompatibility is unvaried, i.e., if

$$\delta a'_{ji} = 0, \delta I'^{ij} = 0.$$

Substituting from (4.5), we have

$$\begin{aligned} \frac{1}{2} \int a'_{ji} \times \delta I'^{ij} dX &= \frac{1}{4} \sum \int a'_{ji} \epsilon^{ikm} \epsilon^{jln} \delta \{ (\partial_k \partial_n w) \partial_l \partial_m v \} dX \\ &= \frac{1}{2} \sum \int B^{klmn} \{ (\partial_k \partial_n \delta w) \partial_l \partial_m v + (\partial_k \partial_n w) \partial_l \partial_m \delta v \} dX \end{aligned} \quad (4.6)$$

where

$$B^{klmn} = \frac{1}{2} a'_{ji} \times \epsilon^{ikm} \epsilon^{jln} = \frac{1}{2} a'_{ji} \times \begin{vmatrix} \delta^{ij} & \delta^{il} & \delta^{in} \\ \delta^{kj} & \delta^{kl} & \delta^{kn} \\ \delta^{mj} & \delta^{ml} & \delta^{mn} \end{vmatrix}. \quad (4.7)$$

By integration by parts, one can transform (4.6) further:

$$\begin{aligned} \frac{1}{2} \int a'_{ji} \times \delta I'^{ij} dX &= \frac{1}{2} \sum \oint \partial_k \delta w B^{klmn} \partial_l \partial_m v dX_n + \frac{1}{2} \sum \oint \partial_l \delta v B^{klmn} \partial_k \partial_n w dX_m \\ &\quad - \frac{1}{2} \sum \oint \delta w \partial_n (B^{klmn} \partial_l \partial_m v) dX_k - \frac{1}{2} \sum \oint \delta w \partial_m (B^{klmn} \partial_k \partial_n w) dX_l \\ &\quad + \frac{1}{2} \sum \int \delta w \partial_k \partial_n (B^{klmn} \partial_l \partial_m v) dX + \frac{1}{2} \sum \int \delta v \partial_l \partial_m (B^{klmn} \partial_k \partial_n w) dX. \end{aligned} \quad (4.8)$$

Also, we have, by substituting from (4.5),

$$\begin{aligned} \frac{1}{2} \int I'^{\times ij} \delta a'_{ji} dX &= \frac{1}{2} \sum \int I'^{\times ij} \{ (\partial_j \delta w) \partial_i v + \partial_j w (\partial_i \delta v) \} dX \\ &= \frac{1}{2} \sum \oint \delta w I'^{\times ij} \delta_i v dX_j + \frac{1}{2} \sum \oint \delta v I'^{\times ij} \partial_j w dX_i \\ &\quad - \frac{1}{2} \sum \int \delta w \partial_j (I'^{\times ij} \partial_i v) dX - \frac{1}{2} \sum \int \delta v \partial_i (I'^{\times ij} \partial_j w) dX. \end{aligned} \quad (4.9)$$

Similarly for

$$\frac{1}{2} \int a'_{ji} \delta I'^{\times ij} dX \text{ and } \frac{1}{2} \int I'^{ij} \delta a'_{ji} \times dX.$$

Inserting these relations (4.8) and (4.9) into (4.2.1), we have

$$\begin{aligned}
& \frac{1}{2} \sum \int \delta w \{ \partial_k \partial_n (B^{klmn} \partial_l \partial_m v) + \partial_j (I'^{\times ij} \partial_i v) \} dX \\
& + \frac{1}{2} \sum \oint \delta w \{ -\partial_n (B^{klmn} \partial_l \partial_m v) - I'^{\times ik} \partial_i v \} dX_k \\
& + \frac{1}{2} \sum \oint \partial_k \delta w B^{klmn} \partial_l \partial_m v dX_n \\
& + \frac{1}{2} \sum \int \delta v \{ \partial_l \partial_m (B^{klmn} \partial_k \partial_n w) + \partial_i (I'^{\times ij} \partial_j w) \} dX \\
& + \frac{1}{2} \sum \oint \delta v \{ -\partial_m (B^{klmn} \partial_k \partial_n w) - I'^{\times ij} \partial_j w \} dX_l \\
& + \frac{1}{2} \sum \oint (\partial_l \delta v) (B^{klmn} \partial_k \partial_n w) dX_m = 0.
\end{aligned} \tag{4.10}$$

Arbitrary values need to be allowed for  $\delta v$ ,  $\delta w$ ,  $\partial_k \delta w$ ,  $\partial_l \delta v$  in the interior and on the boundary of the material body so that their coefficients in the integrands of the volume and surface integrals standing in (4.10) need to vanish separately. Thus we obtain the field equations

$$\boxed{\begin{aligned} \partial_k \partial_n (B^{klmn} \partial_l \partial_m v) + I'^{\times ij} \partial_j \partial_i v &= 0 \\ \partial_l \partial_m (B^{klmn} \partial_k \partial_n w) + I'^{\times ij} \partial_i \partial_j w &= 0 \end{aligned}} \tag{4.11}$$

where non-divergence of  $I'^{\times ij}$  is taken account of, and the associated boundary conditions for free surfaces which are derived from the surface integral of (4.10).

Similarly for the dual restriction (4.2.2), we obtain

$$\boxed{\begin{aligned} \partial_k \partial_n (B^{\times klmn} \partial_l \partial_m v^\times) + I^{\times ij} \partial_j \partial_i v^\times &= 0 \\ \partial_l \partial_m (B^{\times klmn} \partial_k \partial_n w^\times) + I^{\times ij} \partial_j \partial_i w^\times &= 0 \end{aligned}} \tag{4.11.1}$$

where the non-divergence of  $I^{\times ij}$  is taken account of, and the associated free boundary conditions which are derived dually to the foregoing, where

$$B^{\times klmn} = \frac{1}{2} a'_{ji} \epsilon^{ikm} \epsilon^{jln} = \frac{1}{2} a'_{ji} \begin{vmatrix} \delta^{ij} & \delta^{il} & \delta^{in} \\ \delta^{kj} & \delta^{kl} & \delta^{kn} \\ \delta^{mj} & \delta^{ml} & \delta^{mn} \end{vmatrix}. \tag{4.7.1}$$

The equations (4.11) etc. have the same form as the equations of yielding which have been proposed ([16]–[10] etc.) where  $I^{\times ij} = I'^{\times ij}$  plays the role of the critical stress tensor and  $B^{klmn}$  that of the plastic material tensor. The equations (4.11.1) etc. have the same form as the equations of dual yielding which have recently been proposed ([11]–[13] etc.) where  $I^{ij} = I'^{ij}$  plays the role of the critical incompatibility and  $B^{\times klmn}$  that of the dual material tensor for fatigue. As can easily be calculated,

$$B^{klmn} = -2c^{\times[k][l].\delta[m][n]} \quad (4.12)$$

and

$$B^{\times klmn} = -2c^{[k][l].\delta[m][n]} \quad (4.13)$$

where  $c^{\times kl}$  has been defined above and by approximation

$$c^{\times kl} = a^{\times kl} - 1/2a^{\times}\delta^{kl} \quad (4.14)$$

and dually

$$c^{kl} = a'^{kl} - 1/2a\delta^{kl}. \quad (4.14.1)$$

Since the difference of  $a^{mn}$  and  $\delta^{mn}$  ( $a^{\times mn}$  and  $\delta^{\times mn}$ ) is neglected, owing to (1.11) and its dual, we have

$$B^{klmn} = 2k^{[km][ln]} \quad (4.12.1)$$

and

$$B^{\times klmn} = 2k^{\times[km][ln]} \quad (4.13.1)$$

where

$$k^{\times lmnk} = c^{mn}\delta^{kl}.$$

The structures of these material tensors  $B^{klmn}$  and  $B^{\times klmn}$  agree perfectly with the ones obtained by the previous analysis for yielding and dual yielding, as will further be shown for symmetric stress and incompatibility fields.

### IV.3. Reduction to symmetry

In the field equations (4.11) and (4.11.1), only the symmetric parts,  $I^{\times ij}$  and  $I'^{ij}$ , of the primarily asymmetric tensors,  $I^{\times ij}$  and  $I'^{ij}$ , come about, their antisymmetric parts being involved only in the boundary conditions. There can also be a special case in which the antisymmetric features are excluded entirely even in the boundary conditions. A well established geometrical interpretation is associated with this simplified case, as follows.

This is given by

$$v = w \quad (4.15)$$

so that

$$a'_{ji} = a_{ji} = a_{ij}$$

and the initial variational relations (4.2.1) and (4.2.2) are reduced to

$$\frac{1}{2} \int (a^{\times ij} \delta I_{ji} - \delta a_{ji} I^{\times ij}) dX = 0 \quad (4.16)$$

and the initial variational relations (4.2.1) and (4.2.2) are reduced to

$$\frac{1}{2} \int (a^{\times ij} \delta I_{ji} = \delta a_{ji} I^{\times ij}) dX = 0 \quad (4.17)$$

and

$$\frac{1}{2} \int (\delta a_{ji}^{\times} I^{ij} - a^{ij} \delta I_{ji}) dX = 0. \quad (4.18)$$

These can also be transformed, by tracing back the transformations such as from (1.8.1) to (1.13) etc., to:

$$\frac{1}{2} \int (k^{klmn} \delta K_{nmlk} - \delta a_{ji} I^{\times ij}) dX = 0 \quad (4.17.1)$$

etc., where  $k^{klmn}$  etc. have been defined by (1.11) and its dual.

On the other hand, (4.10) is reduced to

$$\begin{aligned} & \sum \int \delta w \{ \partial_k \partial_n (B^{klmn} \partial_l \partial_m) + I^{\times ij} \partial_j \partial_i w \} dX \\ & + \sum \oint \delta w \{ -\partial_n (B^{klmn} \partial_l \partial_m w) - I^{\times ik} \partial_i w \} dX_k \\ & + \sum \oint \partial_k \delta w B^{klmn} \partial_l \partial_m w dX_n = 0 \end{aligned} \quad (4.19)$$

where the symmetric structure of

$$B^{klmn} = B^{[km][ln]} = B^{[ln][km]}$$

is considered. The resulting field equation and the boundary conditions are not at all altered from the foregoing except that only the symmetric

stress enters the equations. By integration by parts, (4.19) can be brought back to

$$\int \{ 2c^{\times[k][l]} \delta^{[m][n]} \sum \partial_n \partial_k \delta w \partial_l \partial_m w - I^{\times ij} \sum (\partial_j w \partial_i \delta w) \} dX = 0$$

or

$$\int \{ k^{mkln} \delta (2H_{[n|[k]} \wedge H_{[l]m]}) - I^{\times ij} \theta_{ji} \} dX = 0 \quad (4.19.1)$$

where

$$\theta_{ji} = 1/2 \partial_j w \partial_i w$$

and

$$H_{nk}{}^\Lambda = \partial_n \partial_k w^\Lambda. \quad (4.20)$$

Comparing (4.17.1) and (4.19.1) we have

$$K_{nlmk} = 2H_{[n|[k]} \wedge H_{[l]m]}. \quad (4.21)$$

The last relation (4.21) has the structure of the well established formulae in Riemannian geometry which expresses the imbedding of the Riemannian manifold in a multidimensional Euclidean space of locally six dimensions. The three-index quantity  $H_{nk}{}^\Lambda$  represents its relative curvature of the Riemannian subspace relative to the enveloping Euclidean space.<sup>6</sup> Formula (4.20) is its approximate expression as far as the deviation of the Riemannian configuration from the Euclidean condition is small and represented by the multidimensional Cartesian coordinates are  $w^\Lambda$ .

It is hardly necessary to point out that the eq (4.7.1) or (4.19.1) is the initial variational criterion with which we have started in our previous formulation of our theory of yielding to define the yield point as a stability limit with the critical condition for the stress at which the material manifold leaves the Euclidean configuration in regard to its strain-incompatibility metric to be curved into the enveloping space obtaining the relative curvature  $H_{nk}{}^\Lambda$ .

In entirely a dual manner, we have formulated our theory of dual yielding to define the dual yield point as another stability limit with the critical condition for the incompatibility at which the material manifold leaves the Euclidean configuration in regard to its stress-function-stress metric.

#### IV.4. Average isotropy

In order to confirm that the foregoing formulation of yielding and dual yielding is not trivial, it is necessary to ascertain that the tensors  $B^{ijkl}$  and  $B^{\timesijkl}$  are not zero tensors.

<sup>6</sup> cf. e.g. references [14], [15] etc.

Some components of  $B^{ijkl}$  and  $B^{\times i j k l}$  vanish identically whatever the reference axes:

$$B^{iiii} = 1/2 (a^{\times ii} \delta^{ii} - a^{\times ii} \delta^{ii} - a^{\times ii} \delta^{ii} + a^{\times ii} \delta^{ii}) = 0,$$

$$B^{iijj} = 1/2 (a^{\times ij} \delta^{ij} - a^{\times ij} \delta^{ij} - a^{\times ij} \delta^{ij} + a^{\times ij} \delta^{ij}) = 0$$

and similarly for  $B^{\times iiii}$  and  $B^{\times iiji}$ . The sole nonzero components are

$$B^{ijji} = 1/2 (a^{\times ii} \delta^{jj} + a^{\times jj} \delta^{ii} - 2a^{\times ij} \delta^{ij}) \quad (4.22)$$

and

$$B^{\times iiji} = 1/2 (a^{ii} \delta^{jj} + a^{jj} \delta^{ii} - 2a^{ij} \delta^{ij}) \quad (4.22.1)$$

where

$$i \neq j. \quad (4.23)$$

Owing to the restriction (4.23), the formulae (4.22) and (4.22.1) are further reduced to

$$B^{ijji} = 1/2 (a^{\times ii} \delta^{ij} + a^{\times ij} \delta^{ii}) \quad (4.22.2)$$

and

$$B^{\times iiji} = 1/2 (a^{ii} \delta^{ij} + a^{jj} \delta^{ii}). \quad (4.22.3)$$

If some restriction is imposed on the structure of the material, further restriction will be entailed. For example, if the material is perfectly isotropic, all the components, i.e., not only  $B^{iiii}$ ,  $B^{ijji}$  etc. but also  $B^{ijkl}$  etc., need to vanish so that the tensors  $B^{ijkl}$  and  $B^{\times i j k l}$  are reduced to zero tensors. Therefore, the foregoing formulation loses its ground for absolutely isotropic materials. It is necessary that the material has some anisotropic or crystalline structure in order that the equations of yielding and dual yielding, (4.11), (4.11.1), etc., are not insignificant.

A drastic implication seems to be connected with this recognition since our previous investigations of various possibilities of types of yielding and dual yielding have mostly been based on the assumption of an isotropic material ([11], [16] ~ [17], etc.). It might appear as if they are all entirely meaningless!

Rescue comes, however, from the microscopically nonuniform structure of the apparently isotropic material, such as mild steel which is polycrystalline. In such a case, the plastic property has to be recognized through, and only through, the average behaviour depending on the statistical average over quite a number of grain crystals which have different orientations from one another (see fig. 1). This is the case, in particular, for the material tensor  $B^{ijkl}$  and/or  $B^{\times i j k l}$ .

Therefore, we have to substitute in the fundamental equations, the average plastic constants,

$$\bar{B}^{\overline{ijkl}} = \frac{1}{2} \sum_{i,j} (a^{+ii} \bar{O}_j^i \bar{O}_j^i \delta^{jj} \bar{O}_j^j \bar{O}_j^j - a^{+jj} \bar{O}_j^j \bar{O}_j^j \delta^{ii} \bar{O}_i^i \bar{O}_i^i) \quad (4.24)$$

etc. where  $O_i^{\bar{i}}$  etc. indicate orthogonal transformations from the axes of  $i, j$  etc. to those of  $\bar{i}, \bar{j}, \bar{k}, \bar{l}$  and the bars indicate the mean values over all possible directions of the latter sets of axes.

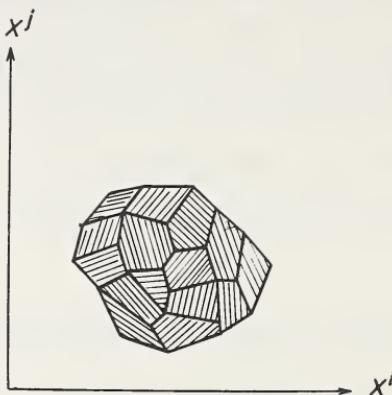


FIGURE 1. Polycrystalline structure

The apparent macroscopic directions indicated by  $\bar{i}, \bar{j}, \bar{k}, \bar{l}$  can be taken along any of the rectangular axes. But the directions indicated by  $i$  and  $j$  are restricted to be mutually orthogonal so that their relations to one and the same fixed mean direction, say of  $\bar{i}$ , are not even statistically the same (cf. fig. 2). Therefore, the first and the second term on the right-hand side of (4.24) need not cancel each other (cf. [18]):

$$\sum_i a^{\times ii} O_i^{\bar{i}} O_i^{\bar{i}} \neq \sum_j a^{\times jj} O_j^{\bar{i}} O_j^{\bar{i}}$$

and

$$\sum_j \delta^{ij} O_j^{\bar{i}} O_j^{\bar{j}} \neq \sum_i \delta^{ii} O_i^{\bar{i}} O_i^{\bar{j}}$$

so that

$$\bar{B}^{\bar{i}\bar{i}\bar{i}\bar{i}} = \text{const.} \left( \sum_i a^{\times ii} O_i^{\bar{i}} O_i^{\bar{i}} - \sum_j a^{\times jj} O_j^{\bar{i}} O_j^{\bar{i}} \right) \delta^{\bar{i}\bar{i}} \neq 0,$$

and

$$\bar{B}^{\bar{i}\bar{j}\bar{i}\bar{j}} = \text{const.} \left( \sum_i a^{\times ii} O_i^{\bar{i}} O_i^{\bar{j}} \right) \left( \sum_j \delta^{ij} O_j^{\bar{i}} O_j^{\bar{j}} - \sum_i \delta^{ii} O_i^{\bar{i}} O_i^{\bar{j}} \right) \neq 0.$$

Similarly for  $\bar{B}^{\times\bar{i}\bar{j}\bar{k}\bar{l}}$ .

It is a straightforward analogy with the theory of elasticity that the four-index tensor  $B^{ijkl}$  which is symmetric with respect to  $i$  and  $k$ ,  $j$  and  $l$  and  $(ik)$  and  $(jl)$  has two, and only two, independent components in

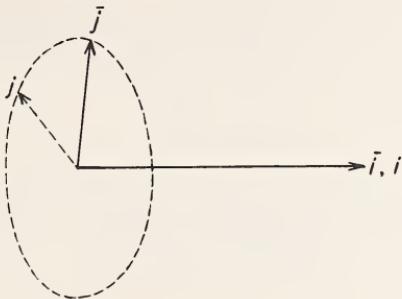


FIGURE 2. Statistical distribution of coordinate axes

the case of isotropy. Hence  $\bar{B}^{iiii}$  and  $\bar{B}^{ijji}$  are sufficient for describing the average macroscopic property.

Writing  $\bar{B}$  for  $\bar{B}^{iiii}$  and  $-\kappa\bar{B}$  for  $\bar{B}^{ijji}$ , we have:

$$\begin{aligned}\bar{U} = & \frac{1}{2} \sum \int \left\{ \bar{B} \sum_{i=1}^3 \left( \partial_{\bar{i}} \partial_i w \right)^2 - 2\kappa \sum_{\bar{i} \neq \bar{j}} \left( \partial_{\bar{j}} \partial_{\bar{i}} w \right) \partial_{\bar{i}} \partial_i w \right. \\ & \left. + 2(1+\kappa) \sum_{j \neq i} \left( \partial_{\bar{j}} \partial_i w \right)^2 \right\} dX.\end{aligned}$$

The equations of yielding are correspondingly simplified to

$$\boxed{\bar{B} \Delta \Delta w + I^{\times} \partial_{\bar{j}} \partial_{\bar{i}} w = 0}$$

and

$$\begin{aligned}(1+\kappa) \bar{B} \partial_{(\nu)} \partial_{(\nu)} \Delta w - \kappa \bar{B} \Delta w &= 0, \\ (2+\kappa) \bar{B} \partial_{(\nu)} \Delta w - (1+\kappa) \bar{B} \partial_{(\nu)} \partial_{(\nu)} \partial_{(\nu)} w + I_{(\nu)}^{\times} \partial_{\bar{i}} w &= 0\end{aligned}$$

etc. where  $\Delta$  is the Laplacian operator.

Similarly for the equations of dual yielding.

It was with these isotropic forms that our previous analysis of yielding and dual yielding has been performed on various special problems.

## V. References

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# DERIVATION OF A CONTINUUM THEORY OF DISLOCATIONS ON THE BASIS OF AN ESTIMATIVE ANALYSIS OF CRYSTAL LATTICES

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Starting from the non-primitive crystal lattice model, a continuum theory is derived by means of an interpolation procedure which takes into account the variability of kinematic and dynamic fields. The non-holonomy of the fields of displacements, energy and entropy is considered in order to elaborate the analysis of dislocation and irreversible effects.

**Key words:** Continuum mechanics; dislocation field theory; statistical methods.

The correspondence between single crystal lattices and continuous models appears to be satisfactory for a limited range of the physical parameters. In the case of more complex lattices or for large ranges of variations of the physical parameters, it seems necessary to estimate the errors of correspondence and to improve the precision of continuous models by means of a more systematic deduction.

Continuous models such as oriented bodies [1-3], multidimensional [4], multipolar [5, 6], and dual media [7] belong to a particular description valid for specific intervals of variation of experimental data. If an interpolation procedure is performed, a more complete modeling can be achieved. A consequence of such procedures is the endowment of the models with non-local features. The non-locality was considered in an early work by Cauchy; afterwards integral constitutive equations were formulated [8] or derived from the adiabatic Born-Oppenheimer approximation for periodic lattices in the frame of linear elasticity [9-13]. The employment of a functional apparatus arises, in the customary way, but difficulties in an effective correspondence, increase sensibly in the case of non-primitive lattices [16-19], not to mention more intricate aspects such as non-linearity, flow and dislocations.

The relatively efficient and simple description of certain structural theories [21-22] which probably can be extended to the analysis of quantum models [23] and the theory of dislocations [24-29] and disclinations [30-34], as well as correlation type theories—for instance connecting the dislocations with plastic strain [35]—suggested under-

taking the present analysis by further taking into account real non-linear behaviour and irreversible processes. As a first step toward this end an interpolation method is developed which utilizes a functional apparatus in a way which tends to avoid the restrictions pointed out above.

The above mentioned theories [21–35] proceed with deductions founded on the assumptions formulated in finite terms, series, or asymptotic expansions [15] (as for instance in non-linear elasticity theories [37–41] and shell theory [42–53]) more or less connected with real lattices. A second type of analysis develops a systematic characterization of the variation of the field values which thereby implies a synthetic extension of the functional apparatus. Finally, as is done here, one can use an approach which identifies the characteristics of the field variable by means of pseudo-differential operators [52–62]. These allow consideration of different types of singularities of motion in the lattice.

The physical properties of the lattices are condensed by using a modified energy tensor which permits a subsequent deduction of constitutive anelastic equations eventually in connection with specific energetic theories postulated by means of conditions of flow [63], activation [64], etc.

The assumptions which have been adopted extend the initial frame of analysis, since no particular potentials or spatial distribution of matter are involved. Meanwhile, the malleable character of the adopted description helps to emphasize the essential features of lattices.

Because of the more extensive analysis given here the treatment tends to be more realistic especially in view of subsequent derivations of particular constitutive equations and of different kinds of incompatibility conditions for kinematic and dynamic fields. The case of non-primitive lattices is also considered in another paper in order to avoid an excessive development.

## I. Structures in a Crystal Lattice

We consider a material structure which corresponds to the physical model of a non-primitive crystal with internal energy dependent on the relative positions of the particles (ions).

According to the model considered, the positions of the ions are to be defined by two sets of points called the *primary* and *secondary* structures ( $\mathcal{P}$  and  $\mathcal{S}$ ) so that any point  $p$  of  $\mathcal{P}$ , referred to a Cartesian coordinate system  $(x^{ip})$ , there is located a particle interacting with a set of other ions located at the points  $s$  belonging to a set  $\mathcal{S}^p$  of  $\mathcal{S}$ .

If it is possible to distinguish a macrostructure  $P$  and a microstructure  $\Pi$  of the primary structure  $\mathcal{P}$  and also a macro and microstructure  $S, \Sigma$  of the secondary structure  $\mathcal{S}$ , we shall consider the coordinates  $x_{\pi}^{ip}$ ,  $x_{\sigma}^{ips}$  of the points  $\pi, \sigma$  of  $\Pi$  and  $\Sigma$ .

More particular structures can easily be defined. For instance, a *cellular* lattice will be characterized by assuming that the microstructures  $\Pi^p, \Pi^q$  of the points  $p, q$  in  $P$  and the microstructures  $\Sigma^s$  and  $\Sigma^r$  of the points  $s, r$  of  $S$  are disjoint sets

$$\Pi^p \cap \Pi^q = 0, (p \neq q); \Sigma^s \cap \Sigma^r = 0, (s \neq r). \quad (1)$$

A *primitive* lattice corresponds to the condition that the sets  $\Pi$  and  $\Sigma$  are empty

$$\Pi = \Sigma = \emptyset. \quad (2)$$

A *non-primitive* lattice is characterized by the condition  $\Pi, \Sigma \neq \emptyset$ . A *coherent* lattice is characterized by a secondary structure which is included in the primary one

$$\mathcal{S} \subset \mathcal{P}. \quad (3)$$

If  $S \subset P, \Sigma \subset P$  the coherence is ordered and if

$$\mathcal{S} \subset \Pi \quad (4)$$

the structure is microcoherent.

If the secondary structure  $\mathcal{S}^p$  associated with a point  $p$  of the primary structure  $\mathcal{P}$  is included in the primary structure:

$$\mathcal{S}^p \subset \mathcal{P}, \quad (5)$$

the lattice is endowed with a non-local field of interactions and if  $\mathcal{S}^p$  is contained in the microstructure of the considered point  $p$ :

$$\mathcal{S}^p \subset \Pi^p \quad (6)$$

the interaction is local.

It is clear that a non-local field corresponds to a coherent lattice and a local field to a micro-coherent lattice. The conditions

$$\Pi \subset P, \Sigma \subset S \quad (7)$$

correspond to lattices with microstructures included in macrostructures (*nuclear* lattices).

If for any subset  $\Pi' \subset \Pi$  of a nuclear lattice, the corresponding primary substructure  $P'$  is included in the primary one:  $P' \subset P$ , then the lattice will be termed *structural nuclear*.

It, can be easily shown that a microcoherent structural nuclear lattice is ordered, since for  $\mathcal{S} \subset \Pi$  it appears that  $\Sigma \subset \Pi$  and hence  $S \subset P$ .

In the next section we shall consider these lattices and more especially the Bravais lattices characterized by the positions of knots and cells

$x^{ip} = p^i a^i$ , ( $p^i = 1, 2, \dots$ );  $x_{\pi}^{ip} \equiv x^{ip} + \xi_{\pi}^{ip}$ , ( $\pi = 1, \dots, s$ ). If the crystal is heterogeneous, similar notations can be used, the indices being replaced by the rows  $p_1 \dots p_n$ ; ( $p_i = 1, \dots, s_i$ ), etc.

## II. Displacements in Crystal Lattices

The relative motions can be described with the aid of the relative macro and micro-coordinates

$$x^{ips} = x^{ip} - x^{is}, \xi_{\pi}^{ip} = x_{\pi}^{ip} - x^{ip}, \xi_{\pi\sigma}^{ips} = \xi_{\pi}^{ip} - \xi_{\sigma}^{is}. \quad (8)$$

Accordingly the macro-displacements will be defined as differences between the actual and initial coordinates

$$u^{i..} = (x(t) - x(0))^{i..}. \quad (9)$$

The micro-displacements are similarly expressed

$$u_{\pi}^{ip} = (\xi(t) - \xi(0))_{\pi}^{ip} = u_{\pi}^{ip} - u^{ip}. \quad (10)$$

In order to characterize the relative displacements, we denote

$$u^{ips} = u^{ip} - u^{is}, u_{\pi\sigma}^{ips} = u_{\pi}^{ip} - u_{\sigma}^{is}. \quad (11)$$

Thus the relative displacement between two arbitrary ions can be decomposed as follows

$$u_{\pi\sigma}^{ips} = u_{\pi}^{ip} - u_{\sigma}^{is} = u^{ips} + u_{\pi\sigma}^{is}. \quad (12)$$

## III. The Modified Energy Tensor

The kinetic energy can be expressed with the aid of the components of velocities defined in the lattice and the masses of the material points

$$T^{(ij)} = \sum_{\mathcal{P}} (mv^i v^j) \frac{u}{\pi}, \quad T^{(i4)} = \sum_{\mathcal{P}} (mv^i) \frac{u}{\pi}, \quad T^{44} = \sum_{\mathcal{P}} m \frac{u}{\pi}, \quad (13)$$

In order to apply the previous definitions, it is more useful to consider the rate tensor (written in an asymmetric form)

$$dT^{ij} = f_{\rho}^{i\pi} du_{\pi}^{jp}, \quad dT^{i4} = m_{\rho}^{\pi} du_{\pi}^{ip}, \quad dT^{44} = 0. \quad (14)$$

The repeated indices in different positions (inferior and superior) imply summation. The absolute forces are denoted by

$$f_{\rho}^{i\pi} = (mw^i) \frac{u}{\pi}, \quad (15)$$

where  $w^i = v^i$  are accelerations. Since the forces are equilibrated by the interactions with the secondary structure  $\mathcal{S}^p$ , following equations of equilibrium must be satisfied:

$$f_p^{i\pi} = \sum_{s, \sigma \in \mathcal{S}} f_{ps}^{i\pi\sigma} + F_p^{i\pi}. \quad (16)$$

Application of the action-reaction principle leads to the conditions concerning the symmetry of interactions with respect to the structural indices

$$f_{ps}^{i\pi\sigma} + f_{sp}^{i\sigma\pi} = 0. \quad (17)$$

After summation of the interactions of a simple cell with the secondary structure

$$f_{ps}^i = \sum_{\Pi, \sigma} f_{ps}^{i\pi\sigma} = -f_{sp}^i, \quad (\pi \in \Pi, \sigma \in \Sigma) \quad (18)$$

and, considering the resulting external forces acting upon the cell

$$F_p^i = \sum_{\pi \in \Pi} F_p^{i\pi}, \quad (19)$$

it will be possible to express the balance equations relative to a cell as

$$f_p^i = \sum_{s \in \mathcal{S}} f_{ps}^i + F_p^i. \quad (20)$$

Here the resulting inertial forces are:

$$f_p^i = \sum_{\pi \in \Pi} f_p^{i\pi}. \quad (21)$$

The forces in the microstructure of  $\mathcal{P}$  can be considered as a superposition of link forces between the crystal and the external bodies ( $\mathcal{N}$ ) or internal coupling forces ( $F$ )

$$F_p^{i\pi} = \sum_{q, \kappa \in \mathcal{P}} F_{pq}^{i\pi\kappa} + \mathcal{N}_p^{i\pi} \quad (22)$$

for

$$F_{pq}^{i\pi\kappa} = -F_{qp}^{i\kappa\pi}. \quad (23)$$

The coupling forces can be considered, if the crystal is heterogeneous, as reactions between the material phases. The resulting forces

$$F_{pq}^i = \sum_{\pi, \kappa \in \Pi} F_{pq}^{i\pi\kappa} = -F_{qp}^i \quad (24)$$

satisfy the equations of equilibrium

$$F_p^i = \sum_{q \in P} F_{pq}^i + \tilde{\delta}_p^i \quad (25)$$

in which the resulting link forces,

$$\tilde{\delta}_p^i = \sum_{\pi} \tilde{\delta}_p^{i\pi}, \quad (26)$$

also occur.

For sake of simplicity, the symbols of summation will henceforth be submitted:  $p, q$  refer to  $P$ ;  $\kappa, \pi$  to  $\Pi$ ;  $s, \sigma$  to  $S$  and  $\Sigma$ , respectively. Equations (10)–(12) and (16)–(26) lead to a reformulation of the rate tensor (14)

$$\begin{aligned} dT^{ij} &= \tilde{\delta}_p^{i\pi} du_{\pi}^{jp} + 1/2 (F_{pq}^{i\pi\kappa} du_{\pi\kappa}^{jpq} + f_{ps}^{i\pi\sigma} du_{\pi\sigma}^{jps}) \\ &= \tilde{\delta}_p^i du^{jp} + \tilde{\delta}_p^{i\pi} du_{\pi}^{jp} \\ &\quad + 1/2 (F_{pq}^{i\pi\kappa} du_{\pi\kappa}^{jpq} + F_{pq}^{i\pi\kappa} du_{\pi\kappa}^{jpq} + f_{ps}^i du^{jps} + f_{ps}^{i\pi\sigma} du_{\pi\sigma}^{jps}) \\ dT^{i4} &= m_p du^{ip} + m_p^{\pi} du_{\pi}^{ip}. \end{aligned} \quad (27)$$

Here the cell-masses are:

$$m_p = \sum_{\pi} m_p^{\pi}. \quad (28)$$

In the case of primitive lattices, terms with greek indices disappear automatically.

We observe that additional rigid motions

$$du^{*jp} = a^j \quad (29)$$

determine a variation of the energy rate tensor

$$dT^{*ij} = \tilde{\delta}_p^i a^j, \quad dT^{*i4} = m a^i. \quad (30)$$

Here

$$\tilde{\delta}_p^i = \sum_p \tilde{\delta}_p^i, \quad m = \sum_p m_p \quad (31)$$

stand for resulting body forces and total mass.

Consequently, if the resulting body forces vanish,  $dT^{ij}$  is invariant under additional rigid motions:

$$dT^{ij} = 0 \text{ for } \tilde{\delta}_p^i = 0. \quad (32)$$

Analogously, if we consider additional rigid rotations

$$du_p^{*i} = b_j^i x_p^j, \quad (b_{ij} = -b_{ji}) \quad (33)$$

$$d\mathfrak{u}_p^{*i} = b_j^i \xi_p^j$$

it follows that

$$\begin{aligned} dT^{*ij} &= \left\{ \sum (\tilde{\delta}^i x^k)_p + \sum (\tilde{\delta}^i x^k)_p^\pi \right. \\ &+ \frac{1}{2} \left( \sum (F^i x^k)_{pq} + \sum (f^i x^k)_{ps} + \dots \right) \} b_k^i \\ dT^{*i4} &= \left\{ \sum (mx^k)_p + \sum (mx^k)_p^\pi \right\} b_k^i. \end{aligned} \quad (34)$$

Hence, in the case of vanishing external forces ( $\tilde{\delta}^i = 0$ ) and if the interactions and coupling forces ( $F$ ) are central forces

$$F_{pq}^i = (\nu^i F)_{pq}, \quad f_{ps}^i = (\nu^i f)_{ps}, \text{ etc.},$$

where

$$\nu^i = x/l, \quad l = (x^j x_j)^{1/2} = \nu_j x^j. \quad (35)$$

Since  $b$  is an antisymmetric tensor, we deduce the invariance condition of the spherical component of the energy rate tensor

$$dT^{*ii} = 0 \quad (36)$$

for additional rigid rotations.

#### IV. The Correlation Between the Dynamic and Kinematic Fields in Crystal Lattices

The interactions  $f_{ps}^{i\pi\sigma}$  can be derived from a potential or generally expressed in terms depending on the relative coordinates  $x_{ps}^i, \xi_{ps}^{i\pi\sigma}$ . This dependence presents more complex features if we take into account the retardation effects, so that variables at different time instants must be considered. Furthermore, in the case of a Van der Waals crystal, since the interactions are not reducible to single central forces, it being necessary to consider interactions between more than two ions to express the polarization effects, the forces are derivable from many-body potentials.

In order to avoid the difficulties which arise from the consideration of the different cases mentioned above, we shall disregard a particular form of potential. The method of description adopted below will be further applied.

The indicial notation  $pt$  will be assigned to particular events which correspond to a position  $x^{ip}$  of the ion  $p$  at an instant  $t$  (or  $x^{pt}$  for the position  $x^{ip}$  at an instant  $t + \tau$ ). The values  $t$  vary continuously or are spread discretely over the time axis. The relations (1)–(7) can be easily transposed in the frame of a “procesual” analysis using instead of the indices  $pt$ , etc. the “chronotopic” indices  $P$ , etc. The double indices

$$PQ \quad (37)$$

stand for an elementary *transition* between anterior events  $P$  and subsequent ones  $Q$ . In (8)–(12), (15) we then substitute the indices

$$p \rightarrow pt \text{ (or } P\text{), etc.} \quad (38)$$

and consider the dependences

$$f_{ps}^i = f_{ps}^i (x_{AB}^j). \quad (39)$$

$AB$  stand for the indices  $ps$  (at an actual instant  $t$ ) and for  $ps$  ( $t \geq \tau \geq t_0$ ). More generally, if non-locality intervenes, the indices correspond to different points and instants.

If  $x_{AB}^j = x_t^j - x_{t_0}^j - (x_t^s - x_{t_0}^s) = u_t^j - u_t^s$ , the interactions depend on the relative displacements. If  $f_{ps}^i(0) = 0$ , then we can reformulate (39) as follows

$$f_{ps}^i = B_{jps}^{iAB} x_{AB}^j + f'_{ps}^i \quad (40)$$

$B$  depends on the relative coordinates and  $f'$  is a residual term which either can be included in the first term of the righthand side member or can be used in order to express a part of the interaction forces which vary in a qualitatively distinct manner (for instance, varying slowly with a low intensity for very distant ions  $p, s$  and increasing rapidly for close distances between  $p$  and  $s$ ) while the first term varies rapidly only for close ions. Considering the usual properties of crystals,  $f'$  stands for a principal term.

We assume that (39) can be solved so that the displacements can be expressed in an analogous form to (40):

$$u^i = A_j^i x^j + u'^i, \quad (p \neq s; i(ps), j(AB)). \quad (41)$$

$x^j$  corresponds to different anterior stages. The residual term  $u'$ , which takes into account the usual physical processes, is a secondary term with rapid variation for small distances and tends to zero for large distances.

The coefficients  $A$  and  $B$  will be termed kinematic and dynamic distortions.

The tensor (27) associated with a primitive lattice takes the form

$$\begin{aligned} \tilde{T}^{ij} = & \sum (v\mathfrak{R}^i du^j)_{4p} + 1/2(vR^i du^j)_{pq} \\ & + 1/2 \sum ((vR_k^i)_{ps} du^k + (\sigma^{ik} dA_k^j + dB_k^i \lambda^{jk})_{ps})_{AB} \\ & + dT'^{ij} + \dots \\ dT^{i4} = & (v\bar{m} du^i)_p. \end{aligned} \quad (42)$$

The non tensorial indices  $p, pq, ps$  are correlated with the tensorial indices  $i, j$  while  $k$  is referred to  $AB$ .  $du^k$  vanishes if  $x_{AB}^i$  are initial relative coordinates.  $v_p$  stands for the volume element of the cell with the knot  $p$  and  $v_{ps} = v_p + v_s$ .

The following notations are also used

$$\begin{aligned} \mathfrak{R}_p^i &= (\mathfrak{F}^i/v)_p, \quad R_{pq}^i = (F^i/v)_{pq}, \quad \bar{m}_p = (m/v)_p \\ R_k^i &= f^i/v_{(i)} A_k^i - (u'^j/v_{(j)}) B_k^i \\ \left\{ \begin{array}{l} \sigma \\ \lambda \end{array} \right\}^{ik} &= \left\{ \begin{array}{l} f \\ -u' \end{array} \right\}^i / v_{(i)} x^k \\ dT'^{ij} &= 1/2 \sum (f'^i du^j), \quad \tilde{T}^{ij} = T^{ij} - 1/2 B_k^i x^k u'^j. \end{aligned} \quad (43)$$

In the last four relations the following correspondences between the indices are considered:  $i, j \leftrightarrow ps$ ,  $k \leftrightarrow AB$  and  $v_{ps} = v_{(i)} - v_{(j)}$ .

We observe that if the dependences concern only initial variables  $x_{AB}^i$ , then  $du^k_{AB} = 0$  and in (42) the terms  $R_k^i$  disappear. For vanishing external link forces  $\mathfrak{F}^i$  we have  $\mathfrak{R}^i = 0$ .  $dT'^{ij}$  are residual parts which can be neglected if the supports of the residual parts of the kinematic and dynamic terms are disjoint or if these parts are of higher order. The first case corresponds to a variation of kinematic and dynamic terms of *complementary* type, in the sense that in the regions where the kinematic terms vary slowly, the dynamic ones vary rapidly. The classical stress model corresponds entirely to an implicit acceptance of this situation. In figure 1 such variations appear simultaneously. From a physical standpoint the situation corresponds to interactions which decrease rapidly with the increase of distance between the ions, while the relative displacements vary slowly, etc.

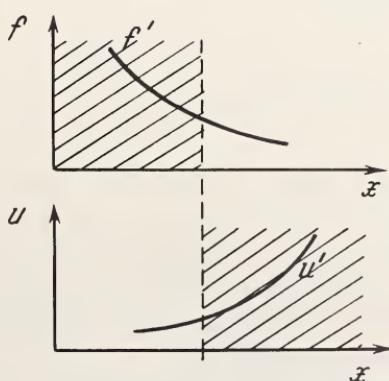


FIGURE 1. Variations of residual forces and displacements.

The coefficients which appear in (42) are of dynamic nature and will be called the distortions of the energy tensor. In a more synthetic treatment it appears as useful to introduce the notations.

$$\alpha = 1, \dots, 9; T^{ij} = T^{\alpha}; \alpha = 10, 11, 12; T^{i4} = T^{\alpha} \quad (44)$$

so that for vanishing dual effects (42) reduces to the conditions

$$dT^{\alpha} = T_{\beta}^{\alpha} dx^{\beta} \quad (45)$$

for

(a)  $\alpha = ij = 1, \dots, 9$

$$\beta = k = 1, \dots, 9; T_{\beta}^{\alpha} = T_{\beta}^{ijk} = \sigma^{ik} \delta_j^i, X = A_k^i, \lambda = psAB$$

$$\beta = k = 10, 11, 12; T_{\beta}^{\alpha} = T_{\beta}^{ij} = v \mathfrak{R}^i \delta_j^i, X = x^k, \lambda = p \quad (46)$$

$$\beta = 13, 14, 15; T_{\beta}^{\alpha} = T_{\beta}^{ij} = v R^i \delta_j^i, X = x^j, \lambda = pq$$

(b)  $\alpha = i = 10, 11, 12$

$$\beta = j = 1, 2, 3; T_{\beta}^{\alpha} = T_j^i = v \bar{m} \delta_j^i, X = u^i, \lambda = p.$$

The relation (35)<sub>2</sub> implies the condition of equilibrium

$$(f^i x^k)_{ps} = (f^k x^i)_{ps} \quad (47)$$

concerning the couples of interactions. Consequently, the "stresses"  $\sigma$  satisfy the identities

$$\sigma^{[ij]x^k] = 0} \quad (48)$$

and admit the decompositions

$$\sigma^{ij} = \sigma^{(ij)} + \sigma^{[ij]} \quad (49)$$

in which appears the additional term

$$\sigma_{psAB}^{[ij]} = (f^{[i} / v)_{ps} (x_{AB}^{j]} - x_{ps}^{j]}). \quad (50)$$

Taking into account (41),  $AB$  does not include the actual couple of indices  $ps$  so that (50) is formulated by means of generalized displacements  $x_{AB}^j - x_{ps}^j$ . If these differences are very small, (50) can be neglected and we obtain a symmetric stress tensor (49).

The equilibrium equations (20), (25) and (18) can be formulated by means of the new defined quantities (43)

$$(vr^i)_p = \sum_{\substack{ps \\ AB}} v_{(i)} \Delta_j \sigma^{ij} + (vR^i)_p \quad (51)$$

$$(vR^i)_p = \sum_q (vR^i)_{pq} + (v\mathfrak{R}^i)_p.$$

Here we have denoted

$$\Delta_j = v_j/l \text{ and} \quad (52)$$

$v_i$  and  $l$  are defined in (35).

## V. Interpretation of the Non-Holonomic Character of the Energy Tensor

For simplicity's sake we assume a plane strain state characterized by three components of the tensor  $A_{(ij)} = e_{ij}$  and three components  $T_{(ij)}$ . Hence, for a strain cycle in the plane  $e_{11}, e_{22}$  there is an open path in the plane  $T_{11}, T_{22}$ , as in figure 2.

The differences  $dT_{11}, dT_{22}$  of the components  $T_{11}, T_{22}$  furnish a measure of the "remanence" or hysteresis during a cycle. In the plane  $T_{11}, T_{22}$  any cycle corresponds in a converse manner to a path in the plane  $e_{11}, e_{22}$ , as in figure 3.

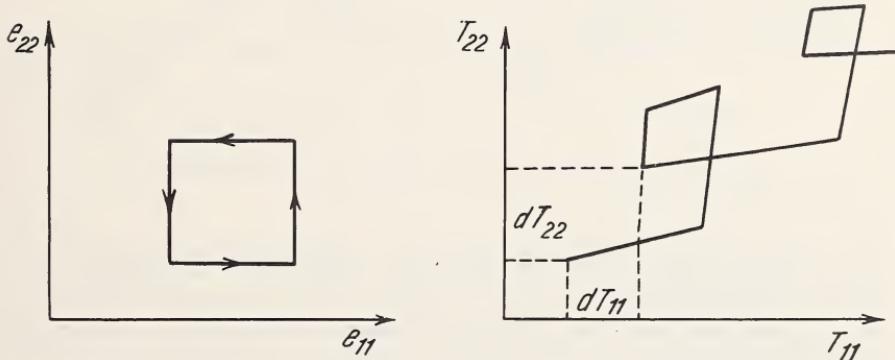


FIGURE 2. Strain cycle and stress path.

The remaining parts  $de_{11}, de_{22}$  give a measure of the remanent strain. If we assume that for  $f(e_{11}, e_{22}, e_{12}) < 1$  the tensor  $T$  is integrable but for  $f(e_{11}, e_{22}, e_{12}) > 1$  it is not integrable, then there exists in the space  $T_{11}, T_{22}, T_{12}$  a curve which separates the domain of variation for the values of  $T$  with reversible or irreversible character, as in figure 4.

For a strain cycle there is a corresponding closed or open path in the  $T_{11}, T_{22}$  plane if it is located on one or the other side of the separation curve. If the curve is replaced by a set of singular points in which  $T$  is

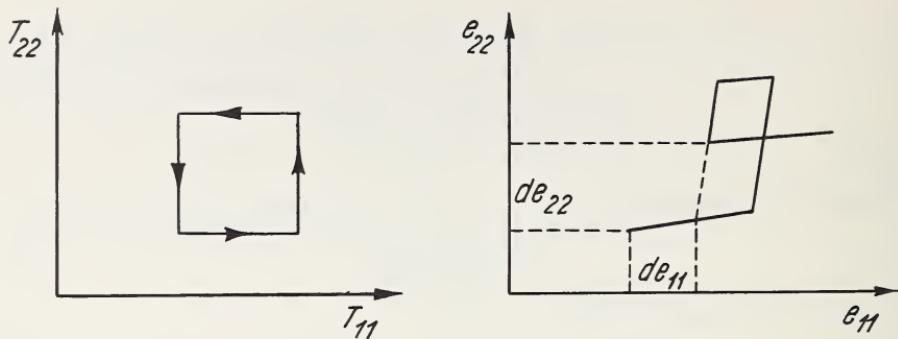


FIGURE 3. Stress cycle and strain path.

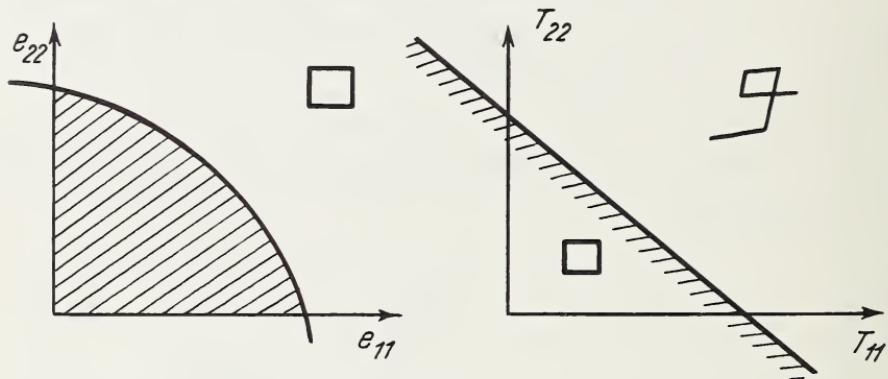


FIGURE 4. Domains of variations for irreversible stress states.

not integrable, the irreversibility takes a more general character. For instance, if on the curve  $\sigma-e$  or  $T-e$  there is located a point which can be crossed over only with loss or gain of energy ( $T$  increases or decreases) in an irreversible manner, then for any strain cycle there are corresponding closed paths or open paths separated by the point (fig. 5).

The unidimensional model sketched in figure 6 illustrates this model.

The spring  $R$  in the box  $C$  has a link  $B$  which at a determined position rubs the threshold  $A$ . If the threshold has a finite length, the singular points must be replaced by a region of accumulated singular points.

In the frame of physics of lattices, such models are correlated with the Taylor model of networks in which hook-effects are produced (fig. 7).

## VI. Interpolation of Physical Fields

Interpolation techniques make use of the step and unit functions:

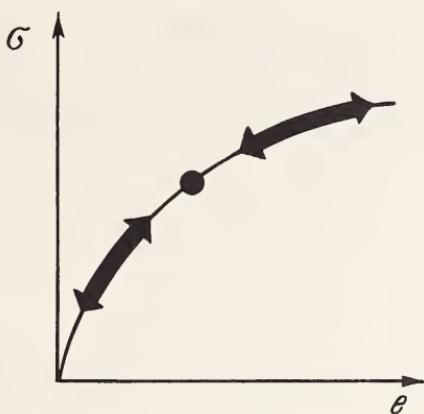


FIGURE 5. Separated branches on the curve  $e-e$  for reversible and irreversible states.

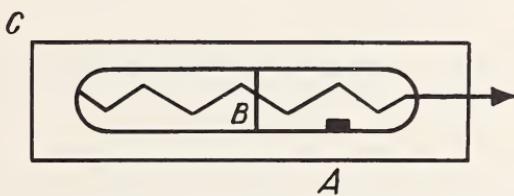


FIGURE 6. Unidimensional irreversible model.

$$\theta(x) = \int_0^\infty \sin kx dx / \pi k = \pm \frac{1}{2}, \quad (x \geq 0)$$

$$0, \quad x < a - b/2$$

$$U_b(x-a) = \theta(x - (a - b/2)) - \theta(x - (a + b/2)) = 1, \quad a - b/2 < x < a + b/2$$

$$0, \quad x < a + b/2$$

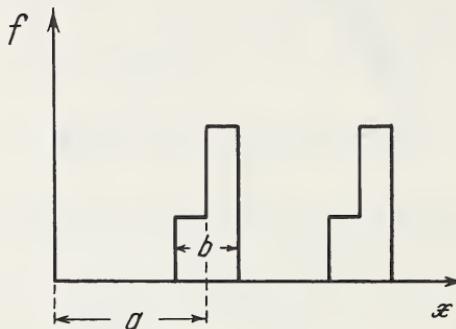
$$\begin{aligned} \mathfrak{H}_b(x-a) &= b(\theta(x-a) - 1/2(\theta(x-(a+b/2)) + \theta(x-(a-b/2)))) \\ &= 0, \quad x > a + b/2, \quad = -b/2, \quad a - b/2 < x < a \\ &= 0, \quad x < a - b/2, \quad = b/2, \quad a < x < a + b/2. \quad (53) \end{aligned}$$

We use the simplified notations  $f = \pi_j f_j$ ,  $(j=1, 2, 3)$ ,  $f = x$ ,  $a$ ,  $U$ , etc. We denote by  $A$  the set of points  $x = a$ .  $B$  stands for the interval  $a - b/2 < x < a + b/2$ . The interpolation is based on the representation of different values  $f_a$  under the unitary form

$$f(x) = \sum_B (f_a^+ U_b(x-a) + f_a' \mathfrak{H}_b(x-a)) \quad (54)$$



FIGURE 7. The hook-model.

FIGURE 8. Noncontinuous variation of the function  $f$ .

for

$$f_a^+ = (f(a + b/2) + f(a - b/2))/2$$

$$f_a' = (f(a + b/2) - f(a - b/2))/2. \quad (55)$$

Figure 8 presents the variation of the function  $f(x)$  compatible with (54).

## VII. Spectral Analysis of the Interpolation Functions

Let us consider the Fourier transformation

$$f(x) = (2\pi)^{-3} \int \exp(-ixs) f^*(s) ds \quad (56)$$

expressed by means of the image function

$$f^*(s) = \int \exp(isx) f(x) dx = \sum_B (f_a^+ U_{ab}^*(s) + f_a' \mathfrak{U}_{ab}^*(s)) \quad (57)$$

and the transforms

$$U_{ab}^*(s) = (\delta(x - a))^* U_b^*(s)$$

$$\mathfrak{U}_{ab}^*(s) = (\delta(x - a))^* \mathfrak{U}_b^*(s) \quad (58)$$

$$(\delta(x-a))^* = e^{isa}, \quad U_b^*(s) = \prod_{j=1}^3 \left( \frac{\sin sb/2}{s/2} \right)_j$$

$$\mathcal{H}_b^*(s) = \prod_{j=1}^3 \left( \frac{b}{2} \frac{(\cos sb/2 - 1)}{is/2} \right)_j.$$

The integrals are taken between the limits  $-1$  and  $\infty$ . For  $b \rightarrow 0$  we have

$$U_b^* \rightarrow \pi^3 \delta(s/2), \quad (59)$$

$\delta(x)$  being the Dirac function. Starting from (53) we consider the identities

$$\begin{aligned} \delta(x) &= (2\pi)^{-3} \int e^{ikx} dx = \theta'(x) = \begin{cases} \infty & , x=0 \\ 0 & , x \neq 0 \end{cases} \\ \int_a^b \delta(x-x') dx' &= 1, (b > x > a); = 0, (x > b \text{ or } x < a) \\ \int_a^b \delta(x-x') f(x') dx' &= f(x), (b > x > a); = 0, (x > b \text{ or } x < a). \end{aligned} \quad (60)$$

In the last equality  $f(x)$  is assumed continuous in the interval  $a < x < b$ . The function  $U_b^*(s)$  in (58) is the transformed unit function, since according to (67)

$$\begin{aligned} U_b(x) &= (2\pi)^{-3} \int_a^b U_b^*(s) \exp(-isx) ds \\ &\rightarrow \int_a^b \delta(s/2) \exp(-isx) d(s/2^3) = \begin{cases} 1, & b > x > a \\ 0, & x > b, x < a. \end{cases} \end{aligned} \quad (61)$$

(59)–(61) imply (57) and (58). We assume  $b \rightarrow 0$ . Since the representation (57) is unique, and (56) stands for the unique correspondence in the frame of the one-dimensional theory of information, the last observation reduces to the Shannon-Kotelnikov theorem.

### VIII. Some Properties of the Interpolation Functions

The functions  $f(x)$  are indefinitely differentiable, vanishing in the exterior of a finite domain of the euclidean space  $E$  (or more generally of a space  $R$ ). The whole set of functions  $f(x)$ , termed *fundamental* functions, constitutes the fundamental space  $K$ .

A continuous linear functional  $g$  over  $K$  is defined by means of real numbers  $(g, f)$  for any fundamental function  $f(x)$ . Hence,  $a$  and  $b$  being real,  $(g, af + bf) = a(g, f) + b(g, f)$ ,  $\lim (f, \varphi_\nu) \rightarrow 0$  for  $\lim_{\nu \rightarrow \infty} \varphi_\nu \rightarrow 0$ , in  $K$ . We also consider the local integrable functions  $g$  (absolutely integrable in any finite domain of  $E$  or  $R$ ) and the numbers

$$(g, f) = \int_{E \text{ or } R} \overline{g(x)} f(x) dx, \quad (62)$$

$f$  being a fundamental function. The integration is performed over the exterior of the domain in which  $f(x)$  vanishes. The functionals  $g \subset K$  are also termed *generalized* functions. If  $g \subset K$  is introduced by means of (62),  $g$  is a functional of regular type, termed a generalized function. If (62) is not valid, the regularity is no longer ensured, the functions being singular. The whole set of these functions belongs to a space  $K$ .

If a generalized function  $g$  does not vanish identically in any neighborhood of a point  $x_0$ , this point is a proper one. The set of proper points constitutes the support of  $g$ . If a set  $B$  of points contains the support of  $g$ , then  $g$  is a functional concentrated over  $B$ . Accordingly,  $f(x)$  in (54) is concentrated over  $aB$ ,  $a$  being the support of  $U_a(x)$  (we assume  $b=0$ ).

Another class of functions, more general than the fundamental ones, is represented by the functions  $f$  with derivatives of any order bounded by finite-order powers of coordinate variables

$$\|x_1^{k_1} x_2^{k_2} x_3^{k_3} \partial^{q_1+q_2+q_3} f(x) / \partial x_1^{k_1} \partial x_2^{k_2} \partial x_3^{k_3}\| \leq C_{k_1 k_2 k_3 q_1 q_2 q_3}. \quad (63)$$

These respective functional space will be denoted by  $S$  and the set of the continuous linear functionals over  $S$  will be denoted  $S'$  (the last one being contained in  $K'$ ). Any function  $f \subset K$  belongs to  $S$ . Now we restrict ourselves to the consideration of generalized functions.

It can be shown that generalized functions possess derivatives which are also generalized functions and satisfy the conditions

$$(\partial f / \partial x^j, g) = (f, -\partial g / \partial x^j). \quad (64)$$

The product of convolution of two generalized functions

$$f(x) \times g(x) = \int f(\xi) g(x - \xi) d\xi \quad (65)$$

has an effective meaning and satisfies the conditions

$$(f \times g, h) = (f(x) \times g(y), h(x+y)) \quad (66)$$

if one of the functionals  $g$  or  $f$  possesses bounded support or if the supports of both functions are bounded by the same side. In these cases the conditions of commutativity, and distributivity as well as the rules of differentiation are satisfied:

$$f \times g = g \times f, (f \times g) \times h = f \times (g \times h)$$

$$D(f \times g) = Df \times g = f \times Dg = D(f \times g) = \dots \\ (D(f \times g), h) = (f \times g, D \times h), \quad (67)$$

$D$  stands for a homogeneous differential operator. Particularly we have

$$\delta \times g = g, \frac{\partial \delta}{\partial x_j} \times g = \frac{\partial g}{\partial x_j}. \quad (68)$$

The transform of Fourier for the fundamental function  $f \subset K$  satisfies the conditions

$$|s_1^{q_1} s_2^{q_2} s_3^{q_3} f(s)| \leq C \exp (q_1 |\tau_1| + q_2 |\tau_2| + q_3 |\tau_3|), \quad (s_j = \sigma_j + i\tau_j) \quad (69)$$

$x_j < a_j$  being a domain outside of which  $f(x)$  vanishes identically. The space of these functions will be denoted  $Z (= S^*)$ .

The Fourier transform of a generalized function  $g$  (over  $K$ ), is the functional  $g(s)$  (over  $Z$ ) satisfying the condition

$$(f^*, g^*) = (2\pi)^3 (f, g), \quad (70)$$

$f^*(s) \subset Z$  being the Fourier transform of the function  $f(x) \subset K'$ . Equation (70) stands for the Parseval formula and can be established directly according to the definitions of the functions  $f$  and  $g$ . Further, the following relations are mentioned

$$P(\partial/\partial x^j) g^* = P(-is) f^*(s) \quad (71)$$

Since  $(f \times g)^* = f^* g^*$ ,  $f \times g = (2\pi)^{-3} \int f^*(s) g^*(s) \exp(-isx) ds$ .

$$f^*(s) = (\bar{f}, \exp(isx)) \quad (72)$$

it results that

$$f^*(0) = (\bar{f}, 1). \quad (73)$$

(71) leads to other identities

$$f^*(0) = (2\pi)^{-3}(\bar{f}, 1), \quad 1^* = (2\pi)^3\delta(s). \quad (74)$$

By the way, the last one follows from (60) and (56). The formulas (52), (59), and (64) will be used for the formulation of the useful relations:

$$\begin{aligned} (f, g) &= \sum_B \left( b\bar{f}_a^+ g_a^+ + \frac{b^3}{4} \bar{f}'_a g'_a \right) \\ &= (2\pi)^{-3} \int f^*(s) g^*(s) ds = (2\pi)^{-3} \int (f \times g)_\kappa^* ds \\ (f, U_b) &= b\bar{f}_a^+, \end{aligned} \quad (75)$$

where

$$b = \int U_b(x) dx = \int_{a-b/2}^{a+b/2} dx.$$

If  $f$  is constant then

$$(1, f) = Bf, \text{ and } B = \sum b. \quad (76)$$

The interpolation formulas (54) and (62), the new representation

$$\begin{aligned} g(x, x') &= \sum_{B, B'} (g_{aa'}^{++} U_b(x-a) U_{b'}(x-a') \\ &+ g_{aa'}'' \mathfrak{H}_b(x-a) \mathfrak{H}_{b'}(x-a') + g_{aa'}^+ U_b(x-a) \mathfrak{H}_{b'}(x-a') \\ &+ g_{aa'}^+ \mathfrak{H}_b(x-a) U_{b'}(x-a')), \end{aligned} \quad (77)$$

and the functionals

$$\begin{aligned} (f, g, h) &= ((\bar{f}, \bar{g}), h) = (2\pi)^{-3} ((\bar{f}, \bar{g})^*, h^*) \\ &= \iint \bar{f}(x) g(x, x') h(x') dx dx' \end{aligned} \quad (78)$$

can be used in order to interpolate more complex expressions

$$(f, g, h) = \sum_{B, B'} (bb' \bar{f}_a^+ g_{aa'}^{++} h_{a'}^+ + \frac{(bh)^3}{16} \bar{f}'_a g_{aa'}'' h_{a'}'). \quad (79)$$

If  $g(x, x') = g(x - x')$ , the results can be directly deduced from the properties (66)–(71) concerning convolution products. The above established formulas represent one to one correspondences between the functional spaces  $K'$  or  $S$  and the space  $F(A)$  of the functions  $f(x)$ . These correspondences (see (75)<sub>1</sub>, (76), (79)) furnish the theoretical basis of the equivalences between the discrete lattices and continuous media.

In connection with determined laws of variation of the values  $f_a$ , the interpolation rules present specific features which can be stressed with the aid of the following parametric developments

$$f^+ = (\epsilon^{p_0} f_0 + \epsilon^{p_1} f_1 + \dots)$$

$$f^- = (\epsilon^{q_0} f_0 + \epsilon^{q_1} f_1 + \dots), \text{ etc.} \quad (80)$$

which correspond to a variation of class  $C(p, q)$ .  $\epsilon$  stands for a small parameter and  $p, q$  or  $(p_0, p_1 \dots; q_0, q_1 \dots)$  are sequences of increasing powers called *indicators of variability*.  $p_0$  and  $q_0$  are positive powers called *indicators of intensity*. The values  $f_i^+, f_i^-$  are assumed independent of  $\epsilon$ . Meanwhile, we assume that the values  $b$  vary according to the development

$$b = \epsilon^{r_0} b_0 + \epsilon^{r_1} b_1 + \dots \quad (81)$$

and the following additional developments are accepted:

$$g^+ = \epsilon^{s_0} g_0^+ + \dots, \quad g' = \epsilon^{t_0} g_0' + \dots$$

Then we deduce the interpolation rules

$$(f, g) = \sum \epsilon^{(p_m + s_n + r_0)} b_0 f_{ma}^+ g_{na}^+ + \sum \frac{1}{2} \epsilon^{(q_m + t_n + r_0 + r_u)} b_0 b_u f_{ma}^+ g_{na}'$$

$$(f, U_b) = \sum \epsilon^{(p_m + r_n)} b_n f_{ma}^+. \quad (82)$$

If the indicators of intensity satisfy the inequality concerning the principal part of the developments

$$q_0 + t_0 > p_0 + s_0 \quad (83)$$

or, more restrictively, if

$$q_0 > p_0 \text{ and } t_0 > s_0 \quad (84)$$

then the values vary slowly so that the principal part (for  $\epsilon = 0$ ) of the parametric developments for  $(f, g)$  depend only on the product of mean

values  $f_{oa}^+$ ,  $g_{oa}^+$ 

$$(f, g)_0 = b_0 f_{oa}^+ g_{oa}^+. \quad (85)$$

Under the same conditions, the following decompositions are valid:

$$(f, U_b) = b_0 (f_a^+)_0 + (f, 1)'$$

$$(f, g) = b_0 (f_a)_0 (g_a)_0 + (f, g)'. \quad (86)$$

The term  $(\cdot)'$  stands for the residual part which can be easily referred to previous considerations.

## IX. The Fundamental Equations of the Theory of Interpolation

The sets of points  $S$ ,  $P$  defined in the first section will be considered as supports of the interpolation function. We assume (83) and instead of  $b$  we consider the volumes  $v$ . Hence (51), after interpolation and application of the relations (75), transform as follows

$$\begin{aligned} r^i &= (1, \partial_j \sigma^{ij}) + R_i, \\ \text{and} \quad R^i &= (1, \rho^i) + \mathcal{R}^i \end{aligned} \quad (87)$$

$\partial_j$  and  $\rho_i$  stand for the ratios  $\Delta_{jAB}/v_p$ ,  $R_{pq}^i/v_p$ . The first integral is performed over the domain  $s \subset S$  and the second one over the set of points  $q \subset Q \subset P \cup S'$ .  $\sigma$  stands for  $\sigma_{psAB}$ .  $r$ ,  $R$  and  $\mathcal{R}^i$  are located at  $p$ .

In order to formulate other elements, we define the functional

$$(a, -, c) = [d], \quad (d = ac) \quad (88)$$

as the double integral

$$\int a(x) c(x') (\cdot)_{x, x'} dx dx'. \quad (89)$$

The notation

$$([d], b) \quad (90)$$

will be used instead of the integral

$$\int a(x) c(x') b(x, x') dx dx'. \quad (91)$$

Consequently the following identity holds true

$$([d], b) = (a, b, c). \quad (92)$$

Further, considering (4) and (41) we have

$$f^i = (b_j^i, x^j) + f^i, u^i = (a_k^i, x^k) + u^i \quad (93)$$

for

$$b_j^i = B_j^i/v_{(j)} \text{ and } a_k^i = A_k^i/v_{(k)}, \quad (94)$$

where the following indices are associated:  $i \leftrightarrow ps, j \leftrightarrow AB, k \leftrightarrow CD$  and are omitted in the notations.

Consequently, in order to interpolate (43), we define the functionals obtained by integration over the volumes  $v_{ps}$  and  $v_{AB}$

$$\begin{aligned} [R^i_k] &= (f^i/v, , a_k^i) - (u^i/v, , b_k^i), \\ [\sigma^{ik}] &= (f^i/v, , x^k), \quad [\lambda^{jk}] = (u^j/v, , x^k). \end{aligned} \quad (95)$$

These functionals are correlated with the values (43) by means of the conditions

$$\begin{aligned} [R^i_k] \delta(x - x_{ps}) \delta(x - x_{AB}) &= R^i_k \\ [\sigma^{ik}] \delta(x - x_{ps}) \delta(x - x_{AB}) &= \sigma^{ik}/v_{AB} \\ [\lambda^{jk}] \delta(x - x_{ps}) \delta(x - x_{AB}) &= \lambda^{jk}/v_{AB}. \end{aligned} \quad (96)$$

Here  $\delta(x) = \prod_1^3 \delta(x_i)$ .

Finally, the rate tensor (42) becomes

$$\begin{aligned} dT^{ij} &= (\mathfrak{R}^i, dx^j)_P + 1/2(R^i, du^j)_{PQ} \\ &\quad + 1/2(([R^i_k], du^k) + ([\sigma^{jk}], da_k^i) + ([\lambda^{jk}], db_k^i)). \end{aligned} \quad (97)$$

The inferior indices specify the range of integration (over the volume elements  $v_p, v_{pq}, v_{AB}$ ).

In a way which tends to extend the iterative methods of elasticity [37-41], or the asymptotic analysis of the theory of shells [42-50], we shall consider the parametric developments analogous to [80]:

$$f_{ps}^i = \sum_m \epsilon^m f_{m,ps}^i, \quad u^{ip} = \sum_m \epsilon^m u_m^i. \quad (98)$$

Any term of these developments corresponds to a distribution of values so that we shall consider the following system of description. To any field

elements defined at the points  $a, b, \dots$  we associate the values  $g_a, g_b$  and the differences  $\Delta_{ab}g = g_b - g_a = \gamma_{ab}(g)g_a$  formulated by means of the ratios  $\gamma_{ab}(g) = \Delta_{ab}g/g_a$ . Using the above mentioned parametric developments, we have

$$\gamma_{ab}(g) = \sum_m \epsilon^m \gamma_{abm} \text{ and } \gamma_{abm} = \Delta_{ab}g_m/g_a. \quad (99)$$

The interval  $ab$  is arbitrary. Further, we derive the relations

$$\begin{aligned} g_b &= G_{ab}g_a, (\text{a fixed}); \\ G_{ab} &= I + \gamma_{ab} = \sum_{m=0, 1, 2, \dots}^{\Theta} \epsilon^m G_{abm} \\ G_{abm} &= \delta_{om} + \gamma_{abm}, \end{aligned} \quad (100)$$

where  $g_a$  and  $G_{abm}$  will be designated as the localized value and the parameteric characteristics of variability. If  $M$  is the minimal power of the parameter  $\epsilon$ , it will be called indicator of intensity and the number  $m - M$  the indicator of order.

Let us also consider (99)<sub>1</sub> put under the form

$$\gamma(g) = \gamma(\epsilon, \gamma_1, \dots, \gamma_m, \dots). \quad (101)$$

If (101) can be solved for  $\epsilon$ , we obtain an expression for the small parameter,  $\epsilon$ , in terms  $\gamma_1, \gamma_2, \dots$  which can be relevant in particular cases. For instance, the exponential law  $g = \exp(\epsilon x/l)$ ,  $\epsilon = l/L < 1$ , can be used in the analysis of boundary layer effects [42-50]. In a different sense the parametric expansions are implicitly considered in the theory of polar media. In this paper we consider a more general case, assuming that the characteristics  $G$  are pseudo-differential operators

$$g_b = G_{ab}g_a = G(b, a)g(a) \quad (102)$$

$g(a)$  being a function of interpolation defined on a differentiable manifold  $\Omega (g \in C_0(\Omega))$ . Then, according to the central theorem mentioned above, there exists a function  $G \in C^\infty(\Omega \times \Omega)$  so that

$$g = (G, \tilde{g}). \quad (103)$$

Here  $\tilde{g} = g(a)$ . Some of the consequences of this assumption in terms of the theory of interpolation may now be given. Thus,

$$\sum_a b_a f_a g_a = (f, G, g) \quad (104)$$

for

$$g_a = G(a, c) \tilde{g}$$

and

$$\sum_{a, b} b_a b_b f_a g_{ab} h_b = (f, G, h, \tilde{g}) \quad (105)$$

for

$$g_{ab} = G(a, b, c) \tilde{g}, \quad \tilde{g} = g(c). \quad (106)$$

Relating these results to (94), we have the laws of variability

$$\begin{aligned} db^j &= \beta_{ij}^k db_k^i, \\ da_j^i &= \alpha_{ij}^k d\tilde{a}_k^i \end{aligned} \quad (107)$$

where ( $\beta, \alpha = 0$  for  $i \neq l, j \neq k$ ) represent characteristics and  $\tilde{b}, \tilde{a}$  values at a point  $c$ ; analogously we assume a variation of relative displacements

$$du^k = \gamma_l^k du^l, \quad (\gamma_l^k = 0 \text{ for } k \neq l). \quad (108)$$

$\alpha, \beta, \gamma$  are considered pseudo-differential operators and  $da, db, du$  functions of class  $C_0^\infty$ . Hence (97)<sub>1</sub> can be reformulated the form

$$\begin{aligned} dT^{ij} &= (\mathfrak{R}^i, dx^j) + 1/2 (R^i, du^j) + 1/2 ((R^i_l, du^l) \\ &\quad + (\sigma^{ijm}_l, d\tilde{a}_m^l) + (\lambda^{ijm}_l, db_m^l)). \end{aligned} \quad (109)$$

where

$$\begin{aligned} \tilde{R}^{ij} &= ([R^i_k], \gamma_l^k), \quad \sigma^{ijm}_l = ([\sigma^{ik}], \alpha_{lk}^{jm}) \\ \lambda^{ijm}_l &= ([\lambda^{jk}], \beta_{lk}^{jm}). \end{aligned} \quad (110)$$

Equation (101) implies a new formulation of the equilibrium equations which will be deduced below, starting from the observation that the equation

$$(f, g) = 1 \quad (111)$$

is satisfied by the function  $g = f^{-1} = \delta(x)/f$  so that

$$[\sigma^{ik}] = \alpha_{mj}^{-1} \sigma^{ijm}. \quad (112)$$

Here we have denoted

$$\alpha^{-1}{}_{mj}^{lk} \alpha_{lp}^{ju} = \delta(x) \delta_m^u \delta_p^k. \quad (113)$$

Thus (87)<sub>1</sub>, taking into account (96), becomes

$$r^i = (1, \partial_{ju}^l, \sigma^{ju}_l)_{ps, AB} + R^i \quad (114)$$

for

$$\partial_{ju}^l = \partial_k \alpha^{-1}{}_{mjps}^{lkAB} \delta(x - x_{ps}) \delta(x - x_{AB}) v_{AB}. \quad (115)$$

(109) and (113) must be further considered in terms of a new formulation of constitutive equations. ( $\tilde{R}$  and  $\lambda$  appear as additional quantities which can be determined by means of the constitutive equations.<sup>1)</sup>

## X. Interpolation Measures of Dislocations

According to the previous notation, we shall consider the following relative coordinates and displacements

$$x^{ip} - x^{iq} = (x^{ir} - x^{is}) = x^{ipq} - x^{irs} = u^{ipqrs} \quad (116)$$

which can be expressed by means of (41) in terms including the kinematic distortions:

$$u^{ipqrs} = A_j^{ipqrs}{}_{LM} x^{jLM}, A_j^{ipqrs}{}_{LM} = A_{jLM}^{ipq} - A_{jLM}^{irs}. \quad (117)$$

If, for instance,  $P = pt$ ,  $Q = qt$ ,  $R = pt_0 = P_0$ ,  $S = qt_0 = Q_0$  then we have

$$u^{ipqp_0q_0} = u^{ipq} = u^{ip} - u^{iq} \quad (118)$$

and for  $P = pt$ ,  $Q = pt_0 = S_0 = P_0$ ,  $R = pt_1 = P_1$ ,  $t > t_0$  ( $t_1$  being the instant of transition from an elastic stage to a plastic one), it follows that

$$\begin{aligned} u^{ipp_0p_1p_0} &= u^{ip} - u_{(e)}^{ip} = u_{(p)}^{ip} = x^{ip} - x^{ip_1} \\ u_{(e)}^{ip} &= x^{ip} - x^{ip_0} = u^{ip_1p_0}, \quad u^{ip'} = x^{ip} - x^{ip_0} = u^{ipp_0}. \end{aligned} \quad (119)$$

Meanwhile (107)–(109) allow us to decompose the displacements and the distortions in parts assigned to the description of elastic and plastic stages

<sup>1)</sup> The terms  $\tilde{R}$  in (101) can be correlated with the interactions and implicitly satisfy the condition of equilibrium which follows from the mentioned ones. However, according to a previous observation,  $\tilde{R}$  will be neglected.

$$\begin{aligned}
u^{iPQ} &= u^{iPQ}{}_{0Q0} = u_{(e)}^{iPQ} + u_{(p)}^{iPQ} = A_{jLM}^{iPQ} x^{jLM} \\
u_{(y)}^{iPQ} &= A_{jLM}^{iPQ} x^{jLM}, \quad (y = p, e) \\
A_{jLM}^{iPQ} &= A_j^{iPQ}{}_{0Q0}{}_{LM} = (A_{(e)} + A_{(p)})_{jLM}^{iPQ} x^{jLM} \\
A_j^{iP1}{}_{0Q1}{}_{Q0} &= A_{jLM}^{iPQ}{}_{(e)}, \quad A_{jLM}^{iPQ}{}_{(p)} = A_j^{iPP1}{}_{QQ1}. \tag{120}
\end{aligned}$$

In (116)–(120) we assign to any set of transitions and displacement  $u^i \dots$  the set  $LM \dots$  and the variables  $x^i \dots$ , the last ones being assumed in the next as belonging to a set  $C^{PQ}$ , that is  $LM \in C^{PQ}$ , etc. Further we shall neglect the residual parts which can be included in the remaining terms.

Let, then,  $P, Q \dots, PQ$  be a chronotopic cycle denoted by  $\mathcal{C}$ . By

$$b^i = \sum_{\mathcal{C}} u_{\mathcal{C}}^{iPQ} \tag{121}$$

we mean the components of a Burgers-type vector for the procesual lattices of chronotopes. Taking into account (120) we can decompose (121) as follows

$$b^i = \sum_{\mathcal{C}} u_{(e)}^{iQ} = \sum_{\mathcal{C}} A_{j(e)AB}^{iPQ} x^{jAB} = 0 \tag{122}$$

which expresses the fact that the eventual existent dislocations cross over the bidimensional region bounded by  $\mathcal{C}$ . If dislocations do not occur, (122) remains still valid.

(121) can be reformulated without loss of generality using a characterization of the variations of plastic distortions starting from a localized value

$$A_{jAB}^{iPQ} - A_{jCD}^{iRS} = A_{jk(p)ABCDEF(p)}^{iPQRS} x^{kEF} \tag{123}$$

$(AB \in C^{PQ}, CD \in C^{RS})$ .

$A_{jk}^i$  is assumed a function of the relative coordinates. We deduce

$$b^i = \sum_{\mathcal{C}} b_{\mathcal{C}}^i + ([S^{jk}], a_{jk(p)}^i) \tag{124}$$

for

$$b_{\mathcal{C}}^i = A_{jCD}^{iRS} \sum_{PQ} \sum_{AB \in C^{PQ}} x^{jAB}, \quad (AB \in C^{PQ}) \tag{125}$$

$$[S^{jk}]^{ABEF} = (x^{jAB}, \dots, x^{kEF})$$

$$a_{jk(p)}^i = A_{jk(p)}^i / v_{(j)} v_{(k)}, \quad v_{(j)} = v_{AB}, \quad v_{(k)} = v_{EF}. \tag{126}$$

If the right-hand side member of (125) vanishes identically, then  $b_{\mathcal{C}}^i = 0$ . This situation occurs, for instance, in the case of isochrone and isotopic

transitions, for  $P=A$ ,  $Q=B$  and hence for  $C^{PQ}=\mathcal{C}$ , when (120) include isochrone and isotopic transitions (relative to a single one). Hence we have

$$\begin{aligned} b^i_{\epsilon} &= \sum (S^{[jk]} A^i_{[jk](p)})_{PQ} \\ S^{[jk]} &= x^{[j} x^{k]}, \quad a^i_{jk} = A^i_{jk}/v_{PQ}. \end{aligned} \quad (127)$$

In order to complete the analysis of vector-like quantities (for instance of the relative coordinates), we consider the variations

$$V^i_{[p]} = V^{i0}_{(p)} + V^i_{j(p)} x^j, \quad i(AB), j(CD) \quad (128)$$

and, in agreement with (120) and (121), we deduce

$$V^i_{(p)} = ((A^{io}_j + A^i_{jk} x^k) (V^{jo} + V^j_{j(p)} x^j))_p \quad (129)$$

and

$$V^i - V^{io} = (A^{io}_j V^j_k + A^i_{jk} V^j) x^k. \quad (130)$$

The possibility of an interpolation being accepted (130) leads to the integral formula

$$\begin{aligned} dV^i &= (a^i_j, V^j_k, x^k) + (V^j, a^i_{jk}, x^k) \\ &= (a^i_j, V^j_k + (V^j, \gamma^j_{lk}), x^k) = V^i - V^i_0 \end{aligned} \quad (131)$$

where

$$a^i_j = A^i_j/v_{(j)}, \quad a^i_{jk} = A^i_{jk}/v_{(j)}v_{(k)},$$

$$(a^i_j, \gamma^j_{lk}) = a^i_{lk}. \quad (132)$$

The last equation defines a functional connexion. The solution

$$\gamma^j_{lk} = (a^{-1j}_m, a^m_{lk}) \quad (133)$$

is expressed by means of the inverse elements  $a^{-1}$  which satisfy the reciprocity conditions

$$(a^i_j, a^{-1j}_k) = (\delta^i_k). \quad (134)$$

$\delta(x)$  stands for the Dirac-type function.

## XI. Thermodynamic Irreversibility and Constitutive Incompatibility

The obtained results can be further developed in the frame of the thermodynamics of irreversible processes (including the fourth principle of the thermodynamics and more adequately the extension of H. B.

Casimir [68]. Equations (42) and (45) shall be considered as a point of departure. The residual terms are disregarded

$$dT^\alpha = T_\beta^\alpha dX^\beta = (t_\beta^\alpha, dX^\beta) \quad (135)$$

$$t_\beta^\alpha = T_\beta^\alpha / v_{(\beta)}.$$

(135) must be decomposed in terms which correspond to reversible and irreversible effects  $dT^\alpha = dT_{(e)}^\alpha + dT_{(p)}^\alpha$ ,  $dT_{(e)}^\alpha = T_{\beta(e)}^\alpha dX^\beta$ . The summation over a closed cycle  $\mathcal{K}$  in the space  $(X)$

$$t^\alpha = \sum_{\mathcal{K}} T_\beta^\alpha dX^\beta \quad (136)$$

represents a measure of the increments of the energy tensor in a cyclic process. If the numbers of indices  $\alpha$  and  $\beta$  are equal,  $t$  appears as a vector analogous with the Burgers vector. Since, by definition

$$\sum_{\mathcal{K}} T_{\beta(e)}^\alpha dX^\beta = 0, \quad (137)$$

we have

$$\sum_{\mathcal{K}} T_{\beta(p)}^\alpha dX^\beta. \quad (138)$$

The following relations

$$T_{\beta(p)}^\alpha = T_{\beta(p)}^{\alpha\alpha} + T_{\beta(p)}^{\alpha\gamma} dX^\gamma \quad (139)$$

correlate in a general way the coefficients  $T_\beta^\alpha$ , which correspond to an actual and a reference state of distortion.

In order to obtain analogous relations with (125) or (127), we replace  $b, A, i, j, k, S$  by  $t, T, \alpha, \beta, \gamma, (dX^{\beta\gamma}, \dots, dX^{\gamma\gamma})$ . In (131) we replace  $\gamma, a, j, l, k$  by  $\tau, t, \alpha, \beta, \gamma$  and we consider a density of constitutive discontinuities

$$t_{\beta\gamma}^\alpha = T_{\beta\gamma}^\alpha / v_{(\beta)} v_{(\gamma)} \quad (140)$$

so that the fundamental measures of dislocations and plastic effects can be deduced in a unitary manner.

We conclude these remarks with the following observation. Equation (137) is satisfied if

$$(dX^\beta, t_{\beta(e)}^\alpha) = dL^\alpha, \sum_{\mathcal{K}} dL^\alpha = 0 \quad (141)$$

$$(t_{\beta}^\alpha = T_{\beta}^\alpha / v_{(\beta)})$$

and hence

$$T_{\beta}^\alpha = \partial L^\alpha / \partial X^\beta, t_{\beta}^\alpha = \partial_{\beta} L^\alpha. \quad (142)$$

$\partial_{\beta}$  is defined by the conditions

$$\partial_{\beta} = \frac{1}{v_{(\beta)}} \frac{\partial}{\partial X^\beta} \text{ or } (dX^\beta, \partial_{\beta} f) = df, \left( \sum_{\mathcal{K}} df = 0 \right), \quad (143)$$

which can be easily analysed by considering the sums of discrete values according to (85).

The analysis of the incompatibility applied to the tensor (135) can be achieved in a more general sense if we resort to an analogous definition of the differential forms starting this time from the equations

$$\rho \dot{\epsilon} = q_{,i}^i + h + \mathcal{L}$$

$$\rho \theta \dot{\eta} - (q_{,i}^i + h) - q^i (\log \theta)_{,i} = \rho \theta \dot{\gamma}, \dot{\gamma} \geq 0 \quad (144)$$

in which

$$\dot{\eta} = \frac{\partial \eta}{\partial t} + \eta_{,i} v^i, \quad \frac{\partial \rho}{\partial t} + (\rho \dot{x}^i)_{,i} = \dot{\rho}. \quad (145)$$

These expressions contain the following functions:  $\rho$  (density),  $\dot{\epsilon}$  (internal energy),  $q$  (heat flux vector),  $h$  (absorption rate of heat),  $\mathcal{L} = \rho \dot{W} = \Sigma T^{ii}$  (rate of mechanical work of distortions),  $\theta$  (temperature),  $\eta$  (entropy referred to the unit undeformed volume),  $\dot{\rho}$  (mass transfer). We assume  $\dot{\rho} = 0$ .

Further we postulate the following dependences

$$d\eta = \eta_0 d\epsilon + \eta_{\bar{\beta}} dX^{\bar{\beta}} = \dot{\eta} dt, \quad dW = W_{\beta} dX^{\beta} = \dot{W} dt \quad (146)$$

$$d\theta = \theta_0 d\epsilon + \theta_{\bar{\beta}} dX^{\bar{\beta}} = \dot{\theta} dt,$$

$$\begin{aligned} dA &= d(\epsilon - \theta\eta) = A_0 d\epsilon + A_{\bar{\beta}} dX^{\bar{\beta}} \\ &= (1 - \theta_0 \eta - \theta \eta_0) d\epsilon - (\theta_{\bar{\beta}} \eta + \theta \eta_{\bar{\beta}}) dX^{\bar{\beta}} = \dot{A} dt. \end{aligned}$$

$dX^{\beta'}$  are hidden variables and  $\bar{\beta}$  stands for indices  $\beta$  and  $\beta'$ . It follows that

$$\begin{aligned} \theta d\gamma &= dW + \theta d\eta - d\epsilon = (\theta \eta_0 - 1) d\epsilon + (W_{\beta} + \theta \eta_{\beta}) dX^{\beta} + \theta \eta_{\beta'} dX^{\beta'} \\ &= g_0 d\epsilon + \gamma_{\bar{\beta}} \cdot dX^{\bar{\beta}} \end{aligned} \quad (147)$$

where

$$g_0 = \theta\eta_0 - 1, \quad W_\beta + \theta_\beta\eta - A_\beta = g_\beta, \quad \theta_{\beta'}\eta - A_{\beta'} = g_{\beta'}. \quad (148)$$

We neglect  $\theta_{\beta'}$  and  $\hat{\rho}$ . A more particular analysis [69] was previously performed for the case of visco-elastic classical continua. We shall proceed in a similar way as before using the condensed formulation

$$\theta d\gamma^A = g_B^A dX^B, \quad (g^A = g, \quad \gamma^A = \gamma) \quad (149)$$

and the decomposition

$$g_B^A = g_{B(e)}^A + g_{Bc}^A dX^C. \quad (150)$$

Hence  $g_B^A$  play the role of distortions (of entropic nature) and represent irreversible thermodynamic forces.  $g_{B(e)}$  are generalized phenomenological coefficients and  $g_{Bc}^A$  are elastic parts so that

$$\sum_{\mathcal{K}'} g_{B(e)}^A dX^B = 0, \quad (151)$$

$\mathcal{K}'$  being a closed cycle in  $(X)$ . Thus we deduce an analogous form to (138) for the generalized Burgers vector assigned to the entropy.  $g_{Bc}^A$  vanish identically if the Onsager's reciprocity principle is accepted. In the case of isochrone and isotopic dependences, this quantity vanishes. The plastic effects can be correlated with non-vanishing entropic Burgers-type vector.

## XII. Final Remarks

(a) The decomposition (137), leads to the below deduced equations which contain as an elastic part the terms (140), and as an irreversible part (139). From (42), (100), or (142) it is possible to obtain equivalent equations. Using (132) we obtain in the frame of a linear theory,

$$T_{\beta(e)}^\alpha = (c_{\beta\gamma}^\alpha, X^\gamma), \quad (152)$$

$c_{\beta\gamma}^\alpha$  being elastic constants. A similar result follows from (151). Further, (139) correlates the symbols  $T$  with the analysis of irreversible processes, since these symbols lead to a definition of torsion and curvature of the respective connexion, which constitute measures of a constitutive incompatibility. The consistent development of the theory will be analysed elsewhere.

(b) We observe that the Taylor expansions can be applied only by including systematically terms of the same order of magnitude in the sense of the above mentioned estimative analysis. For instance, if the characteristics of variability (see (96)) can be approximated by simple differential operators, the distributions in (42) take the form

$$A_{kAB}^{ips} = (A_k^i)_{ps} + (A_{k,l})_{ps} x_{AB}^l. \quad (153)$$

It follows that the energetic terms including the kinematic distortions can be expressed in the form

$$1/2 (\bar{\sigma}^{ik} dA_k^i + \sigma^{i(kl)} dA_{(k,l)}^i) = 1/2 ((\sigma^{ik}, da_k^i) + (\sigma^{i(kl)}, da_{(kl)}^i)) \quad (154)$$

for

$$\sigma_{ps}^{ikl} = \sum_{AB} f_{ps}^i (x^k x^l)_{AB}, \quad \bar{\sigma}_{ps}^{ik} = \sum_{AB} \sigma_{psAB}^{ik}.$$

It is obvious that the corresponding model which results only in the frame of a local theory constitutes an extension of the symmetric continuum (for  $x_{AB}^k \equiv x_{ps}^k$ ) and if non-primitivity is taken into account, a more general analysis leads to a Cosserat like continuum which is endowed with more general features then usually considered.

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# THE ELASTIC GENERALIZED COSSERAT CONTINUUM WITH INCOMPATIBLE STRAINS

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Considered is a continuum with deformable directors. Dislocations are regarded as sources of incompatibilities and internal strains. Established are the relations between the dislocation density tensor and the gradients of directors. The conservation law for dislocations (i.e. the law that the dislocation lines cannot end inside a body) appears as the integrability condition for the dislocation density – gradients of directors relation. In a linearly connected space  $L_3$  in which the directors of a dislocated medium represent fields of absolutely parallel vectors the equality of the dislocation density tensor with the torsion tensor of the space  $L_3$  follows as an immediate consequence. It is also proved that the geometry of  $L_3$  is equivalent to the geometry of the linearly connected space  $L_3$  which is defined in terms of the distortions, introduced in the theories based on the non-oriented continuum models. From the principle of virtual work are derived the general (non-linear) relations for stress and hyperstress. The stress tensor is not symmetric. In the appendix are presented the modified divergence theorem and the expressions for the variations of the gradients of directors in the absence of a displacement field, i.e., in the case when the compatibility conditions for the strain tensor are not satisfied.

Key word: Continuum mechanics: Cosserat continua; dislocation field theory; oriented media.

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## I. Introduction

A configuration  $\theta_t$  of a generalized Cosserat continuum representing a body  $\theta$  at an instant  $t$  of time is characterized by the position  $x^k(\mathbf{X}, t)$  of the particles  $\mathbf{X}$  of the body, and by the directors  $\mathbf{d}^{(\lambda)}(\mathbf{X}, t)$ ,  $\lambda = 1, 2, 3$ , attached to each point of the body. If  $X^K$ ,  $K = 1, 2, 3$  are material, and  $x^k$  the spatial coordinates of points of the body, and if  $\mathbf{D}^{(\lambda)}$  are the directors in the initial configuration,

$$\mathbf{D}^{(\lambda)} = \mathbf{D}^{(\lambda)}(\mathbf{X}), \quad (1.1)$$

the equations of motion are

$$x^k = x^k(X^1, X^2, X^3; t), \quad (1.2)$$

$$d_k^{(\lambda)} = d_k^{(\lambda)}(D_1^{(\lambda)}, D_2^{(\lambda)}, D_3^{(\lambda)}; \mathbf{X}, t). \quad (1.3)$$

The theory of elasticity of this medium is discussed in a number of papers; for references see [1].

In the present paper we are concerned with the problem of internal stresses in the generalized Cosserat continuum. We assume that the state of stress can not be associated with a strain tensor which satisfies the compatibility conditions. Therefore, there are no analytic mappings of the form (1.2), (1.3) which bring the body considered from a stressed configuration  $(D)$  to an unstressed configuration  $(I)$ . In general, a body may be released from internal stresses only through the violation of its continuity, e.g., by cutting. It is possible, however, to consider a certain non-Euclidean configuration  $(N)$  in a non-Euclidean space  $L_3$  in which the body is free from stresses and its continuity is preserved. If  $u^\lambda$ ,  $\lambda = 1, 2, 3$  are coordinates of points of the body  $\theta$  in the configuration  $(N)$ , in the space  $L_3$ , the mapping  $(N) \rightarrow (D)$  is given by the non-integrable relations

$$du^\lambda = \phi_i^{(\lambda)} dx^i, \quad (1.4)$$

where  $\phi_i^{(\lambda)}$  are elastic distortions. The strain tensor corresponding to this deformation does not satisfy the compatibility conditions.

For non-oriented bodies the general theory of incompatible deformations in elasticity is elaborated by Stojanović, Vujošević, and Djurić [2, 3]. To establish the stress relations we shall follow the method and ideas of [2].

As sources of incompatibilities we regard dislocations. In section II of this paper, we establish the connection between the dislocation density tensor (which we consider as given) and the gradients or directors. The integrability conditions for the dislocation density – director gradients relations yield some geometric implications, which we discuss in section III. The conservation law for the dislocation density tensor (i.e., the theorem that the dislocation lines cannot end inside a body), and the equality of the torsion tensor of the space  $L_3$  with the dislocation density tensor follow as immediate consequences of these geometric implications. The stress relations are derived in section IV.

## II. Dislocations and the Deformations of Directors

Let us regard simultaneously a crystal lattice with dislocations and the corresponding perfect reference lattice. The lattice vectors  $\mathbf{D}^{(\lambda)}$  of the

perfect crystal are determined by the lattice points and if the crystal is subjected to a deformation, the lattice vectors are deformed as material vectors. Hence, the lattice vectors of a perfect crystal can not be considered as directors of a Cosserat medium. The lattice vectors in the perfect undeformed crystal represent fields of parallel vectors in the Euclidean sense.

If we refer the reference lattice to a coordinate system  $X^k$ , and the dislocated lattice to a coordinate system  $x^k$ , it is impossible to determine the lattice points of the dislocated crystal by the mappings of the form

$$x^k = x^k(\mathbf{x}) \quad (2.1)$$

and the lattice vectors  $\mathbf{d}^{(\lambda)}$  of the dislocated crystal can not be regarded as deformed lattice vectors  $\mathbf{D}^{(\lambda)}$  of the reference crystal, i.e., there are no relations of the form

$$d_k^{(\lambda)} = D_k^{(\lambda)} X_{;k}^{\lambda}. \quad (2.2)$$

If  $P$  is a lattice point of the dislocated crystal and if  $D_i^{(\lambda)}$  are components of the lattice vectors of the reference crystal transported parallel to  $P$ , for the components of the lattice vectors  $d_i^{(\lambda)}$  we may write

$$d_i^{(\lambda)} = D_i^{(\lambda)} + \Delta_i^{(\lambda)}. \quad (2.3)$$

The vectors  $\Delta^{(\lambda)}$  vanish if the directors  $d_i^{(\lambda)}$  deform as material vectors.

An infinitesimal displacement along the lattice vector  $\mathbf{d}^{(\lambda)}$  is represented by the expression

$$dr^\lambda = d_i^{(\lambda)} dx^i. \quad (2.4)$$

Let  $l$  be a closed contour passing over lattice points in the “good” region of a dislocated crystal and surrounding a dislocation line (or a zone with dislocations). The contour integral

$$\Delta b^{(\lambda)} = \oint_l dr^\lambda = \oint_l (D_i^{(\lambda)} + \Delta_i^{(\lambda)}) dx^i \quad (2.5)$$

determines the components of the Burgers vector in the directions of the lattice vectors  $\mathbf{d}^{(\lambda)}$ . The Burgers vectors  $\Delta \mathbf{b}$  corresponding to the dislocations surrounded by  $l$  is given by the components

$$\Delta b^i = \Delta b^\lambda d_{(\lambda)}^i, \quad (2.6)$$

where  $d_{(\lambda)}$  are vectors of the reciprocal director triad,  $d_{(\lambda)}^i d_j^{(\lambda)} = \delta_j^i$ .

For an infinitesimal region  $\Delta\mathbf{F}$  encircled by  $l$  we have from (2.5)

$$\begin{aligned}\Delta b^\lambda &= \int \int_{\Delta\mathbf{F}} (D_{[j, i]}^{(\lambda)} + \Delta_{[j, i]}^{(\lambda)}) dF^{ij} \\ &\approx (D_{[j, i]}^{(\lambda)} + \Delta_{[j, i]}^{(\lambda)}) \Delta F^{ij}.\end{aligned}\quad (2.7)$$

Since the vectors  $D_i^{(\lambda)}$  represent fields of parallel vectors, the gradients  $D_{j, i}^{(\lambda)}$  vanish and we have

$$\Delta b^\lambda = \Delta_{[j, i]}^{(\lambda)} \Delta F^{ij}. \quad (2.8)$$

When  $\Delta\mathbf{F} \rightarrow 0$ , we obtain from (2.6) and (2.8) for the dislocation density tensor  $\alpha_{ij}^{jk}$  the expression

$$\alpha_{ij}^{jk} = d_{(\lambda)}^k \lim_{\Delta\mathbf{F} \rightarrow 0} \frac{\Delta b^\lambda}{\Delta F^{ij}} = d_{(\lambda)}^k \Delta_{[j, i]}^{(\lambda)}. \quad (2.9)$$

This relation, or its equivalent

$$\alpha_{ij}^{jk} = d_{(\lambda)}^k d_{[j, i]}^{(\lambda)} = b^{kl} \alpha_{ijl} \quad (2.10)$$

where the fundamental metric tensor  $\mathbf{b}$  of the Euclidean space is used for the raising and lowering of indices, represents the basic relation between the distribution of dislocations and the gradients of directors [1, 4].

The existence of the directors  $\mathbf{d}^{(\lambda)}$  for a given distribution of dislocations depends on the integrability of the equations (2.10), which we write in the form

$$\partial_i d_j^{(\lambda)} - \partial_j d_i^{(\lambda)} = 2\alpha_{ij}^{kl} d_l^{(\lambda)}. \quad (2.11)$$

Differentiating this relation with respect to  $x^k$  and alternating the indices  $ijk$  we obtain

$$\partial_{[k} \partial_{i]} d_{j]}^{(\lambda)} = d_{l(\lambda)}^{(\lambda)} \partial_{[k} \alpha_{ij]}^{l]} + \alpha_{[ij}^{l]} \partial_{k]} d_l^{(\lambda)}. \quad (2.12)$$

The left-hand side of (2.12) vanishes because of the commutativity of partial derivatives, and the integrability conditions reduce to the relations

$$\partial_{[k} \alpha_{ij]}^{l]} = - [d_{l(\lambda)}^{(\lambda)} (\partial_{k]} d_l^{(\lambda)}) \alpha_{ij]}^{l]}]_{[ijk]}. \quad (2.13)$$

The indices  $ijk$  involved in the alternation in (2.13) must all have different values and hence there are only three independent relations (2.13),

for  $l=1, 2, 3$ . Nothing will be lost if we transvect these relations with the alternating Ricci tensor  $\epsilon_b^{ijk}$  formed with respect to the Euclidean metric tensor **b**. Writing

$$\frac{1}{2} \epsilon_b^{ijk} \alpha_{ij}^l = \alpha^{kl}, \quad (2.14)$$

and

$$d_{(\lambda)}^l \partial_k d_l^{(\lambda)} = - d_l^{(\lambda)} \partial_k d_{(\lambda)}^l \equiv D_{kl}, \quad (2.15)$$

the integrability conditions (2.13) obtain the form

$$\partial_k \alpha^{kl} + b_{km}^k \alpha^{ml} = - D_{mt}^l \alpha^{mt}. \quad (2.16)$$

Here  $b_{kl}^m$  are the Christoffel symbols of the first kind for the tensor **b**, and  $b_{km}^m = \partial_k \ln \sqrt{b}$ .

### III. Geometry

In the continuum theory of dislocations the stress-free state ( $N$ ) of a dislocated crystal is considered in a linearly connected metric space with torsion [5, 6, 7]. If  $g_{ij}$  is the fundamental tensor of this space and  $S_{ij}^k$  the torsion tensor, the coefficients of connection  $\Gamma_{ij}^k$  are given by

$$\Gamma_{ij}^k = g_{ij}^{'k} + h_{ij}^{::k}, \quad (3.1)$$

where  $g_{ij}^{'k}$  are the Christoffel symbols of the second kind for the tensor **g** and

$$\begin{aligned} h_{ij}^{::k} &= S_{ij}^{::k} - S_{ji}^k + S_{ki}^j, \\ S_{ij}^{::k} &\equiv \Gamma_{[ij]}^k. \end{aligned} \quad (3.2)$$

Writing

$$g_{ijk} \equiv \frac{1}{2} \left( \overset{b}{\nabla}_i g_{jk} + \overset{b}{\nabla}_j g_{ki} - \overset{b}{\nabla}_k g_{ij} \right), \quad (3.3)$$

where  $\overset{b}{\nabla}_m$  denotes the covariant differentiation with respect to the Euclidean metric tensor **b** [7], the coefficients  $\Gamma_{ij}^k$  may be expressed by the relations

$$\Gamma_{ij}^k = b_{ij}^k + g^{kl} g_{ijl} + h_{ij}^{::k} \equiv b_{ij}^k + G_{ij}^{::k}. \quad (3.4)$$

If we assume that the lattice vectors of a dislocated crystal represent fields of parallel vectors in the space  $L_3$ , they have to be covariant constant with respect to the connection  $\Gamma_{ij}^k$ ,

$$\overset{\Gamma}{\nabla}_i d_j^{(\lambda)} = \partial_i d_j^{(\lambda)} - \Gamma_{ij}^k d_k^{(\lambda)} = 0, \quad (3.5)$$

and from this and (2.15) it follows that

$$\Gamma_{ij}^k = D_{ij}^k = d_{(\lambda)}^k \partial_i d_j^{(\lambda)}. \quad (3.6)$$

Hence, the geometry of the non-Euclidean space  $L_3$  is completely determined by the directors  $\mathbf{d}^{(\lambda)}$ , i.e., by the lattice vectors of the dislocated crystal.

From (2.10) and (3.6) we see that the torsion tensor  $S_{ij}^{;k}$  of  $L_3$  is equal to the dislocation density tensor,

$$S_{ij}^{;k} = \alpha_{ij}^{;k}. \quad (3.7)$$

The integrability condition (2.16) may be brought to a more familiar form. If we substitute partial derivatives by the covariant derivatives with respect to the Euclidean metric  $\mathbf{b}$ , i.e.,

$$\partial_k \alpha^{kl} \equiv \overset{b}{\nabla}_k \alpha^{kl} - b_{km}^k \alpha^{ml} - b_{km}^l \alpha^{km}, \quad (3.8)$$

and if we use the expression (3.4) for the coefficients of connection, the expression (2.16) reduces to

$$\overset{b}{\nabla}_k \alpha^{kl} = - G_{km}^{;l} \alpha^{km}. \quad (3.9)$$

Using the fundamental tensor  $g_{ij}$  of  $L_3$  for the raising and lowering of the indices, so that

$$\alpha^{kl} g_{ij} = \alpha^{kj}. \quad (3.10)$$

the integrability conditions obtain the form

$$\overset{b}{\nabla}_k \alpha_{ij}^k = g^{kl} G_{ijk} \alpha_{il}. \quad (3.11)$$

This coincides with Kröner's and Seeger's [7] generalization to the non-linear case of the conservation law for the dislocation density tensor, given in the linear theory by Nye [9].

In the treatment of the continuously distributed dislocations Kondo [6] and Kröner and Seeger [7, 8] consider the space  $L_3$  corresponding to the  $(N)$ -configuration of a dislocated crystal with the coefficients of connection determined in terms of the distortions  $\phi_l^{(\lambda)}$ ,

$$\tilde{\Gamma}_{lm}^k = \phi_{(\lambda)}^k \partial_l \phi_m^{(\lambda)}. \quad (3.12)$$

The coefficients  $\Gamma_{lm}^k$  determined in terms of the directors  $\mathbf{d}^{(\lambda)}$  were introduced first by Bilby et al. [5] (for detailed references, see [10, 11]. However, the geometries of the two spaces,  $L_3$  and  $\tilde{L}_3$ , are equivalent. In  $L_3$  the dislocation density tensor is also equal to the torsion tensor of the space,

$$\alpha_{lm}^{::k} = \tilde{\Gamma}_{[lm]}^k = \phi_{(\lambda)}^k \partial_{[l} \phi_{m]}^{(\lambda)}. \quad (3.13)$$

The integrability condition of (3.13) reads

$$\overset{b}{\nabla}_k \alpha^{kl} + b_{km}^k \alpha^{ml} = - \tilde{\Gamma}_{mt}^l \alpha^{ml}. \quad (3.14)$$

Comparing this with (2.16) we see that the coefficients of connection  $\Gamma_{ij}^k$  and  $\tilde{\Gamma}_{ij}^k$  of the spaces  $L_3$  and  $\tilde{L}_3$  are equal, which makes the geometries equivalent.

#### IV. Stress Relations and the Equilibrium Conditions

To obtain the stress relations, the equations of equilibrium, and the boundary conditions we shall use the principle of virtual work. In statics this principle has the form

$$\delta E = A, \quad (4.1)$$

where  $E$  is the total internal energy of a body  $\theta$ ,

$$E = \int_{\theta} \rho w d\theta,$$

and  $w$  is the energy density.  $A$  is the virtual work of all forces acting on the body.

In analogy with [1] we shall assume that the internal energy is a function of the distortions  $\phi_{(\lambda)}^l$  and of the gradients of directors,  $d_{l,m}^{(\lambda)}$ .

$$w = w(\phi_{(\lambda)}^l, d_{l,m}^{(\lambda)}). \quad (4.2)$$

We assume further that the independent variations are  $\delta x^i$  and  $\delta d_i^{(\lambda)}$ , and the expression for the virtual work may be written in the form

$$A = \int_v \rho (f_i \delta x^i + g_{(\lambda)}^i \delta d_i^{(\lambda)}) dv + \int_s (F_i \delta x^i + G_{(\lambda)}^i \delta d_i^{(\lambda)}) da \quad (4.3)$$

where  $f_i$  is the volume force,  $g_{(\lambda)}^i$  are the director forces,  $F_i$  and  $G_{(\lambda)}^i$  are surface tractions.

Variation of the total energy gives

$$\delta E = \int_v \rho \left( \frac{\partial w}{\partial \phi_{(\lambda)}^i} \delta \phi_{(\lambda)}^i + \frac{\partial w}{\partial d_{i,j}^{(\lambda)}} \delta d_{i,j}^{(\lambda)} \right) dv. \quad (4.4)$$

To transform this expression to the form which involves only the independent variations  $\delta x^i$  and  $\delta d_{(\lambda)}^i$  we have to apply the modified divergence theorem (see Appendix, eq (A.13)). By (A.18) the expression (4.4) becomes

$$\delta E = \int_v \rho \left[ \left( \frac{\partial w}{\partial \phi_{(\lambda)}^i} - \frac{\partial w}{\partial d_{i,l}^{(\mu)}} d_{i,j}^{(\mu)} \phi_j^{(\lambda)} \right) \delta \phi_{(\lambda)}^i + \frac{\partial w}{\partial d_{i,j}^{(\mu)}} (\delta d_{i,j}^{(\mu)})_{,j} \right] dv. \quad (4.5)$$

Writing

$$\rho \left( \frac{\partial w}{\partial \phi_{(\lambda)}^i} - \frac{\partial w}{\partial d_{i,n}^{(\mu)}} d_{i,j}^{(\mu)} \phi_j^{(\lambda)} \right) \phi_{(\lambda)}^j = t_l^j, \quad (4.6)$$

$$\rho \frac{\partial w}{\partial d_{i,j}^{(\mu)}} = h_{(\mu)}^{ij}. \quad (4.7)$$

and applying (A.13) and the divergence theorem to (4.5), we obtain for the variation of the internal energy the expression

$$\delta E = - \int_v (t_{l,j}^j \delta x^l + h_{(\mu),j}^{ij} \delta d_{i,j}^{(\mu)}) dv + \oint_s (t_l^j \delta x^l + h_{(\mu),j}^{ij} \delta d_{i,j}^{(\mu)}) da_j. \quad (4.8)$$

The principle of virtual work gives now the equilibrium equations

$$t_{l,j}^j + \rho f_l = 0, \quad (4.9)$$

$$h_{(\mu),j}^{ij} + \rho g_{(\mu)}^i = 0, \quad (4.10)$$

and the conditions on the bounding surfaces of the body,

$$t_l^j n_j = F_l, \quad (4.11)$$

$$h_{(\mu),j}^{ij} n_j = G_{(\mu)}^i. \quad (4.12)$$

The relations (4.6) and (4.7) represent the stress relations, where  $t_l^i$  is the stress tensor and  $h_{(\mu)}^{ij}$  are three tensors of the stresses of orientation.

The internal energy function  $w$  must be invariant under rigid motions. If  $x^k$  are Cartesian coordinates, the function  $w$  has to be invariant under the transformations of the group of orthogonal transformations (cf. [10], p. 884).

$$\bar{x}^k = (\delta_l^k + \omega_l^k) x^l. \quad (4.13)$$

where  $\omega$  is an antisymmetric tensor of infinitesimal rotation. The invariance requirement yields three partial differential equations in  $9 + 27 = 36$  variables  $\phi_{(\lambda)}^i$  and  $d_{i,j}^{(\lambda)}$ ,

$$\left[ b^{il} \left( \frac{\partial w}{\partial \phi_{(\lambda)}^l} \phi_{(\lambda)}^j - \frac{\partial w}{\partial d_{m,j}^{(\mu)}} d_{m,l}^{(\mu)} - \frac{\partial w}{\partial d_{j,m}^{(\mu)}} d_{l,m}^{(\mu)} \right) \right]_{[ij]} = 0. \quad (4.14)$$

This system admits  $36 - 3 = 33$  independent integrals:

$$C_{\lambda\mu} = C_{\mu\lambda} = b_{lm} \phi_{(\lambda)}^l \phi_{(\mu)}^m, \quad (4.15)$$

$$F_{\lambda\mu}^{(\alpha)} = d_{l,m}^{(\alpha)} \phi_{(\lambda)}^l \phi_{(\mu)}^m, \quad (4.16)$$

and  $w$  is an arbitrary function of these integrals,

$$w = w(C_{\lambda\mu}, F_{\lambda\mu}^{(\alpha)}). \quad (4.17)$$

Instead of the stress of orientation tensors we may introduce one single hyperstress tensor  $h_i^{jk}$ ,

$$h_i^{jk} \equiv h_{(\mu)}^{jk} d_i^{(\mu)}. \quad (4.18)$$

From (4.8) and (4.14) for the antisymmetric part of the stress tensor we obtain

$$t^{[ij]} = \rho \left( b^{il} \frac{\partial w}{\partial d_{j,m}^{(\mu)}} d_{l,m}^{(\mu)} \right)_{[ij]}, \quad (4.19)$$

which, using now (4.10) and (4.18), reduces to the simple form

$$t^{[ij]} = h_{,m}^{[ij]m} + d^{(\mu)[i} g_{(\mu)}^{j]}. \quad (4.20)$$

The tensor  $d^{(\mu)[i} g_{(\mu)}^{j]} \equiv l^{[ij]}$  represents some extrinsic couples which act on the particles of the body.

From (4.19) and (4.20) we see that the antisymmetric part of the stress tensor depends exclusively on the hyperstress and extrinsic couples, i.e., on the deformations of the directors, and not on the distortions.

Since the energy function  $w$  depends only on the tensors  $\mathbf{C}$  and  $\mathbf{F}$ , using (4.15) and (4.16) we obtain for the symmetric part of the stress tensor and for the stress of orientation tensors from (4.6) and (4.7) the following relations:

$$t^{(ij)} = 2\rho \frac{\partial w}{\partial C_{\lambda\mu}} \phi_{(\lambda)}^i \phi_{(\mu)}^j + h_{,m}^{(ij)m} + l^{(ij)}, \quad (4.21)$$

$$(l^{ij} \equiv d^{(\mu)i} g_{(\mu)}^j)$$

$$h_{(\mu)}^{ij} = \rho \frac{\partial w}{\partial F_{\alpha\beta}^{(\mu)}} \phi_{(\alpha)}^i \phi_{(\beta)}^j. \quad (4.22)$$

In [4] we assumed, that the hyperstress  $h^{ijk}$  is an antisymmetric tensor,  $h^{ijk} = -h^{jik}$ , completely determined by the given dislocation density tensor. If, moreover, we assume that the director forces act only through the couples  $l^{[ij]}$  and that  $l^{(ij)} = 0$ , the symmetric part of the stress tensor will depend only on the elastic distortions.

## V. Appendix

Since there are no integrable mappings of a non-Riemannian configuration ( $N$ ) on the Euclidean configuration ( $D$ ), a straightforward application of the divergence theorem to the surface integral

$$\oint_s (t_i^j \delta x^i + h_{(\lambda)}^{ij} \delta d_i^{(\lambda)}) da_j \quad (A.1)$$

is impossible.

The Pfaffians

$$dx^i = \phi_{(\lambda)}^i du^\lambda, \quad du^\lambda = \phi_i^{(\lambda)} dx^i \quad (A.2)$$

represent mappings of infinitesimal elements  $dx^i$  of the Euclidean space on the corresponding elements  $du^\lambda$  of the non-Euclidean space. Let  $\mathbf{x}_1$  and  $\mathbf{x}_2 = \mathbf{x}_1 + \Delta \mathbf{x}$  be two points in  $E_3$ , then

$$x_2^i - x_1^i = \Delta x^i = \phi_{(\lambda)}^i \Delta u^\lambda; \quad \Delta u^\lambda = \phi_i^{(\lambda)} \Delta x^i. \quad (A.3)$$

The ( $N$ )-configuration is fixed and  $\Delta u^\lambda$  remain unchanged when we compare different possible configurations ( $D$ ).

Virtual displacements of any two points are  $\delta x_1^i$  and  $\delta x_2^i$  and if they are sufficiently near to one another, according to (A.3), we may write

$$\Delta \delta x^i = \delta x_2^i - \delta x_1^i = \delta \Delta x^i = \delta \phi_{(\lambda)}^i \Delta u^\lambda. \quad (A.4)$$

Here  $\Delta \delta x^i$  represents the difference of virtual displacements of the two points, and  $\delta \Delta x^i$  is the virtual change of  $\Delta x^i$  when the points  $x_1$  and  $x_2$  undergo displacements  $\delta x_1$  and  $\delta x_2$ . From (A.3) we have

$$\Delta \delta x^i = \delta \phi_{(\lambda)}^i \phi_i^{(\lambda)} \Delta x^i. \quad (A.5)$$

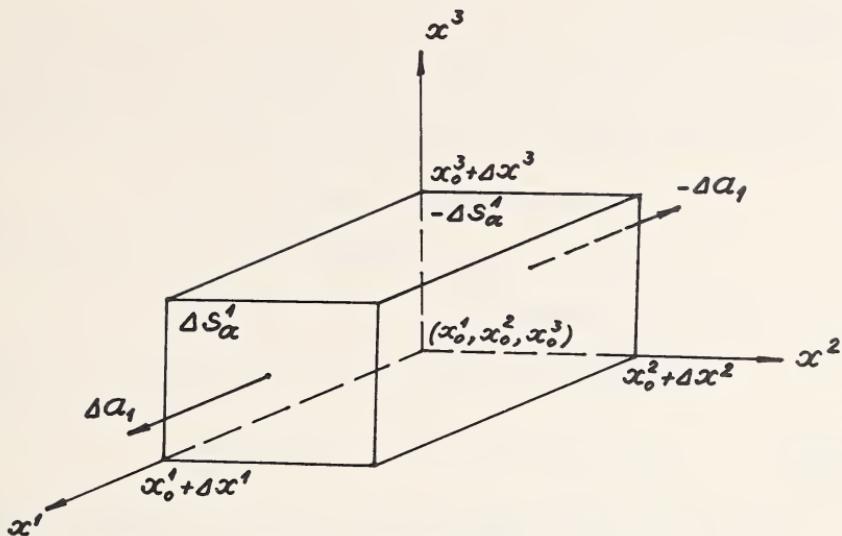


FIGURE 1

Let now  $T_i^j$  be any regular and differentiable tensor field in  $E_3$  and let us consider the integral

$$J = \oint \oint_{s_{\mathfrak{A}}} T_i^j \delta x^i da_j, \quad (\text{A.6})$$

where  $s$  is the surface enveloping a volume  $v$  of a body  $\theta$ . The whole region  $v$  may be divided into a number of small elements  $\Delta v_{\mathfrak{A}}$  with enveloping surface  $\Delta s_{\mathfrak{A}}$ , and we have

$$J = \sum_{\mathfrak{A}} J_{\mathfrak{A}} = \sum_{\mathfrak{A}} \oint \oint_{s_{\mathfrak{A}}} T_i^j \delta x^i da_j. \quad (\text{A.7})$$

For Cartesian coordinates  $x^i$  we may chose  $\Delta v_{\mathfrak{A}}$  to be cuboids with edges  $\Delta x^1, \Delta x^2, \Delta x^3$ . Then, if we put  $T_i^j \delta x^i \equiv T^j$  we have

$$\begin{aligned} J_{\mathfrak{A}} = & \int \int_{\Delta s_{\mathfrak{A}}^1} T^1 da_1 + \int \int_{\Delta s_{\mathfrak{A}}^2} T^2 da_2 + \int \int_{\Delta s_{\mathfrak{A}}^3} T^3 da_3 + \int \int_{-\Delta s_{\mathfrak{A}}^1} T^4 (-da_1) \\ & + \int \int_{-\Delta s_{\mathfrak{A}}^2} T^2 (-da_2) + \int \int_{-\Delta s_{\mathfrak{A}}^3} T^3 (-da_3). \end{aligned} \quad (\text{A.8})$$

On  $\Delta s_{\mathfrak{A}}^1$  we have ( $x \equiv x^1, y \equiv x^2, z \equiv x^3$ )

$$\Delta s_{\mathfrak{A}}^1: \quad T^1 = T^1(x_0 + \Delta x, y, z);$$

and on  $-\Delta s_{\mathfrak{A}}^1$ :

$$-\Delta s_{\mathfrak{A}}^1: \quad T^1 = T^1(x_0, y, z).$$

Similarly

$$\begin{aligned}\Delta s_{\mathfrak{A}}^2: \quad T^2 &= T^2(x, y_0 + \Delta y, z), \\ -\Delta s_{\mathfrak{A}}^2: \quad T^2 &= T^2(x, y_0, z), \\ \Delta s_{\mathfrak{A}}^3: \quad T^3 &= T^3(x, y, z_0 + \Delta z), \\ -\Delta s_{\mathfrak{A}}^3: \quad T^3 &= T^3(x, y, z_0).\end{aligned}$$

Hence, for the pair of integrals

$$J_{\mathfrak{A}}^1 \equiv \iint_{\Delta s_{\mathfrak{A}}^1} T^1 da_1 - \iint_{-\Delta s_{\mathfrak{A}}^1} T^1 da_1 = \iint_{\Delta s_{\mathfrak{A}}^1} \Delta T^1 da_1 \quad (\text{A.9})$$

we have

$$J_{\mathfrak{A}}^1 = \int_{y_0}^{y_0 + \Delta y} \int_{z_0}^{z_0 + \Delta z} [T^1(x_0 + \Delta x, y, z) - T^1(x_0, y, z)] dy dz. \quad (\text{A.10})$$

However, for the regular field  $T_i^j$  we have

$$T_i^1(x_0 + \Delta x, y, z) = T_i^1(x_0, y, z) + \partial_1 T_i^1 \Delta x + \dots, \quad (\text{A.11})$$

and for the variations we have from (A.5)

$$\delta x^i|_{(x_0 + \Delta x, y, z)} = \delta x^i|_{x_0} + \Delta \delta x^i = \delta x^i + \delta \phi_{(\lambda)}^i \phi_1^{(\lambda)} \Delta x. \quad (\text{A.12})$$

The difference  $\Delta T^1$  in (A.7) obtains now the form

$$\Delta T^1 = (T_i^1 \delta \phi_{(\lambda)}^i \phi_1^{(\lambda)} + \partial_1 T_i^1 \delta x^i) \Delta x. \quad (\text{A.13})$$

For infinitesimal elements  $\Delta V_{\mathfrak{A}}$  the mean-value theorem may be applied to the integrals  $J_{\mathfrak{A}}^1$ , which yields

$$J_{\mathfrak{A}}^1 = (T_i^1 \delta \phi_{(\lambda)}^i \phi_1^{(\lambda)} + \partial_1 T_i^1 \delta x^i) \Delta x \Delta y \Delta z$$

and, in general,

$$J_{\mathfrak{A}} = (T_i^j \delta \phi_{(\lambda)}^i \phi_j^{(\lambda)} + \partial_j T_i^j \delta x^i) dv. \quad (\text{A.14})$$

When  $\Delta v \rightarrow 0$  and  $A \rightarrow \infty$ , the sum (A.5) becomes the volume integral over  $v$  and for any curvilinear system of coordinates we may finally write

$$J = \oint_s \oint_v T_i^j \delta x^i da_j = \iint_v (\nabla_j T_i^j \delta x^i + T_i^j \delta \phi_{(\lambda)}^i \phi_j^{(\lambda)}) dv. \quad (\text{A.15})$$

For the directors we assume that they are continuous and differentiable functions of position in  $E_3$ . If  $P\{\mathbf{x}\}$  and  $Q\{\mathbf{x} + \Delta\mathbf{x}\}$  are two infinitesimally near points of the body  $\theta$ , the difference of the components of the directors at  $P$  and  $Q$  is in the first approximation given by the relation

$$d_i^{(\lambda)}\{Q\} - d_i^{(\lambda)}\{P\} \equiv \Delta d_i^{(\lambda)} - d_{i,j}^{(\lambda)}\Delta x^j + \dots \quad (A.16)$$

The variation of this difference gives

$$\begin{aligned} \delta d_i^{(\lambda)}\{Q\} - \delta d_i^{(\lambda)}\{P\} &= \Delta \delta d_i^{(\lambda)} = \delta \Delta d_i^{(\lambda)} \\ &= (\delta d_{i,j}^{(\lambda)}) \Delta x^j + d_{i,j}^{(\lambda)} \delta \Delta x^j. \end{aligned} \quad (A.17)$$

But we also have

$$\delta \Delta d_i^{(\lambda)} = \delta d_i^{(\lambda)}\{Q\} - \delta d_i^{(\lambda)}\{P\} = (\delta d_i^{(\lambda)})_{,j} \Delta x^j, \quad (A.18)$$

and from (A.3), (A.15), and (A.16) it follows that

$$(\delta d_i^{(\lambda)})_{,j} \Delta x^j = (\delta d_{i,j}^{(\lambda)}) \Delta x^j + d_{i,j}^{(\lambda)} \phi_i^{(\mu)} \delta \phi_{(\mu)} \Delta x^j. \quad (A.19)$$

This expression must be valid for any  $\Delta x^i$  and we finally have

$$(\delta d_i^{(\lambda)})_{,j} = \delta(d_{i,j}^{(\lambda)}) + d_{i,j}^{(\lambda)} \delta \phi_{(\mu)} \phi_j^{(\mu)}. \quad (A.20)$$

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## Discussion on Papers by E. Kröner, and E. Kröner and B. K. Datta.

ERINGEN: I have three questions I would like to put to our Chairman.

One is: What are the equations of motion and the boundary conditions in his non-local theory? The second one is: In a non-local theory why use the deformation gradients? The third one is: What can be said about the stability of the elastic continuum? That is, what restrictions does the non-negative energy function place on the constitutive functionals?

KRÖNER: As regards the first question, the equations of motion are integro-differential equations. Actually, one can write them down immediately: one starts with the equations of motion of the local theory in the form which contains the stress tensor and then replaces the stress by the displacement via the non-local constitutive law connecting stress and strain. Now, the second question was why we use the displacement gradient  $\beta_{ij}$ . Do you mean instead of using the strain or the strain gradient?

ERINGEN: No, I think that, in general, the deformation of all points in the body should be used. Why the deformation gradient only?

KRÖNER: We always use the strain in elasticity theory and also here.

ERINGEN: But here we are dealing, of course, with non-local theory.

KRÖNER: This doesn't really matter because the strain still is a local concept. The strain describes the change in distance of neighboring atoms, for instance, and this is the same in non-local as in local theories. The non-locality has to do with the range of the forces, and so appears not in the strain but in the crystal.

ERINGEN: Perhaps I could explain that a little further. If we remember, in continuum mechanics dependence of stress on the deformation gradient arises from the near neighborhood hypothesis. Since you don't have a local theory, I think that perhaps you have to formulate it in terms of a displacement functional. In other words, why favor the first gradient of the deformation?

KRÖNER: [At this point Professor Kröner gave a short discussion at the blackboard which was not recorded.] One other comment: If we develop the strain in the stress-strain law in terms of a Taylor series around the point  $r$ , then we would get a whole series of terms and these would be strain gradients. So, if you take a strain gradient theory up to infinite order it would be equivalent to this theory, and so you see that the first strain gradient approach is a very poor approximation of this non-local theory.

ERINGEN: With this process, can you get not only the strain gradients, but also higher order strains, third, fourth order strains, etc., which are not expressible as gradients of the deformation at the point  $r$ ?

KRÖNER: In my opinion this has nothing to do with non-locality. This is something which comes in if you have a structure of the body as in your materials. Your materials are primarily not non-local materials. You can introduce non-locality in addition, but that is a different story.

ERINGEN: The boundary conditions. Do you have any idea about that?

KRÖNER: Again one just writes the local equations and replaces the stress by the displacements via the non-local stress-strain law. In this way one obtains the boundary conditions in integral form.

ERINGEN: One other thing: I am wondering whether we can call your theory a non-local constitutive theory, because Cauchy's equations of motion are assumed to be valid rather than a more general set of equations incorporating the balances of other points.

KRÖNER: Well, this is a functional equation. The integral equation is a simple kind of functional equation.

ERINGEN: Right, but the motion of a given point is affected by the motions of others. In other words you have only an ordinary partial differentiation for the stress tensor at the point under consideration, which does not reflect the non-local character of the field.

KRÖNER: I have no objection if you call this theory a non-local constitutive theory. About the stability I cannot say much, but, of course, there are restrictions on the form of these tensors. This has to be explored.

DE WIT: Equation 12 in your non-local review paper looks just like the strain in a Cosserat continuum. Can you perhaps comment on whether there is any relation to Cosserat theory here or not?

KRÖNER: Well, there are some similarities between the Cosserat theory and the continuous dislocation theory, of course, but I know these are only similarities. There are also important differences, and I think this again is a rather long story. Perhaps we could speak of this in the final panel.

DE WIT: You still maintain there is a basic difference.

KRÖNER: Yes.

BARNETT: In reply to Professor Eringen's questions, which I think were very good: If you recognize that in developing this non-local theory, you try merely to reproduce the lattice mechanics—which may or may not be correct, but probably is to a certain approximation—you find that the gradient of the displacement field enters naturally into the represen-

tation in this quasi-continuum. You don't really care about that because it is somewhat artificial; you have a choice of solving the equation in either of the two representations, direct or reciprocal, and if you go to the Fourier representation, which is probably the most natural to do from the lattice, then you are talking about a displacement. You don't really ever have to worry about displacement gradients—unless, perhaps, you went to higher order terms in the expansion, in other words the anharmonic terms; then you might pick up the higher gradients of the displacement field. At any rate, if you remain with the Fourier representation, you really only have to worry about the displacement field as far as the harmonic approximation is concerned. Secondly, from some work I have started I think this question of stability is one which is very important, and it is still open to discussion. We tried to look at this from a stand-point of investigating these integral equations in terms of generalized functions. It turns out that you run into some very difficult problems because positive definite operators are defined only with respect to particular types of functions which we really don't encounter in any of these physical situations, so that was a very good question which we cannot answer right now.

One thing I would like to interject is that I think there is a fundamental difference between approaching the non-local theory from trying to reconstruct the lattice mechanics using Kunin and Krumhansl's interpolation schemes,<sup>1</sup> and trying to develop the non-local theory by continuizing the lattice through the Euler-MacLaurin formula. You can show that you do run into all sorts of difficulties or differences when you try to construct solutions for point force loadings, and if you don't take account of the cut-off in  $k$  space and the fact that the Brillouin zone is bounded, then if you wish to develop non-local mechanics along the same lines that lattice mechanics have been developed, you have to change things. If you represent a point defect by a dilatation center, you have to spread out the dilatation center over a certain volume of space in order to obtain an admissible solution. So there are many questions that are still open and I don't think it is really clear how these two approaches differ and how they are similar, but I think there are some very fundamental differences.

KRÖNER: If I may just answer this. First, I did not think we had any difficulty with the dilatation center in this formulation of the theory, and second, of course, it is true that you can extract all the solutions of lattice

<sup>1</sup> Krumhansl, J. A., in *Lattice Dynamics*, R. F. Wallis, Ed. (Pergamon Press, Oxford, 1965); Kunin, I. A., *PMM*, **31**, 889 (1967); Vdovin, V. E., and Kunin, I. A., *Soviet Physics—Solid State*, **10**, 297 (1968); Kosilova, V. G., Kunin, I. A., and Sosnina, E. G., *Soviet Physics—Solid State*, **10**, 291 (1968); Kunin, I. A., in *Mechanics of Generalized Continua*, E. Kröner, Ed. (Springer-Verlag, Berlin, 1968).

theory from a continuum theory, but only part of these solutions have physical meaning because of this cut-off, etc. Now I think the selection of physically meaningful solutions is probably another problem which makes obtaining solutions from the two formulations equally difficult.

[Written contribution] Having thought over Dr. Barnett's comment once more, I am quite sure that his "very fundamental differences" of the two formulations are just the usual differences between ordinary space and Fourier space representation of a theory. It then depends on the problem itself which formulation is to be preferred.

ERINGEN: I would like to insert a small comment. I thought that I was playing here the Devil's Advocate in bringing this stability back which I discussed with Professor Kröner sometime ago, trying to induce him to look into this publicly as we discussed privately. Perhaps I owe an apology for this. In regard to the problem of non-locality, I think it is a very good start. I do approve that. I had some misgiving myself in a paper sometime in 1965, where I used a purely formal way of introducing this. I have been puzzled ever since then precisely about these three questions I raised.

MARADUDIN: My question is prompted more by my background as a crystal physicist than as an elastician, but it seems to me that the chief advantage of elasticity theory was its generality and freedom from model building. The general properties of the elastic constants followed either from the symmetry requirements of the point group of the crystal or from more general invariance conditions, rotational invariance and things of this sort. There were few independent parameters of the theory and everything went well. Once you abandon locality in continuum theory and introduce non-locality, it seems to me that you have given up these desirable features of local theory, and you are then faced with all the complications, such as the determining of the  $C_{ijkl}$  for example as a function of  $r$  and  $r'$ , that you have inherent in the lattice theory. I guess my question to Professor Kröner and Dr. Barnett would be: What, then, is the advantage of a continuum non-local theory as opposed to starting directly from a lattice formulation?

KRÖNER: Maybe, I could refer to an allegory which is roughly like this: Somebody has to get up the mountain and there is one plateau here, another one higher up, and a third one just on top. One gets something out for his efforts when he comes to the first plateau, he gets something better at the second plateau, and he obtains the best on top. Now it is relatively easy to come to the lowest plateau, this would correspond to conventional elasticity theory. Climbing to the second plateau would mean using non-local elasticity theory. Finally one has to do much more to come to the peak, i.e. to apply lattice theory, except if trivial solutions

are concerned. If one compares the calculation of the dilatation center of Dr. Bullough and the non-local calculation, there is no doubt that the latter one is much simpler.

Besides this fact it is not at all clear to me that one really gets much more out from lattice theory because this could only be the case with phenomena on a rather atomic scale. As is well-known, classical theories are not too reliable in this region, one rather should use quantum mechanics. In spite of this clear recognition we often prefer the classical theory, putting simplicity over accuracy. I doubt that in these cases the lattice approximation comes much closer to the truth than the non-local approximation. At least, there exist cases where the solutions in the non-local theory are obtained more easily than in the lattice theory. To learn more about this we should start solving problems now.

BEN-ABRAHAM: I would say that as a physicist I much prefer lattice theory. However, it so happens that we are geared and conditioned by a few hundred years to prefer continuous functions. I believe Dr. Barnett showed it very convincingly that the non-local theory is a representation for just this kind of mathematics that we are used to, and we can, then, use Kunin's representation, or Krumhansl's for that matter, and find a physical interpretation around the level of lattice theory. Also, as Professor Kröner pointed out when we go to atomic distances then classical theory is rather doubtful.

BULLOUGH: Actually, I think there is quite a lot more in the lattice theory—in a sense—because, for example, perhaps you could explain how you would put volume dependent forces into a non-local framework. Is this a feasible thing to do?

KRÖNER: I should think that this is possible. In fact, this theory could be expanded in such a way as to consider many-body forces and it should be possible to use also volume dependent forces. I have not thought about this in any detail. Incidentally, the inclusion of many-body forces would make the theory non-linear.

BULLOUGH: I am a little puzzled that you think integro-differential equations are simpler than difference equations.

AUDIENCE: General laughter.

KRÖNER: With the same argument you could wipe away the conventional elasticity theory by saying that difference equations are simpler than differential equations. Notwithstanding, it is a fact that some of your finite sums are much more complicated to calculate than our integrals.

BULLOUGH: I don't see this. We just performed an absolute summation over the reciprocal lattice vectors of the reduced zone. That is just a quadrature, after all, just as you are involved with integral quadratures.

The fact that our result was obtained through the use of a computer does not dirty it.

KRÖNER: Before having really compared the whole calculation you made and we made, you and I cannot say too much. Even in the particular case in which you consider you had to make so little effort, the non-local theory has been much simpler than the lattice theory. Of course, it could be different in other situations. I think we can discuss it tomorrow in the "Future Directions" panel.

BULLOUGH: I just object to having lattice theory at the top of the hill, that's all.

BARNETT: In answer to Professor Maradudin, all I want to point out is in this theory [the interpolation theories referred to previously] you merely use the continuum representation. It can't tell you anything more than the lattice theory would tell you; it tells you exactly the same thing. It is just a different representation, but it does allow you to use a formulation which permits solving very simple problems like point defects and straight dislocations. I think you very quickly reach a point where it becomes more efficient to do the lattice theory than the non-local theory for the simple reason that you begin with the lattice equations and then rig up a continuum scheme which takes you to either a continuum or quasi-continuum representation, and then, when you have a difficult problem—and you will if you just put in a boundary—you must go back and solve the thing numerically to get some numbers out of it. You have to do this with a set of difference equations. So, effectively you are going from lattice mechanics to continuum mechanics, and to get an answer you go back to lattice mechanics again and go to the computer. So the question you should really ask yourself is: Why not stay with the lattice mechanics all the way? I feel there are instances where a continuum approach might be preferable for very simple problems, otherwise probably not.

KRÖNER: [Written contribution] I should like to remind Dr. Barnett that replacing complicated continuum equations by difference equations is only one way of obtaining numerical results. Other possibilities may well be preferable in certain situations, in particular if the step width must be one atomic distance. Having gained now some distance of time from the conference, this whole discussion forced upon me seems to be what in Germany is called a "Streit um Kaisers Bart" (quarrel about emperor's beard).

It should be evident to everybody who has studied *both* approaches that it depends on the problem itself which method one utilizes with advantage. Fortunately, such choices exist in many parts of physics. Nobody disputes any more whether Heisenberg's or Schrödinger's quantum mechanics is "better."

# A DYNAMIC THEORY OF DISLOCATIONS AND ITS APPLICATIONS TO THE THEORY OF THE ELASTIC-PLASTIC CONTINUUM

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The starting point of this study is a paper by Kröner (J. Math. Phys., **42**, p. 27, 1963), who proposed the replacement of the loading history variables in the yield criterion and in the work-hardening equation by state variables, such as the dislocation density and the density of dislocation loops.

The first part of the work summarizes the formulation recently given by the author for the dynamic non-linear theory of dislocations in anisotropic media. The relations connecting the continuum kinematic quantities to the discrete dislocation arrangement and to the dislocation velocities are emphasized.

To construct a theory of the elasto-plasticity, the system of kinematic equations is completed by postulating a yield condition and a work-hardening equation, which contain as independent variables the stress, the dislocation density, the density of dislocation loops, and the temperature.

Making constitutive assumptions for the free energy, the specific entropy, and the heat conduction vector, and using the principle of material indifference and the thermodynamical restrictions, a definite theory of the elastic-plastic continuum is obtained.

**Key words:** Anisotropic elasticity: anisotropic plasticity dislocations: constitutive relations; dislocation dynamics; non-linear elasticity.

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The starting point of this study is a paper by Kröner [1], who proposed the replacement of the loading history variables in the yield condition and in the work-hardening equation by internal state variables such as the dislocation density and the density of dislocation loops.

Recently, Fox [2] generalized the work of Green and Naghdi [3] on the theory of the elastic-plastic continuum. He replaced their linear composition between the material plastic and elastic symmetric strains by the

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non-linear matrix rule of composition used in the continuum theory of dislocations for the non-symmetric elastic and plastic distortions. Fox showed that the elastic distortion is equivalent to a dipolar displacement field as defined by Green and Rivlin [4]. This permitted the utilization of the formalism of multipolar continua. However, Fox introduced in the yield condition the plastic distortion, which is not a state quantity.

The object of the present work is the construction of a non-linear dislocation theory of the elastic-plastic behaviour for single crystals. To this end we use the formalism of the continuum mechanics and the thermodynamic principles adding to the state variables the dislocation density and formulating a supplementary constitutive equation for the dislocation flux.

Section 1 contains a new formulation of the non-linear kinematics of the elastic-plastic deformation, which includes in a natural way the dislocation density and flux. The basic *non-linear* kinematic equations were obtained for the first time by Günther [5], by means of a four-dimensional formalism and of the analogy with the theory of relativity. The present approach is grounded on purely continuum mechanical considerations, being related to a paper by Eckart [11], who introduced the notion of moving local natural configurations.

In section 2 the kinematic equations are linearized and the main geometric differences between the plastic and the elastic deformation are pointed out.

Section 3 comprises the analysis of the dislocation density and flux associated with isolated moving dislocation lines or to other microscopic dislocation arrangements and motions, in the framework of the linear theory.

In section 4 it is shown that in the case of uniformly moving dislocation lines, or groups of dislocation lines, the dislocation flux is completely determined by the dislocation density and the velocity of the dislocations with respect to the material.

In section 5 we return to the general theory. The kinematical equations are supplemented by the balance laws for the mass, linear momentum, and energy. To construct a theory of the elasto-plasticity, we postulate an yield condition and an work-hardening equation, which contain as state variables the stress, the dislocation density, the temperature, and the dislocation flux. Making constitutive assumptions for the stress, the specific free energy, the specific entropy, the heat conduction vector, and the dislocation flux, and using the principle of material indifference and the thermodynamical restrictions, a rate-type theory of the elastic-plastic continuum is obtained. The paper by Green and Naghdi mentioned above is used as a guide in constructing the continuum theory, but their formulation is modified by considering internal state variables which describe the dislocation arrangement and kinematics.

Section 6 contains a discussion of the theory proposed and of the possibilities to refine it by considering more microscopic details of the dislocation arrangement and motion.

The basic tensor equations employed throughout the paper, the equivalences between the direct notation and the component form, as well as some elements of the theory of  $\delta$ -functions defined on lines and surfaces, are included in appendix 1.

Appendix 2 comprises a new derivation of Mura's formulae [6] for the determination of the self-stress and of the particle velocity field when the dislocation density and flux are known, in the framework of the linear theory and using Green's functions.

Finally, appendix 3 gives the principal equivalences between the notations employed in the present paper and other notations used in the literature.

## I. Continuum Kinematics of the Elastic-Plastic Deformation

The body  $\mathcal{B}$  is considered in a *reference configuration* ( $k_0$ ) at time  $t=0$ , which need not be a natural state, and a *current configuration* ( $k$ ) at time  $t$ .  $\mathbf{x}$  and  $\mathbf{x}_0$  denote the position vectors of a material particle  $X$  in the reference and current configurations (fig. 1).<sup>1</sup> Identifying the particles by their position vectors in the reference configuration, we denote the *motion* of the body by

$$\mathbf{x} = \chi(\mathbf{x}_0, t) \quad (1.1)$$

and the particle *velocity* field by

$$\mathbf{v} \equiv \dot{\mathbf{x}} \equiv \frac{\partial}{\partial t} \chi(\mathbf{x}_0, t). \quad (1.2)$$

The *deformation gradient* associated with the motion (1.1) is

$$\mathbf{F} \equiv \text{grad}_0 \chi(\mathbf{x}_0, t) \equiv \frac{\partial}{\partial \mathbf{x}_0} \chi(\mathbf{x}_0, t). \quad (1.3)$$

We assume that the body contains dislocations. Therefore, a *global natural configuration*, i.e., a stress-free configuration of the whole body, does not exist. Let  $N(X)$  denote the set of particles in a neighbourhood of the particle  $X$ . In order to determine the elastic deformation undergone by  $N(X)$  at time  $t$ , we may, at least in principle, cut out of the body this

<sup>1</sup> We shall employ the same names,  $\mathbf{x}$  and  $\mathbf{x}_0$ , for the spatial points occupied by the particle  $X$  at times  $t=0$  and  $t$ . The right-hand operators curl, divergence, and gradient, taken with respect to the particle positions in the configurations ( $k$ ) and ( $k_0$ ), will be denoted by curl, div, grad, and curl<sub>0</sub>, div<sub>0</sub>, grad<sub>0</sub>, respectively.

neighbourhood and allow it to relax. We denote by  $(\kappa)$  the *local natural configuration* obtained in this way.

We refer  $(k)$  to a system of general co-ordinates  $x^k$  and  $(\kappa)$  to a local frame of rectangular Cartesian co-ordinates  $\xi^\kappa$ , fixed with respect to the particle. To simplify the further formulation of the constitutive equations, we choose the local frames so that they have the same orientation with respect to the preferred crystallographic axes. Let now  $Y$  be another particle of  $N(X)$ . We denote by  $d\mathbf{x}$  and  $d\xi$  the position vectors of  $Y$  with respect to  $X$  in the configurations  $(k)$  and  $(\kappa)$ , and define the *elastic distortion*,  $\mathbf{A}$ , by the relation

$$dx^k = A^k{}_\kappa d\xi^\kappa, \quad (1.4)$$

where  $dx^k$  and  $d\xi^\kappa$  are the components of  $d\mathbf{x}$  and  $d\xi$  in the co-ordinate systems  $x^k$  and  $\xi^\kappa$ .

We assume that, for sufficiently small neighbourhoods  $N(X)$ , the so-defined value of  $\mathbf{A}$  does not depend on the choice of the neighbourhood  $N(X)$  and of the particle  $Y \in N(X)$ . Consequently, by repeating the same procedure for all particles  $X \in \mathcal{B}$  and times  $t$ , we may define the field  $\mathbf{A}(\mathbf{x}, t)$ . In the presence of dislocations,  $\mathbf{A}$  cannot be written in general as a global deformation gradient, although it may be further interpreted as the gradient at  $X$  of the function describing the local deformation around  $X$ , that is the deformation of  $N(X)$  from  $(\kappa)$  to  $(k)$  (see e.g., Teodosiu and Seeger [7]).

Since the local frames are fixed with respect to the material,  $\mathbf{A}$  does not depend on the rotation of  $N(X)$ . In order to simplify the shifting of the tensor components from  $(k)$  to  $(\kappa)$ , or inversely, we may then assume that the local frames are rotated together with the corresponding neighbourhoods so that their axes become parallel to a time-independent rectangular Cartesian frame with axes  $z^k$  (for a two-dimensional representation see fig. 1). Consequently, if the relation between the general co-ordinates  $x^k$  and the Cartesian co-ordinates  $z^\kappa$  is

$$x^k = x^k(z^\kappa), \quad z^\kappa = z^\kappa(x^k),$$

then the shifting of the tensor components from  $(k)$  to  $(\kappa)$  and inversely may be done by using the formulae

$$\varphi_{\cdot \cdot \cdot \kappa \cdot \cdot \cdot}^{\cdot \cdot \cdot} g_k^\kappa = \varphi_{\cdot \cdot \cdot k \cdot \cdot \cdot}^{\cdot \cdot \cdot}, \quad \varphi_{\cdot \cdot \cdot k \cdot \cdot \cdot}^{\cdot \cdot \cdot} g_\kappa^k = \varphi_{\cdot \cdot \cdot \kappa \cdot \cdot \cdot}^{\cdot \cdot \cdot},$$

where the shifters  $g_k^\kappa$  and  $g_\kappa^k$  are defined by

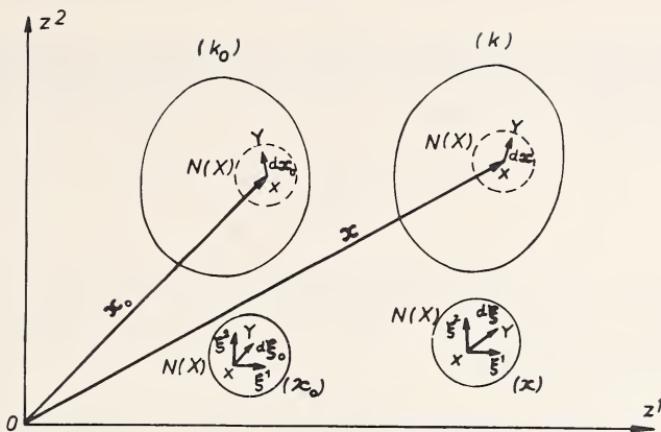


FIGURE 1. Two-dimensional representation of the motion and of the elastic-plastic deformation.

$$g_k^\kappa = \frac{\partial z^\kappa}{\partial x^k}, \quad g^\kappa_k = \frac{\partial x^k}{\partial z^\kappa}.$$

Let us follow now the material vector linking the particles  $X$  and  $Y \in N(X)$  throughout the motion. We denote by  $\mathbf{A}_0$ ,  $d\mathbf{x}_0$ , and  $d\xi_0$ , the values of the fields  $\mathbf{A}$ ,  $d\mathbf{x}$ , and  $d\xi$ , at time  $t = 0$ , i.e., those corresponding to the reference configuration, and define the *plastic distortion*  $\mathbf{P}(\mathbf{x}, t)$  by the relation

$$d\xi^\kappa = P^\kappa_\lambda d\xi_0^\lambda. \quad (1.5)$$

We assume that the fields  $\mathbf{F}$ ,  $\mathbf{A}$ , and  $\mathbf{P}$ , are continuously differentiable and admit *for every fixed time*  $t$  the inverses  $\mathbf{F}^{-1}$ ,  $\mathbf{A}^{-1}$ , and  $\mathbf{P}^{-1}$ , hence

$$\mathbf{F}\mathbf{F}^{-1} = \mathbf{F}^{-1}\mathbf{F} = \mathbf{1}, \quad \mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{1}, \quad \mathbf{P}\mathbf{P}^{-1} = \mathbf{P}^{-1}\mathbf{P} = \mathbf{1}, \quad (1.6)$$

where  $\mathbf{1}$  is the unit tensor.

From the above definitions we infer that the deformation gradient  $\mathbf{F}$ , which will be also called *total distortion*, may be expressed as

$$\mathbf{F} = \mathbf{A}\mathbf{P}\mathbf{A}^{-1}. \quad (1.7)$$

We remark also that in our considerations the choice of the reference configuration does not play a special role, because we have not assumed that this configuration represents a natural state of the body. It is true that from (1.5) it follows  $\mathbf{P}(\mathbf{x}, 0) = \mathbf{1}$ , i.e., the plastic distortion is measured with respect to the reference configuration. However, as only the time derivative of  $\mathbf{P}$  will be essential for the theory, the choice of the reference configuration is in fact immaterial. One may dispose of this arbitrariness by choosing as reference configuration an unloaded state of the body.

Let us consider now a smooth surface  $s$ , bounded by the closed line  $c$ , and containing the point  $\mathbf{x}$ . The *true Burgers vector*,  $\bar{\mathbf{b}}$ , of the dislocations piercing through  $s$  is defined by

$$\bar{\mathbf{b}} \equiv \oint_c d\boldsymbol{\xi}. \quad (1.8)$$

It is important to note that in the integral (1.8), the vector  $d\boldsymbol{\xi}$  is considered as function of  $\mathbf{x}$  and  $t$ . Substituting (1.4) into (1.8) and applying Kelvin's transformation (A.22) gives

$$\bar{\mathbf{b}} = \oint_c \mathbf{A}^{-1} d\mathbf{x} = - \int_{s'} (\operatorname{curl} \mathbf{A}^{-1}) \mathbf{n} ds = \int_s \bar{\boldsymbol{\alpha}} \mathbf{n} ds, \quad (1.9)$$

where  $\mathbf{n}$  is the unit normal to  $s$ , and the positive sense on  $c$  is chosen clockwise when sighting down along  $\mathbf{n}$ . The tensor

$$\bar{\boldsymbol{\alpha}} \equiv -\operatorname{curl} \mathbf{A}^{-1}, \quad \bar{\alpha}^{\lambda m} = -\epsilon^{rsm} \bar{A}^{\lambda}{}_{r,s}, \quad (1.10)$$

is usually called the *true dislocation density*. If  $\bar{\boldsymbol{\alpha}}$  is a continuous function and  $s$  is infinitesimal, we may write (1.9) as

$$d\bar{\mathbf{b}} = \bar{\boldsymbol{\alpha}} \mathbf{n} ds, \quad d\bar{b}^{\kappa} = \bar{\alpha}^{\kappa m} n_m ds, \quad (1.11)$$

where  $d\bar{\mathbf{b}}$  is the infinitesimal true Burgers vector of the dislocations threading  $ds$ .<sup>2</sup>

We may define now the infinitesimal *local Burgers vector*,  $d\mathbf{b}$ , and the *local dislocation density*,  $\boldsymbol{\alpha}$ , at  $\mathbf{x}$ , by the relations

$$d\mathbf{b} \equiv \mathbf{A} d\bar{\mathbf{b}}, \quad db^k \equiv A^k{}_n d\bar{b}^n \quad (1.12)$$

$$\boldsymbol{\alpha} \equiv \mathbf{A} \bar{\boldsymbol{\alpha}}, \quad \alpha^{kl} \equiv A^k{}_{\kappa} \bar{\alpha}^{\kappa l} \quad (1.13)$$

From these two definitions follows also

$$d\mathbf{b} = \boldsymbol{\alpha} \mathbf{n} ds, \quad db^k = \alpha^{kl} n_l ds. \quad (1.14)$$

<sup>2</sup> For the time being there is no system of definitions and sign conventions generally adopted in the continuum theory of dislocations. The present author tried to employ a system of notations close to those frequently used nowadays in continuum mechanics. The sign conventions will be mentioned explicitly. A table of equivalences with the notations used by other authors is given in appendix 3.

Along with the well-known true and local dislocation densities,  $\bar{\alpha}$  and  $\alpha$ , we shall make use of another dislocation density,  $\tilde{\alpha}$ , first considered by Noll [8], and defined by

$$\bar{\alpha} \equiv j \tilde{\alpha} \mathbf{A}^T, \quad \bar{\alpha}^{\kappa m} = j A^m{}_\mu \tilde{\alpha}^{\kappa \mu}, \quad (1.15)$$

where

$$j \equiv |\det \mathbf{A}^{-1}|. \quad (1.16)$$

In order to understand the significance of Noll's dislocation density let us consider first an oriented material surface element,  $\mathbf{n}ds$ , through the particle  $X$ , in the current configuration ( $k$ ). By releasing a neighbourhood  $N(X)$  of  $X$  containing the surface element, the magnitude and the orientation of the vector  $\mathbf{n}ds$  will change to  $\tilde{\mathbf{n}}d\tilde{s}$ , say, and we have (see e.g., Truesdell and Toupin [9], p. 249)

$$\tilde{\mathbf{n}}d\tilde{s} = j \mathbf{A}^T \mathbf{n}ds, \quad \tilde{n}_\lambda d\tilde{s} = j A^l{}_\lambda n_l ds. \quad (1.17)$$

Substituting (1.17) and (1.15) into (1.11) yields

$$d\bar{\mathbf{b}} = \bar{\alpha} \tilde{\mathbf{n}}d\tilde{s}, \quad d\bar{b}^\kappa = \bar{\alpha}^{\kappa\lambda} n_\lambda d\tilde{s}. \quad (1.18)$$

Since the true Burgers vector  $d\bar{\mathbf{b}}$  and the oriented surface element in the local natural configuration  $\tilde{\mathbf{n}}d\tilde{s}$  do not depend on the elastic distortion,  $\bar{\alpha}$  does not either, in contradistinction to the true and local dislocation densities which vary under superimposed elastic deformations.

Equation (1.10) was called by Kröner [10] the fundamental geometric equation of the continuum theory of dislocations. When the dislocation densities  $\bar{\alpha}$  or  $\alpha$  are known and time-independent, this equation allows the determination of the self-stresses produced by dislocations, when combined with the equilibrium equations, the elastic constitutive equations, and the boundary conditions.

Let us consider now the kinematic of the elastic-plastic deformation. Differentiating (1.5) with respect to  $t$  gives

$$\dot{\bar{\mathbf{d}\xi}} = \dot{\mathbf{P}} d\xi_0. \quad (1.19)$$

Since

$$d\xi_0 = \mathbf{P}^{-1} d\xi = \mathbf{P}^{-1} \mathbf{A}^{-1} d\mathbf{x}, \quad (1.20)$$

we may write (1.19) in the alternative forms

$$\dot{d}\tilde{\xi} = \tilde{\mathbf{I}} d\xi = \bar{\mathbf{I}} d\mathbf{x}, \quad (1.21)$$

where the tensors  $\tilde{\mathbf{I}}$  and  $\bar{\mathbf{I}}$ , called dislocation fluxes,<sup>3</sup> are defined by the relations

$$\tilde{\mathbf{I}} \equiv \bar{\mathbf{I}} \mathbf{A} \equiv \dot{\mathbf{P}} \mathbf{P}^{-1}, \quad \tilde{I}^{\lambda}_{\mu} = \bar{I}^{\lambda}_{\mu} A^{\mu}_{\nu} = \dot{P}^{\lambda}_{\sigma} \bar{P}^{\sigma}_{\mu} \quad (1.22)$$

By analogy to the names given above to the dislocation densities, we call  $\bar{\mathbf{I}}$  *true dislocation flux* and define also a *local dislocation flux*,  $\mathbf{I}$ , by the identity

$$\mathbf{I} \equiv \mathbf{A} \bar{\mathbf{I}}, \quad I^k_l \equiv A^k_{\mu} \bar{I}^{\mu}_l \quad (1.23)$$

From (1.21) and (1.8), considering that  $c$  is a material line, follows

$$\dot{b} = \oint_c \bar{\mathbf{I}} d\mathbf{x}. \quad (1.24)$$

This relation shows that the dislocation flux characterizes completely the transport of the Burgers vector through a material line.

If we denote by  $\text{grad}$  and  $\text{grad}_0$  the gradients taken with respect to the particle positions in the configurations  $(k)$  and  $(k_0)$ , we derive successively from (1.1)–(1.3)

$$\begin{aligned} \text{grad}_0(\cdot) &= [\text{grad}(\cdot)] \mathbf{F}, \\ \dot{\mathbf{F}} &= \text{grad}_0 \mathbf{v} = (\text{grad} \mathbf{v}) \mathbf{F}, \\ \text{grad} \mathbf{v} &= \dot{\mathbf{F}} \mathbf{F}^{-1} \end{aligned} \quad (1.25)$$

By taking into account (1.7) and (1.22) the last relation becomes

$$\text{grad} \mathbf{v} = (\dot{\mathbf{A}} \mathbf{P} \mathbf{A}_0^{-1} + \mathbf{A} \dot{\mathbf{P}} \mathbf{A}_0^{-1}) \mathbf{A}_0 \mathbf{P}^{-1} \mathbf{A}^{-1},$$

from this follows

$$\text{grad} \mathbf{v} = \mathbf{A} \bar{\mathbf{I}} + \dot{\mathbf{A}} \mathbf{A}^{-1}, \quad v^k_{,l} = A^k_{\mu} \bar{I}^{\mu}_l + \dot{A}^k_{\mu} A^{\mu}_{,l} \quad (1.26)$$

If the dislocation flux  $\bar{\mathbf{I}}$  and the dislocation density  $\bar{\alpha}$  are known, as

<sup>3</sup> This denomination will be justified by the considerations in section 3.

for instance in the case of a uniformly moving dislocation, the eqs (1.10) and (1.26) together with the usual equilibrium equations, the elastic constitutive equations, and the boundary conditions, allow again the determination of the self-stresses produced by dislocations, as shown by Mura [6] (see also app. 2). However,  $\bar{\mathbf{I}}$  and  $\bar{\alpha}$  cannot be assigned arbitrarily. In order for the eqs (1.10) and (1.26) to be compatible, the following conditions must be satisfied

$$\operatorname{div} \bar{\alpha} = 0, \quad \bar{\alpha}^{\kappa m}{}_{,m} = 0, \quad (1.27)$$

$$\operatorname{curl} (\mathbf{A} \bar{\mathbf{I}} + \dot{\mathbf{A}} \bar{\mathbf{A}}^{-1}) = 0. \quad (1.28)$$

To eliminate  $\mathbf{A}$  from the last equation we shall write it first in its component form<sup>4</sup>

$$\epsilon^{lsm} (A^k{}_\kappa \bar{I}^\kappa{}_l + \dot{A}^k{}_\kappa \bar{A}^\kappa{}_l)_{,s} = 0.$$

By performing the differentiation of the first term in the parenthesis, multiplying the result by  $\bar{A}_k{}^{-1}$ , and taking into account (1.6)<sub>2</sub>, we obtain

$$\epsilon^{lsm} A^k{}_\kappa{}_{,s} \bar{A}^\lambda{}_k \bar{I}^\kappa{}_l + \epsilon^{lsm} (\dot{A}^k{}_\kappa \bar{A}^\kappa{}_l)_{,s} = -\epsilon^{lsm} \bar{I}^\lambda{}_l{}_{,s}. \quad (1.29)$$

By (1.6)<sub>2</sub> and (1.26), the first term of this equation may be transformed as follows:

$$\begin{aligned} \epsilon^{lsm} A^k{}_\kappa{}_{,s} \bar{A}^\lambda{}_k \bar{I}^\kappa{}_l &= -\epsilon^{lsm} \bar{A}^\lambda{}_{k,s} A^k{}_\kappa \bar{I}^\kappa{}_l \\ &= -\epsilon^{lsm} \bar{A}^\lambda{}_{k,s} v^k{}_{,l} + \epsilon^{lsm} \bar{A}^\lambda{}_{k,s} \bar{A}^k{}_\kappa \bar{A}^\kappa{}_l. \end{aligned}$$

Equation (1.29) becomes

$$-\epsilon^{lsm} \bar{A}^\lambda{}_{k,s} v^k{}_{,l} + \epsilon^{lsm} (\dot{A}^k{}_\kappa \bar{A}^\kappa{}_l \bar{A}^\lambda{}_k)_{,s} = -\epsilon^{lsm} \bar{I}^\lambda{}_l{}_{,s}. \quad (1.30)$$

Using (1.6)<sub>2</sub>, (1.10), and (A.23), we have

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<sup>4</sup> When using the component form of the tensor equations we write for convenience the non-tensorial subscripts underneath the kernel index, and the non-tensorial superscripts above the kernel index.

$$\begin{aligned}
\epsilon^{lsm}(\dot{A}^k \bar{A}^\kappa \bar{A}^\lambda \bar{A}^\lambda)_{,s} &= -\epsilon^{lsm} \left[ \frac{d}{dt} (\bar{A}^\lambda) \right]_{,s} \\
&= -\epsilon^{lsm} \frac{d}{dt} (\bar{A}^\lambda)_{,s} - \epsilon^{lsm} \bar{A}^\lambda_{,k} v^k_{,s} \\
&= \dot{\alpha}^{\lambda m} + \epsilon^{lsm} \bar{A}^\lambda_{s,k} v^k_{,l}
\end{aligned}$$

and eq (1.30) takes the form

$$\dot{\alpha}^{\lambda m} - 2\epsilon^{lsm} \bar{A}^\lambda_{k,s} v^k_{,l} = -\epsilon^{lsm} \bar{I}^\lambda_{l,s}.$$

From (1.10) follows

$$\bar{A}^\lambda_{k,s} = -\epsilon_{ksp} \bar{\alpha}^{\lambda p}. \quad (1.31)$$

Hence, we get finally

$$\dot{\alpha}^{\lambda m} - \bar{\alpha}^{\lambda l} v^m_{,l} + \bar{\alpha}^{\lambda m} v^l_{,l} = -\epsilon^{lsm} \bar{I}^\lambda_{l,s}, \quad (1.32)$$

which is the required compatibility condition for  $\bar{I}$ .

There is also another more indirect but much simpler way of demonstrating (1.32). By applying Kelvin's transformation (A.22) we derive from (1.23)

$$\dot{\mathbf{b}} = - \int_s (\operatorname{curl} \bar{\mathbf{I}}) \mathbf{n} ds, \quad (1.33)$$

where  $s$  is the material surface bounded by  $c$ . On the other hand, by applying the formula for the rate of change of the surface integrals (see e.g., Truesdell and Toupin [9], p. 346), we deduce from (1.9)

$$\dot{\mathbf{b}} = \int_s \{ \dot{\alpha} - \bar{\alpha} (\operatorname{grad} \mathbf{v})^T + \bar{\alpha} \operatorname{div} \mathbf{v} \} \mathbf{n} ds. \quad (1.34)$$

By comparing (1.33) and (1.34) and taking into account that  $s$  may be arbitrarily chosen we obtain the equation

$$\dot{\alpha} - \bar{\alpha} (\operatorname{grad} \mathbf{v})^T + \bar{\alpha} \operatorname{div} \mathbf{v} = -\operatorname{curl} \bar{\mathbf{I}}, \quad (1.35)$$

which coincides with (1.32).

Equations (1.10), (1.26), (1.27), and (1.35) are the basic kinematic equations of the non-linear dislocation dynamics. They were obtained for the

first time by Günther [5], by using a four-dimensional formalism and the analogy between the theory of dislocations and the theory of relativity. The present approach has in author's opinion the advantage of being based on more elementary and direct considerations and on methods which are currently employed in continuum mechanics.

Before closing this section we shall mention another formula giving the rate of the plastic change of a material length element. Let  $dl^2$  be the square length of the vector element  $d\xi$ , linking the particles  $X$  and  $Y \in N(X)$  in the configuration  $(\kappa)$ . We have

$$dl^2 = \delta_{\kappa\lambda} d\xi^\kappa d\xi^\lambda. \quad (1.36)$$

Hence, by using (1.21) we obtain

$$\dot{\bar{dl}^2} = 2\tilde{I}_{(\kappa\lambda)} d\xi^\kappa d\xi^\lambda. \quad (1.37)$$

The last formula was obtained for the first time by Eckart [11]. The tensor

$$\tilde{\mathbf{J}} \equiv 1/2 (\tilde{\mathbf{I}} + \tilde{\mathbf{I}}^T), \quad \tilde{J}_{\kappa\lambda} \equiv \tilde{I}_{(\kappa\lambda)}, \quad (1.38)$$

appearing in this relation, was called by Eckart *anelasticity tensor* and by Truesdell and Toupin ([9], p. 372) *slippage tensor*.

## II. Linearized Kinematic Equations

In order to linearize the kinematic equations deduced in the preceding section, we write

$$\mathbf{F} = \mathbf{1} + \boldsymbol{\beta}^G, \quad \mathbf{P} = \mathbf{1} + \boldsymbol{\beta}^P, \quad \mathbf{A} = \mathbf{1} + \boldsymbol{\beta}, \quad \mathbf{A}_0 = \mathbf{1} + \boldsymbol{\beta}_0, \quad (2.1)$$

assume that the magnitudes of the tensors  $\boldsymbol{\beta}^G$ ,  $\boldsymbol{\beta}^P$ ,  $\boldsymbol{\beta}$ ,  $\boldsymbol{\beta}_0$ , as well as those of their material derivatives<sup>5</sup>  $\dot{\boldsymbol{\beta}}^G$ ,  $\dot{\boldsymbol{\beta}}^P$ ,  $\dot{\boldsymbol{\beta}}$  are "small," and neglect their products in the linear approximation.

We obtain successively from (1.6)<sub>2</sub>, (1.22), (1.23), and (1.25),

$$\mathbf{A}^{-1} \approx \mathbf{1} - \boldsymbol{\beta}, \quad (2.2)$$

$$\mathbf{I} \approx \tilde{\mathbf{I}} \approx \bar{\mathbf{I}} \approx \dot{\boldsymbol{\beta}}^P, \quad (2.3)$$

$$\text{grad } \mathbf{v} \approx \dot{\boldsymbol{\beta}}^G. \quad (2.4)$$

<sup>5</sup> Following Kröner [10], we shall call  $\boldsymbol{\beta}^G$ ,  $\boldsymbol{\beta}^P$ , and  $\boldsymbol{\beta}$ , respectively, *total*, *plastic*, and *elastic distortion*, employing thus for them the same nomenclature as that already used for  $\mathbf{F}$ ,  $\mathbf{P}$ , and  $\mathbf{A}$ . We use for the total distortion the superscript  $G$ , from the German word "gesamt", to avoid the confusion with the transpose of  $\boldsymbol{\beta}$ .

From (1.13) and (1.15) we deduce also that in the linear approximation all the dislocation densities previously defined coincide, i.e.,

$$\tilde{\alpha} \approx \bar{\alpha} \approx \alpha, \quad \tilde{\mathbf{b}} \approx \mathbf{b}. \quad (2.5)$$

Furthermore, we assume that for all kinematic quantities considered the material derivatives may be approximated by the partial time derivatives, that is,

$$\frac{d}{dt} (\cdot) = \frac{\partial}{\partial t} (\cdot) + [\text{grad} (\cdot)] \mathbf{v} \approx \frac{\partial}{\partial t} (\cdot).$$

This assumption is justified whenever the gradients of the quantities involved and the velocity  $\mathbf{v}$  are sufficiently small.

By introducing (2.1)–(2.6) into the basic equations (1.10), (1.26), (1.27), and (1.35), we get the linearized kinematic equations

$$\text{curl } \boldsymbol{\beta} = \boldsymbol{\alpha}, \quad \epsilon^{pst} \beta^m{}_{p,s} = \alpha^{mt}, \quad (2.7)$$

$$\text{grad } \mathbf{v} = \mathbf{I} + \frac{\partial \boldsymbol{\beta}}{\partial t}, \quad v^k{}_{,r} = I^k{}_{r} + \frac{\partial \beta^k_r}{\partial t}, \quad (2.8)$$

$$\text{div } \boldsymbol{\alpha} = 0, \quad \alpha^{km}{}_{,m} = 0. \quad (2.9)$$

$$\frac{\partial \boldsymbol{\alpha}}{\partial t} = -\text{curl } \mathbf{I}, \quad \frac{\partial \alpha^{mt}}{\partial t} = -\epsilon^{pst} I^m{}_{p,s} \quad (2.10)$$

This system must be supplemented by eqs (2.3) and (2.4), which, in view of (2.6), become

$$\mathbf{I} = \frac{\partial \boldsymbol{\beta}^P}{\partial t}, \quad (2.11)$$

$$\text{grad } \mathbf{v} = \frac{\partial \boldsymbol{\beta}^G}{\partial t} \quad (2.12)$$

The system of kinematic equations (2.7)–(2.12), or some of these equations, were employed in various linear theories of the dislocation dynamics developed by Holländer [12], Amari [13], Kosevich [14, 15], Mura [6], and Bross [16] (see also the critical discussion by Günther [5]).

It is worthwhile to illustrate here the qualitative geometric distinction between the infinitesimal plastic and elastic distortions (see Kröner [10], p. 18). To this end, let us consider the neighbourhood  $N(X)$  in the configuration  $(\kappa_0)$ , i.e., in the local natural configuration at time  $t=0$ . Starting

from  $(\kappa_0)$  we may consider a *pure elastic distortion*  $\beta_0$  of  $N(X)$ , to the configuration  $(k_0)$ , and a *pure plastic distortion*  $\beta^P$  of  $N(X)$ , to the local natural configuration  $(\kappa)$ , at a fixed time  $t$ . To simplify the graphical representations let us assume that  $\beta_0$  and  $\beta^P$  are constant in  $N(X)$ , so that both distortions are homogeneous.

If we denote by  $\tilde{\mathbf{E}}$ ,  $\tilde{\mathbf{E}}^P$ , the infinitesimal elastic and plastic strain tensors, and by  $\tilde{\mathbf{R}}$ ,  $\tilde{\mathbf{R}}^P$ , the infinitesimal elastic and plastic rotation tensors, we have the formulae

$$\beta_0 = \tilde{\mathbf{E}}_0 + \tilde{\mathbf{R}}_0, \quad \beta^P = \tilde{\mathbf{E}}^P + \tilde{\mathbf{R}}^P, \quad (2.13)$$

which represent the invariant decomposition of the infinitesimal elastic and plastic distortions in their symmetric and antisymmetric parts.

Introducing (2.13) and (2.1) into (1.5) and then into the eq (1.4), written for  $t=0$ , yields

$$d\mathbf{x}_0 - d\xi_0 = (\tilde{\mathbf{E}}_0 + \tilde{\mathbf{R}}_0) d\xi_0, \quad (2.14)$$

$$d\xi - d\xi_0 = (\tilde{\mathbf{E}}^P + \tilde{\mathbf{R}}^P) d\xi_0. \quad (2.15)$$

For sake of simplicity we refer also the global configuration  $(k_0)$  to Cartesian co-ordinates and consider only the following typical cases

(a).  $\tilde{\mathbf{E}}_0 = 0$ ,  $\tilde{R}_{12} = -\tilde{R}_{21} > 0$ , all other components of  $\tilde{\mathbf{R}}_0$  are zero (pure elastic rotation, fig. 2a),

(b).  $\tilde{\mathbf{R}}_0 = 0$ ,  $\tilde{E}_{12} = \tilde{E}_{21} > 0$ , all other components of  $\tilde{\mathbf{E}}_0$  are zero (pure elastic strain, fig. 2b),

(c).  $\tilde{\mathbf{E}}^P = 0$ ,  $\tilde{R}_{12}^P = -\tilde{R}_{21}^P > 0$ , all other components of  $\tilde{\mathbf{R}}^P$  are zero (pure elastic strain, fig. 2b),

(d).  $\tilde{\mathbf{R}}^P = 0$ ,  $\tilde{E}_{12}^P = \tilde{E}_{21}^P > 0$ , all other components of  $\tilde{\mathbf{E}}^P$  are zero (pure plastic strain).

Furthermore, we take

$$d\xi_1 = d\xi_2 = 0, \quad d\xi_3 = 0,$$

so that the vectors  $d\xi_0$ ,  $d\mathbf{x}_0$ , and  $d\xi$ , all lie in  $\xi^3$ -planes. Moreover, in the case of the pure strains considered above, the chosen direction of the vector  $d\xi_0$  coincides with that of the principal positive extension, hence it undergoes merely an elongation.

We consider first the elastic distortion. By pure elastic rotation, the vector  $d\xi_0$  undergoes a variation perpendicular to itself, and its length remains constant in the linear approximation. The lattice is rotated together with  $N(X)$  (fig. 2a). The pure elastic strain results in the deformation of the lattice together with  $N(X)$ . Due to its particular orientation, our vector

$d\xi_0$  maintains its orientation but its length is increased (fig. 2b). In both cases of pure elastic rotation and pure elastic strain, we indicated by dashed lines the directions which would be taken by the axes  $\xi^1$  and  $\xi^2$  if they were material lines.

Next consider the plastic distortion. To facilitate the comparison with the elastic distortion, we have taken in fig. 2c, d,  $\tilde{\mathbf{R}}^P = \tilde{\mathbf{R}}_0$ ,  $\tilde{\mathbf{E}}^P = \tilde{\mathbf{E}}_0$ , so that the material vector  $d\xi_0$  suffers the same rotation and elongation as

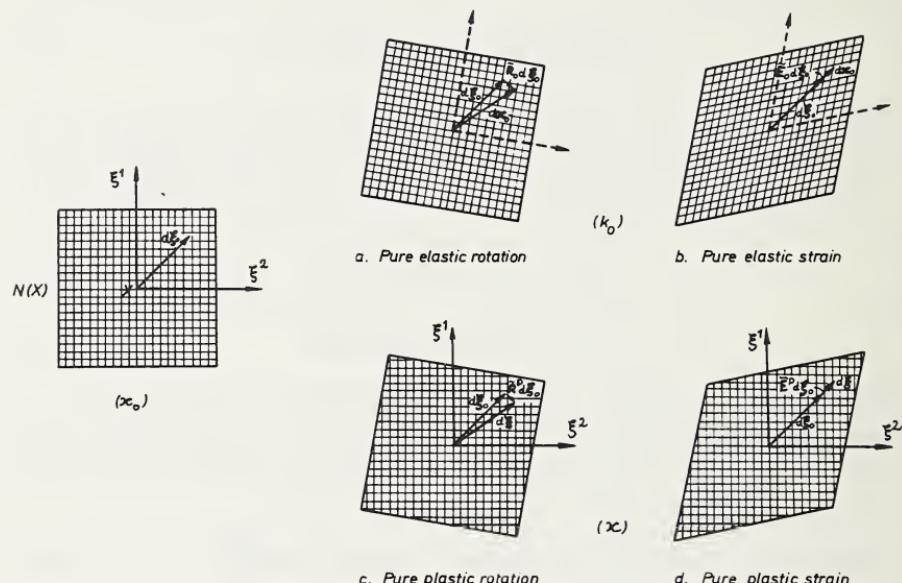


FIGURE 2. On the geometric distinction between the infinitesimal plastic and elastic distortions.

in figure 2a, b. However, in contradistinction to the case of the elastic distortion, the lattice does *not* rotate and deform together with  $N(X)$ .

### III. The Dependence of the Dislocation Density and of the Dislocation Flux on the Microscopic Arrangement and Kinematics of the Dislocation Lines

For completeness we write down the expression of the dislocation density and flux for an isolated dislocation. Such expressions may be found in different papers and books but because of the differences in notations and sign conventions it is better to make precise those conventions that are in agreement with the definitions used in sec. 1 for the continuous distributions of dislocations.

We begin by the convention used to determine the Burgers vector. Assume that the dislocation loop occupies the spatial line  $L$ . Choose a positive sense on  $L$ , and denote the corresponding tangent unit vector to

$L$  by  $\mathbf{l}(\mathbf{x}_L)$ , where  $\mathbf{x}_L$  is the position vector of a current point on  $L$ . To determine the Burgers vector of the dislocation in a small neighbourhood of  $\mathbf{x}_L$ , make the Burgers circuit in a sense that appears *clockwise* when looking down the dislocation line along  $\mathbf{l}(\mathbf{x}_L)$ . Make the corresponding Burgers circuit in an ideal crystal. The vector which completes the circuit and is drawn from the beginning point to the end point is the *true Burgers vector*.

It is easily seen that the above convention coincides with the continuum definition (1.8) if we choose the positive signs on all dislocation lines piercing through  $s$ , so that the scalar product  $\mathbf{n} \cdot \mathbf{l}$  be positive for all dislocations in the points where they intersect  $s$ . For an isolated dislocation we have

$$\bar{\alpha}(\mathbf{x}) = \bar{\mathbf{b}} \otimes \delta(L) = \bar{\mathbf{b}} \otimes \mathbf{l}(\mathbf{x}_L) \delta(L), \quad \bar{\alpha}^{\kappa m}(\mathbf{x}) = \bar{b}^{\kappa} l^m(\mathbf{x}_L) \delta(L). \quad (3.1)$$

Indeed, if we take a smooth surface  $s$  that intersects  $L$  in only one point, where  $\mathbf{n} \cdot \mathbf{l} > 0$ , we have by (A.30)

$$\int_s \bar{\alpha} \mathbf{n} ds = \bar{\mathbf{b}} \int_s \delta(L) \cdot \mathbf{n} ds = \bar{\mathbf{b}}, \quad (3.2)$$

which coincides with the definition (1.9) of  $\bar{\alpha}$ .

For a straight infinite edge dislocation whose line  $L$  is parallel to the  $z^3$  axis of a Cartesian system of co-ordinates (fig. 3), and has the equation

$$z^1 = z_L^1, \quad z^2 = z_L^2, \quad (3.3)$$

we have

$$\bar{\mathbf{b}} = -\bar{b} \mathbf{e}_1, \quad \delta(L) = \delta(z^1 - z_L^1) \delta(z^2 - z_L^2).$$

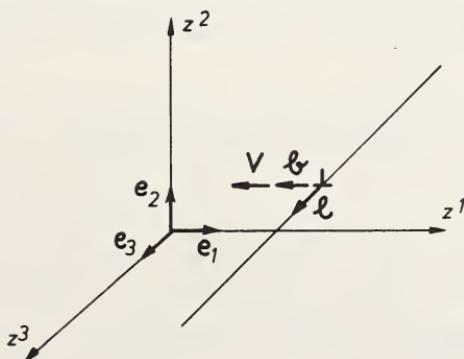


FIGURE 3. Straight edge dislocation.

If the positive orientations on  $L$  and on the  $z^3$  axis coincide,  $\mathbf{1}$  is equal with the unit vector  $\mathbf{e}_3$  of this axis and by (3.1) we deduce

$$\bar{\alpha}(z^1, z^2, z^3) = -\bar{b}\delta(z^1 - z_L^1)\delta(z^2 - z_L^2)\mathbf{e}_1 \oplus \mathbf{e}_3. \quad (3.4)$$

$$\bar{\alpha}_{13}(z^1, z^2, z^3) = -b\delta(z^1 - z_L^1)\delta(z^2 - z_L^2). \quad (3.5)$$

Consider now a moving planar dislocation loop, which occupies at time  $t$  the spatial line  $L_t$ , situated in a plane with unit normal  $\mathbf{n}$ . Denote by  $\mathbf{V}(\mathbf{x}_{L_t})$  the velocity of the dislocation line at  $\mathbf{x}_{L_t}$ , and by  $S_t$  the planar spatial surface encircled by the dislocation loop at time  $t$ . We assume that  $\mathbf{V}(\mathbf{x}_{L_t})$  and  $\mathbf{b}$  lie in the plane of the loop (the glide plane) and attempt to determine the plastic distortion produced when the size of the loop increases from a point to that of  $S_t$ . In the remaining part of this section we shall use the linear approximation presented in sec. 2 (formulae (2.2)–(2.6)). Consequently, we neglect the velocity of the material particles with respect to the dislocation velocity and the elastic deformation of  $S_t$  together with the material.

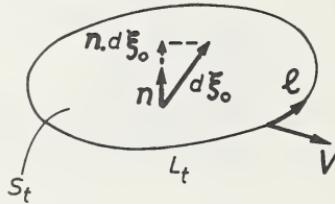


FIGURE 4. On the plastic distortion produced by the expansion of a dislocation loop.

Let  $d\xi_0$  be a vector element at time  $t=0$  (fig. 4). If  $d\xi_0$  does not intersect the glide plane, it remains invariant during the motion of the dislocation loop, hence  $d\xi = d\xi_0$ . If  $d\xi_0$  intersects the glide plane, the component of  $d\xi_0$  parallel to the glide plane remains unchanged during the motion of the dislocation loop, and the component normal to  $S_t$  changes by  $\mathbf{b}$ . In the general case we have

$$d\xi = d\xi_0 + \mathbf{b}(\mathbf{n} \cdot d\xi_0)\delta(S_t), \quad (3.6)$$

or, equivalently,

$$d\xi = (\mathbf{1} + \mathbf{b} \otimes \mathbf{n}\delta(S_t))d\xi_0. \quad (3.7)$$

Comparing (3.7) with (1.5) and (2.1)<sub>2</sub> we deduce

$$\mathbf{P} = \mathbf{1} + \mathbf{b} \otimes \mathbf{n}\delta(S_t), \quad (3.8)$$

$$\beta' = \mathbf{b} \otimes \mathbf{n} \delta(S_t). \quad (3.9)$$

Finally, by (A.36) we derive the expression of the dislocation flux for the glide of an isolated planar dislocation loop in the linear approximation

$$\mathbf{I}(\mathbf{x}, t) \approx \frac{\partial \beta'}{\partial t} = \mathbf{b} \otimes \mathbf{V}(\mathbf{x}_{L_t}) \times \delta(\mathbf{L}_t), \quad (3.10)$$

or, in component form,

$$I_{kl}(\mathbf{x}, t) \approx b_k \epsilon_{lmn} V^m(\mathbf{x}_{L_t}) l^n(\mathbf{x}_{L_t}) \delta(L_t). \quad (3.11)$$

By examining (3.7) and figure 4 we deduce also the rule for determining the plastic distortion produced by the expansion of a dislocation loop. Arbitrarily choose one of the unit normals to  $S_t$  as the positive unit normal  $\mathbf{n}$ . Choose the positive sense on the dislocation loop  $L_t$  clockwise when looking down along  $\mathbf{n}$ . As the loop increases its size from zero, the displacement of the part of the crystal into which  $\mathbf{n}$  points, with respect to the part situated on the other side of  $S_t$ , is equal in magnitude and direction to the Burgers vector.

For the isolated straight edge dislocation represented in figure 3, moving in  $-z^1$  direction with the velocity  $V(t)$ , we have:

$$\mathbf{V} = -V(t) \mathbf{e}_1, \quad \mathbf{b} = -b \mathbf{e}_1, \quad \delta(\mathbf{L}_t) = \delta(z^1 - z_L^1(t)) \delta(z^2 - z_L^2(t)) \mathbf{e}_3,$$

and by (3.10) we obtain the flux corresponding to this motion

$$\mathbf{I}(\mathbf{x}, t) = -bV(t) \delta(z^1 - z_L^1(t)) \delta(z^2 - z_L^2(t)) \mathbf{e}_1 \otimes \mathbf{e}_2 \quad (3.12)$$

whose only non-zero component is

$$I_{12}(\mathbf{x}, t) = -bV(t) \delta(z^1 - z_L^1(t)) \delta(z^2 - z_L^2(t)).$$

The formula (3.11) may be also used to determine the dislocation flux associated with various microscopic arrangements and motions of the dislocation lines. To illustrate the necessary procedure, we give here a particular example of *single glide*.

Assume that plastic distortion is produced by the creation and expansion of circular dislocation loops, generated by Frank-Read sources, and moving in parallel glide planes. When the number of the loops per unit volume is very large we may assume that it is a continuously differentiable function of  $\mathbf{x}$  and  $t$ . We denote by  $N(\mathbf{x}, t)$  the number of the activated Frank-Read sources per unit volume, by  $n(\mathbf{x}, t)$  the mean number of dislocation loops emitted by each Frank-Read source, and by  $R(\mathbf{x}, t)$

the mean radius of the dislocation loops. For the sake of simplicity we do not write explicitly the dependence on  $\mathbf{x}$  in the following considerations.

We choose a system of Cartesian co-ordinates which has its  $z^1$  and  $z^3$  axes parallel to the glide planes, and the  $z^2$  axis perpendicular to the glide planes. Let us determine first the flux of the loops generated by a Frank-Read source situated in the plane  $z^2 = z_0^2$ . By hypothesis, all dislocation loops are circular and remain so during the expansion. Consequently the velocity has a constant magnitude along every dislocation loop, has a radial direction, and depends on the radius  $r(t)$  of the loop  $L_t$  and possibly on time. We denote this velocity by  $\hat{\mathbf{V}}(r(t), t)$ .

Let  $(z_0^1, z_0^2, z_0^3)$  be the co-ordinates of the common centre of the loops produced by the Frank-Read source considered, and

$$\rho(z^1, z^3; z_0^1, z_0^3) = \{(z^1 - z_0^1)^2 + (z^3 - z_0^3)^2\}^{1/2}. \quad (3.13)$$

Since

$$\hat{\mathbf{V}}(r(t), t) \times \mathbf{1}(\mathbf{x}_{L_t}) = \hat{V}(r(t), t) \mathbf{n}, \quad (3.14)$$

where now  $\mathbf{n} = \mathbf{e}_2$ , we deduce from (3.11) the flux of the dislocation loop  $L_t$

$$\mathbf{I}(t) = \mathbf{b} \otimes \mathbf{n} \hat{V}(r(t), t) \delta(\rho - r(t)) \delta(z^2 - z_0^2). \quad (3.15)$$

We assimilate now the dislocation loops produced by the Frank-Read source by a continuous distribution, introducing the number of dislocation loops per unit length measured radially,  $\hat{n}(r(t), t)$ . The total flux of the dislocation loops generated by a Frank-Read source situated in the plane  $z^2 = z_0^2$  is by (3.15)

$$\begin{aligned} \mathbf{I}(t) &= \mathbf{b} \otimes \mathbf{n} \delta(z^2 - z_0^2) \int_0^\infty \hat{V}(r, t) \hat{n}(r, t) \delta(\rho - r) dr \\ &= \mathbf{b} \otimes \mathbf{n} \delta(z^2 - z_0^2) \hat{V}(\rho, t) \hat{n}(\rho, t). \end{aligned} \quad (3.16)$$

We can now derive the flux of all the dislocation loops at  $\mathbf{x}$  and  $t$ , by taking into account the definition of  $\mathbf{N}(\mathbf{x}, t)$  and by integrating (3.16) over the whole space. We obtain

$$\mathbf{I}(t) = \mathbf{b} \otimes \mathbf{e}_2 N(t) \int_{-\infty}^{\infty} \delta(z^2 - z_0^2) dz_0^2 \int_0^\infty \hat{V}(\rho, t) \hat{n}(\rho, t) 2\pi \rho d\rho. \quad (3.17)$$

Finally, if we define the mean radial velocity  $V(t)$  of the dislocation loops at  $\mathbf{x}$  and  $t$ , by<sup>6</sup>

$$\int_0^{\infty} \hat{V}(\rho, t) \hat{n}(\rho, t) \rho d\rho = R(t) V(t) n(t), \quad (3.18)$$

we get

$$\mathbf{I} = 2\pi R V n \mathbf{b} \otimes \mathbf{n}, \quad (3.19)$$

where all quantities except  $\mathbf{b}$  and  $\mathbf{n}$  depend in general on  $\mathbf{x}$  and  $t$ .

Formulae similar to (3.19) were already used (see for instance Seeger [17] and Kronmüller [18]) in order to construct dislocational models of the work-hardening.

#### IV. Uniformly Moving Dislocations

For certain physical problems it is interesting to study the uniform motion of a straight dislocation or of a pile-up of straight dislocations.<sup>7</sup> In such cases we have

$$\bar{\alpha}(\mathbf{x}, t) = \bar{\alpha}_0(\mathbf{x} - \mathbf{V}t), \quad (4.1)$$

where  $\alpha_0$  is Noll's dislocation density at time  $t=0$ , and  $\mathbf{V}$  is the *constant* velocity of the dislocation group considered.

The dislocation densities  $\bar{\alpha}$  and  $\alpha$  do not satisfy in general a similar relation, because they do depend on the deformation of the material surface and linear elements. However, if the medium is *infinite*, and the elastic distortion produced by all other causes are zero or *constant*, then

$$j(\mathbf{x}, t) = j_0(\mathbf{x} - \mathbf{V}t), \quad \mathbf{A}(\mathbf{x}, t) = \mathbf{A}_0(\mathbf{x} - \mathbf{V}t), \quad (4.2)$$

where  $j_0$  and  $\mathbf{A}_0$  are the values of  $j$  and  $\mathbf{A}$  at time  $t=0$ , and from (1.15) follows

$$\bar{\alpha}(\mathbf{x}, t) = \bar{\alpha}_0(\mathbf{x} - \mathbf{V}t), \quad \bar{\alpha}^{\kappa m}(\mathbf{x}, t) = \bar{\alpha}_0^{\kappa m}(\mathbf{x} - \mathbf{V}t). \quad (4.3)$$

In the remaining part of this section we shall explore the consequences of this relation and demonstrate that, under the above mentioned hy-

<sup>6</sup> The integral (3.18) is obviously finite, because  $\hat{n}(\rho, t) = 0$  when  $\rho$  is larger than the maximum radius of the dislocation loops.

<sup>7</sup> The uniform expansion of a dislocation loop represents a more complicated situation. Although the expansion velocity  $\mathbf{V}$  has a constant magnitude, its direction varies along the dislocation line.

potheses, the dislocation flux is completely determined by the dislocation density at time  $t=0$  and by the constant dislocation velocity  $\mathbf{V}$ .

From (4.3) we deduce

$$\frac{\partial \bar{\alpha}^{\kappa m}}{\partial t} + \bar{\alpha}^{\kappa m, l} V^l = 0, \quad (4.4)$$

hence

$$\begin{aligned} \frac{d\bar{\alpha}^{\kappa m}}{dt} &= \frac{\partial \bar{\alpha}^{\kappa m}}{\partial t} + \bar{\alpha}^{\kappa m, l} v^l \\ &= \bar{\alpha}^{\kappa m, l} (v^l - V^l). \end{aligned} \quad (4.5)$$

Introducing (4.5) into (1.32) yields

$$\bar{\alpha}^{\kappa m, l} (v^l - V^l) - \bar{\alpha}^{\kappa l} v^m, l + \bar{\alpha}^{\kappa m} v^l, l = -\epsilon^{lrm} \bar{I}^{\kappa l, r}.$$

By using (1.27) and remembering that  $\mathbf{V}$  is constant, hence  $V^l, l = 0$ , we may write the last equation in the form

$$\{\bar{\alpha}^{\kappa m} (v^l - V^l)\}_{,l} - \{\bar{\alpha}^{\kappa l} (v^m - V^m)\}_{,l} = -\epsilon^{lrm} \bar{I}^{\kappa l, r},$$

or, equivalently,

$$\epsilon^{rml} \{\epsilon_{rts} \bar{\alpha}^{\kappa t} (v^s - V^s) - \bar{I}^{\kappa r}\}_{,l} = 0. \quad (4.6)$$

If  $\mathbf{V} = \mathbf{v}$ , the dislocations do not move with respect to the material. There is no plastic deformation, therefore,  $\bar{I} = 0$ . Consequently, from (4.6) we deduce

$$\bar{I} = -\bar{\alpha} \times (\mathbf{V} - \mathbf{v}), \quad \bar{I}^{\kappa r} = -\epsilon_{rts} \bar{\alpha}^{\kappa t} (V^s - v^s), \quad (4.7)$$

and, by (1.13) and (1.22), we have also

$$\mathbf{I} = -\alpha \times (\mathbf{V} - \mathbf{v}), \quad I^{\kappa r} = -\epsilon_{rts} \alpha^{\kappa t} (V^s - v^s), \quad (4.8)$$

Relation (4.8) replaces the constitutive equation which must relate the dislocation flux to the stress, by a supplementary kinematic condition valid for uniformly moving dislocations. If the dislocation density at time  $t=0$ ,  $\bar{\alpha}(\mathbf{x}, t)$ , and the dislocation velocity  $\mathbf{V}$ , are known, then we know  $\bar{\alpha}(\mathbf{x}, t)$  and  $\mathbf{I}(\mathbf{x}, t)$  from (4.3) and (4.7) and we may determine completely the self-stress and the particle velocity field by using the usual field equations and the boundary conditions of the theory of elasticity (see Teodosiu and Seeger [7]).

If the particle velocity field  $\mathbf{v}$  may be neglected with respect to the dislocation velocity, we obtain from (4.8)

$$\mathbf{I} = -\alpha \times \mathbf{V}. \quad (4.9)$$

Finally, for an isolated dislocation line  $L_t$  we have by (3.1),

$$\alpha(\mathbf{x}, t) = \mathbf{b} \otimes \delta(\mathbf{L}_t), \quad (4.10)$$

and we get from (4.9)

$$\mathbf{I}(\mathbf{x}, t) = \mathbf{b} \otimes \mathbf{V} \times \delta(\mathbf{L}_t), \quad (4.11)$$

so recovering (3.10) for a constant velocity.

## V. Theory of an Elastic-Plastic Continuum

In formulating the constitutive equations and in exploring the consequences of the thermodynamical restrictions we shall follow the paper by Green and Naghdi [3]. However, our thermodynamical variables will include the dislocation density and the dislocation flux.

The thermodynamic process must be compatible with the law of *balance of linear momentum*

$$\operatorname{div} \mathbf{T} + \rho \mathbf{f} = \rho \dot{\mathbf{v}}, \quad (5.1)$$

and the law of *balance of energy*

$$\rho \dot{\epsilon} - \mathbf{T} \cdot \operatorname{grad} \mathbf{v} + \operatorname{div} \mathbf{q} = \rho r. \quad (5.2)$$

Here  $\mathbf{T} = \mathbf{T}^r$  is the *stress tensor*,  $\mathbf{f}$  is the specific *body force* per unit mass,  $\epsilon$  is the specific *internal energy* per unit mass,  $\mathbf{q}$  is the *heat flux vector*, and  $r$  is the *heat supply* per unit mass and unit time, all quantities being functions of  $X$  and  $t$ , or, alternatively, of  $\mathbf{x}$  and  $t$ .

Introducing the *second Piola-Kirchoff stress tensor*,  $\tilde{\mathbf{T}}$ , defined by the relation

$$\mathbf{T} = j \tilde{\mathbf{A}} \mathbf{A}^T, \quad T^{kl} = j A^k{}_\kappa A^k{}_\lambda A^l{}_\lambda \tilde{T}^{k\lambda}, \quad (5.3)$$

and taking into account (1.26) and (1.22) we deduce

$$\begin{aligned} \mathbf{T} \cdot \operatorname{grad} \mathbf{v} &= (j \tilde{\mathbf{A}} \mathbf{A}^T) \cdot (\mathbf{A} \mathbf{I} \mathbf{A}^{-1} + \dot{\mathbf{A}} \mathbf{A}^{-1}) \\ &= j A^k{}_\kappa A^l{}_\lambda \tilde{T}^{k\lambda} (A_{k\mu} \tilde{I}^\mu{}_\sigma \tilde{A}^\sigma{}_l + \dot{A}_{k\mu} \tilde{A}^\mu{}_l) \\ &= j A^k{}_\kappa A_{k\mu} \tilde{T}^{k\lambda} \tilde{I}^\mu{}_\lambda + j \tilde{T}^{k\lambda} A^k{}_\kappa \dot{A}_{k\lambda}. \end{aligned}$$

Furthermore, by using the *elastic strain tensor*

$$\mathbf{E} = 1/2 (\mathbf{A}^T \mathbf{A} - \mathbf{I}), \quad E_{\kappa\lambda} = 1/2 (A_{k\kappa} A^k{}_\lambda - \delta_{\kappa\lambda}), \quad (5.4)$$

and the symmetry of  $\tilde{\mathbf{T}}$ , we may write the last relation in the form

$$\mathbf{T} \cdot \text{grad } \mathbf{v} = j(\mathbf{A}^T \mathbf{A} \tilde{\mathbf{T}}) \cdot \tilde{\mathbf{I}} + j\tilde{\mathbf{T}} \cdot \dot{\mathbf{E}}. \quad (5.5)$$

Substituting now (5.5) into (5.2) yields

$$\rho\dot{\epsilon} - j(\mathbf{A}^T \mathbf{A} \tilde{\mathbf{T}}) \cdot \tilde{\mathbf{I}} - j\tilde{\mathbf{T}} \cdot \dot{\mathbf{E}} = \rho r, \quad (5.6)$$

or, in component form,

$$\rho\dot{\epsilon} - jA^k{}_\kappa A_{k\mu} \tilde{T}^{\kappa\lambda} \tilde{I}^{\mu\lambda} - j\tilde{T}^{\kappa\lambda} \dot{\mathbf{E}}_{\kappa\lambda} = \rho r.$$

Let  $\rho$ ,  $\rho_0$ ,  $\tilde{\rho}$ , and  $\tilde{\rho}_0$  denote the mass densities in the configurations  $(k)$ ,  $(k_0)$ ,  $(\kappa)$ , and  $(\kappa_0)$ , respectively. The usual law of the *balance of mass*,

$$\rho = j\rho_0, \quad (5.7)$$

or, alternatively,

$$\dot{\rho} + \rho \text{ div } \mathbf{v} = 0, \quad \dot{\rho} + \rho v^l,_l = 0, \quad (5.8)$$

must be supplemented by the law governing the change of the mass density on account of the plastic deformation. To obtain this law we start from the relation analogous to (5.7),

$$\tilde{\rho}/\tilde{\rho}_0 = |\det \mathbf{P}^{-1}|, \quad (5.9)$$

which results from (1.5). Differentiating (5.9) with respect to  $t$  by using the formula for the differentiation of a determinant gives

$$\dot{\tilde{\rho}}/\tilde{\rho}_0 = \mathbf{P} \cdot \dot{\mathbf{P}}^{-1} |\det \mathbf{P}^{-1}|,$$

wherefrom we derive with the help of (1.22), (A.13), and (5.9),

$$\dot{\tilde{\rho}} + \tilde{\rho} \text{ tr } \tilde{\mathbf{I}} = 0, \quad \dot{\tilde{\rho}} + \tilde{\rho} \tilde{I}_{\lambda\lambda} = 0. \quad (5.10)$$

As it is well-known, the change of the mass density produced by the plastic deformation is in general very small. Hence we may consider that the dislocation flux is a deviatoric tensor, i.e.,

$$\text{tr } \tilde{\mathbf{I}} = 0. \quad (5.11)$$

In the case of an isolated straight dislocation, this relation has a very simple meaning. Let us substitute the linear relation (3.11) into (5.11), by taking into consideration that  $\mathbf{I} \approx \tilde{\mathbf{I}}$ . We get

$$\epsilon_{kmn} b^k V^m l^n = \mathbf{V} \cdot (\mathbf{l} \times \mathbf{b}) = 0, \quad (5.12)$$

i.e.,  $\mathbf{V}$  lies in the glide plane (the plane determined by  $\mathbf{l}$  and  $\mathbf{b}$ ). The only case in which the condition (5.12) is not fulfilled is that of the climbing of an edge dislocation ( $\mathbf{V}$  perpendicular to the glide plane), which plays a significant role merely by high temperatures.

The laws (5.1), (5.6), (5.8), and (5.11) must be supplemented by the elastic-plastic constitutive equations, whose study will cover the remaining part of this section.

We assume that the *yield condition* for the material under consideration may be written as

$$f(\tilde{\mathbf{T}}, \tilde{\boldsymbol{\alpha}}, \theta) = K, \quad (5.13)$$

where  $f$  is a continuously differentiable function of its arguments<sup>8</sup> and  $\theta > 0$  is the absolute temperature. The time-variation of  $K$  characterizes the *work-hardening* of the material. The rate of  $K$  depends in general on the stress, temperature, and on the arrangement, production, and motion of the dislocations. We expect, therefore, that  $\dot{K}$  will be a definite function of  $\tilde{\mathbf{T}}$ ,  $\tilde{\boldsymbol{\alpha}}$ ,  $\theta$ , and  $\tilde{\mathbf{I}}$ . If the dislocation arrangement remains constant, hence  $\tilde{\mathbf{I}} = 0$ , no work-hardening takes place. We may assume, therefore, in the first approximation, that

$$\dot{K} = \mathbf{W}(\tilde{\mathbf{T}}, \tilde{\boldsymbol{\alpha}}, \theta) \cdot \tilde{\mathbf{I}}. \quad (5.14)$$

Suppose the body is initially at rest, at a constant temperature and free of external loads. There is a certain range of variation of  $\tilde{\mathbf{T}}$  and  $\theta$  around this state, where the response of the material may be considered as *elastic*. Consequently, we may assume that there is a value of  $K$ , say  $K^*$ , such that

$$\tilde{\mathbf{I}} = 0 \text{ for } f < K^*. \quad (5.15)$$

In fact, even for loadings and temperatures satisfying the condition  $K < K^*$ , certain anelastic effects are produced by the reversible bowing out of the dislocation lines between the nodes. However, we shall neglect these effects in the present approach.

If  $f = K^*$ , the process of the dislocation production and glide begins.

<sup>8</sup> The more general case when the surface (5.13) is piecewise smooth does not present particular difficulties, but will not be considered here.

We assume that the dislocation flux associated with this process is given by a constitutive equation of the form

$$\tilde{\mathbf{I}} = \hat{\mathbf{I}}(\tilde{\mathbf{T}}, \dot{\tilde{\mathbf{T}}}, \tilde{\boldsymbol{\alpha}}, \theta, \dot{\theta}). \quad (5.16)$$

Suppose we know the function  $\hat{\mathbf{I}}$ . It is then possible to determine the variation of  $K$  through (5.14) and the new form of the surface (5.13) in the space of the stress components and temperature.

The surfaces (5.13) are usually called *yield surfaces* or *loading surfaces* and the sequence of points in the space of the stress components and temperature, corresponding to the variation of the stress and temperature, is called *loading path*.

For states of stress and temperature on the loading surface, we say that *loading*, *unloading*, or *neutral loading* takes place according to whether the vector tangent to the loading path is directed outward, inward, or along the tangent to the loading surface.

Since

$$\dot{f} = \frac{\partial f}{\partial \tilde{\mathbf{T}}} \cdot \dot{\tilde{\mathbf{T}}} + \frac{\partial f}{\partial \tilde{\boldsymbol{\alpha}}} \cdot \dot{\tilde{\boldsymbol{\alpha}}} + \frac{\partial f}{\partial \theta} \dot{\theta},$$

loading, unloading, or neutral loading takes place for a given point on the loading surface ( $f = K$ ) and for a given  $\tilde{\boldsymbol{\alpha}}$ , if the expression

$$\frac{\partial f}{\partial \tilde{\mathbf{T}}} \cdot \dot{\tilde{\mathbf{T}}} + \frac{\partial f}{\partial \theta} \dot{\theta} \quad (5.17)$$

is  $>0$ ,  $<0$ , or  $=0$ , respectively.

We neglect in the present formulation the dislocation flux corresponding to the dislocation rearrangement during unloading or neutral loading. Consequently, we assume that

$$\tilde{\mathbf{I}} = \hat{\mathbf{I}}(\tilde{\mathbf{T}}, \dot{\tilde{\mathbf{T}}}, \tilde{\boldsymbol{\alpha}}, \theta, \dot{\theta}), \text{ when } f = K, \frac{\partial f}{\partial \tilde{\mathbf{T}}} \cdot \dot{\tilde{\mathbf{T}}} + \frac{\partial f}{\partial \theta} \dot{\theta} > 0 \quad (\text{loading}), \quad (5.18)$$

$$\tilde{\mathbf{I}} = 0, \quad \text{when } f = K, \frac{\partial f}{\partial \tilde{\mathbf{T}}} \cdot \dot{\tilde{\mathbf{T}}} + \frac{\partial f}{\partial \theta} \dot{\theta} \leq 0 \quad (\text{unloading or neutral loading}), \quad (5.19)$$

or when  $f < K$  (elastic range).

Equation (5.18) must be independent of the time scale used to compute the rate of change, so that  $\hat{\mathbf{I}}$  is homogeneous of degree one in  $\dot{\mathbf{T}}$  and  $\dot{\theta}$ .

If we assume in addition that  $\hat{\mathbf{I}}$  is a linear function of  $\dot{\mathbf{T}}$  and  $\dot{\theta}$ , whose coefficients depend on  $\tilde{\mathbf{T}}$ ,  $\tilde{\alpha}$ , and  $\theta$ , and if we require the continuity of  $\tilde{\mathbf{I}}$  throughout stress and temperature space, we may derive from (5.18) the constitutive equation for loading

$$\tilde{\mathbf{I}} = \Lambda \left( \frac{\partial f}{\partial \tilde{\mathbf{T}}} \cdot \dot{\mathbf{T}} + \frac{\partial f}{\partial \theta} \dot{\theta} \right) \mathbf{H}, \quad (5.20)$$

where  $\Lambda$  is a scalar-valued function and  $\mathbf{H}$  is a tensor-valued function of  $\tilde{\mathbf{T}}$ ,  $\tilde{\alpha}$ , and  $\theta$ .

We complete now the set of constitutive equations, by assuming that the *free energy*

$$\psi = \epsilon - \theta \eta, \quad (5.21)$$

the *specific entropy*  $\eta$ , the Piola-Kirchoff stress tensor  $\tilde{\mathbf{T}}$ , and the heat flux  $\mathbf{q}$ , depend on  $\mathbf{A}$ ,  $\tilde{\alpha}$ ,  $\theta$ , and  $\text{grad } \theta$ . Using the principle of material objectivity (invariance of the constitutive equations with respect to the rigid-body motions), we conclude that  $\mathbf{A}$  and  $\text{grad } \theta$  must be replaced in the constitutive equations by the strain tensor  $\mathbf{E}$  and by the vector  $\mathbf{g} = \mathbf{A}^T \text{grad } \theta$ . Consequently, we adopt the following constitutive assumptions:

$$\psi = \hat{\psi} (\mathbf{E}, \tilde{\alpha}, \theta, \mathbf{g}), \quad (5.22)$$

$$\eta = \hat{\eta} (\mathbf{E}, \tilde{\alpha}, \theta, \mathbf{g}), \quad (5.23)$$

$$\tilde{\mathbf{T}} = \hat{\mathbf{T}} (\mathbf{E}, \tilde{\alpha}, \theta, \mathbf{g}), \quad (5.24)$$

$$\mathbf{q} = \hat{\mathbf{q}} (\mathbf{E}, \tilde{\alpha}, \theta, \mathbf{g}), \quad (5.25)$$

where the sign “ $\hat{\cdot}$ ” is used to distinguish the functions  $\hat{\psi}$ ,  $\hat{\eta}$ ,  $\hat{\mathbf{T}}$ , and  $\hat{\mathbf{q}}$  from their values.

Let us investigate the restrictions imposed on the constitutive equations (5.20), (5.22)–(5.25) by the second principle of thermodynamics, expressed by the Clausius-Duhem inequality

$$\rho \dot{\eta} - \frac{\rho r}{\theta} + \text{div} \left( \frac{\mathbf{q}}{\theta} \right) \geq 0. \quad (5.26)$$

Eliminating  $r$  between (5.6) and (5.26) and taking into account (5.7) and (5.21) we obtain

$$-\rho_0 \dot{\psi} - \rho_0 \dot{\theta} \eta + (\mathbf{A}^T \mathbf{A} \tilde{\mathbf{T}}) \cdot \tilde{\mathbf{I}} + \tilde{\mathbf{T}} \cdot \mathbf{E} - (j\theta)^{-1} \mathbf{q} \cdot \text{grad } \theta \geq 0. \quad (5.27)$$

From (5.22) follows

$$\dot{\psi} = \frac{\partial \hat{\psi}}{\partial \mathbf{E}} \cdot \dot{\mathbf{E}} + \frac{\partial \hat{\psi}}{\partial \tilde{\boldsymbol{\alpha}}} \cdot \dot{\tilde{\boldsymbol{\alpha}}} + \frac{\partial \hat{\psi}}{\partial \theta} \dot{\theta} + \frac{\partial \hat{\psi}}{\partial \mathbf{g}} \cdot \dot{\mathbf{g}}, \quad (5.28)$$

and (5.27) becomes

$$\begin{aligned} \left( \tilde{\mathbf{T}} - \rho_0 \frac{\partial \hat{\psi}}{\partial \mathbf{E}} \right) \cdot \dot{\mathbf{E}} - \rho_0 \left( \eta + \frac{\partial \hat{\psi}}{\partial \theta} \right) \dot{\theta} - \rho_0 \frac{\partial \hat{\psi}}{\partial \mathbf{g}} \cdot \dot{\mathbf{g}} - \rho_0 \frac{\partial \hat{\psi}}{\partial \tilde{\boldsymbol{\alpha}}} \cdot \dot{\tilde{\boldsymbol{\alpha}}} \\ + (\mathbf{A}^T \mathbf{A} \tilde{\mathbf{T}}) \cdot \tilde{\mathbf{I}} - (j\theta)^{-1} \mathbf{q} \cdot \text{grad } \theta \geq 0. \end{aligned} \quad (5.29)$$

In order for the inequality (5.29) to be satisfied for arbitrary fields  $\dot{\mathbf{E}}$ ,  $\dot{\theta}$ , and  $\dot{\mathbf{g}}$ , it is necessary that

$$\tilde{\mathbf{T}} = \rho_0 \frac{\partial \hat{\psi}}{\partial \mathbf{E}}, \quad (5.30)$$

$$\eta = -\frac{\partial \hat{\psi}}{\partial \theta}, \quad (5.31)$$

$$\frac{\partial \hat{\psi}}{\partial \mathbf{g}} = 0. \quad (5.32)$$

Equation (5.32) entails the dropping of  $\mathbf{g}$  from (5.22), and by (5.30) and (5.31) also the dropping of  $\mathbf{g}$  from (5.23) and (5.24). We have, therefore,

$$\psi = \hat{\psi}(\mathbf{E}, \tilde{\boldsymbol{\alpha}}, \theta), \quad (5.33)$$

and the functions  $\hat{\eta}$  and  $\tilde{\mathbf{T}}$  are completely determined by the gradients of  $\hat{\psi}$ . The remaining part of (5.29) is

$$-\rho_0 \frac{\partial \hat{\psi}}{\partial \tilde{\boldsymbol{\alpha}}} \cdot \dot{\tilde{\boldsymbol{\alpha}}} + (\mathbf{A}^T \mathbf{A} \tilde{\mathbf{T}}) \cdot \tilde{\mathbf{I}} - (j\theta)^{-1} \mathbf{q} \cdot \text{grad } \theta \geq 0, \quad (5.34)$$

for loading, and

$$\mathbf{q} \cdot \text{grad } \theta \leq 0 \quad (\tilde{\mathbf{I}} = 0), \quad (5.35)$$

for neutral loading, unloading, and the elastic range. The general dissipation inequality (5.34) may be decomposed under certain restrictive assumptions into an internal dissipation inequality and a heat-conduction inequality, as has been done by Coleman and Gurtin [23].

In (5.34) the tensors  $\tilde{\alpha}$  and  $\tilde{\mathbf{I}}$  are not independent of each other. They are related by the compatibility condition (1.35) in which  $\tilde{\alpha}$  and  $\tilde{\mathbf{I}}$  must be replaced by  $\dot{\alpha}$  and  $\tilde{\mathbf{I}}$  using the definitions (1.15) and (1.22).

By (5.21), (5.28), and (5.30)–(5.32), the law of the balance of energy (5.6) may be written in the form

$$\rho_0 \theta \dot{\eta} + \rho_0 \frac{\partial \hat{\psi}}{\partial \tilde{\alpha}} \cdot \dot{\alpha} - (\mathbf{A}^T \mathbf{A} \tilde{\mathbf{T}}) \cdot \tilde{\mathbf{I}} + (\rho_0 / \rho) \operatorname{div} \mathbf{q} = \rho_0 r \quad (5.36)$$

for loading, and

$$\rho \theta \dot{\eta} + \operatorname{div} \mathbf{q} = \rho r, \quad (5.37)$$

for neutral loading, unloading, and initial elastic range.

We make use finally of the simplifying assumption that during unloading and within the elastic range, the behaviour of the medium is purely elastic, i.e.,  $\partial \hat{\psi} / \partial \mathbf{E}$  and  $\partial \hat{\psi} / \partial \theta$  are independent of  $\tilde{\alpha}$ . Consequently, the specific free energy must have the special form

$$\hat{\psi}(\mathbf{E}, \tilde{\alpha}, \theta) = \hat{\psi}'(\mathbf{E}, \theta) + \hat{\psi}''(\tilde{\alpha}), \quad (5.38)$$

and the constitutive equations (5.30) and (5.31) become

$$\tilde{\mathbf{T}} = \rho_0 \frac{\partial \hat{\psi}'}{\partial \mathbf{E}}, \quad (5.39)$$

$$\eta = -\frac{\partial \hat{\psi}'}{\partial \theta}. \quad (5.40)$$

We obtained so a complete set of constitutive equations which, together with the kinematic equations and the balance laws, represent the basic field equations of the elastic-plastic behaviour in the present theory. In the next section we shall analyse the principal features of this theory.

## VI. Discussion of the Theory Proposed

For convenience we collect here the basic field equations of the theory, namely the *kinematic equations* (1.10), (1.15), (1.22), (1.26), (1.27), (1.35), and (5.4):

$$\operatorname{curl} \mathbf{A}^{-1} = \bar{\boldsymbol{\alpha}}, \quad (6.1)$$

$$\operatorname{grad} \mathbf{v} = \mathbf{A} \bar{\mathbf{I}} + \dot{\mathbf{A}} \mathbf{A}^{-1}. \quad (6.2)$$

$$\operatorname{div} \bar{\boldsymbol{\alpha}} = 0, \quad (6.3)$$

$$\dot{\bar{\boldsymbol{\alpha}}} - \bar{\boldsymbol{\alpha}} (\operatorname{grad} \mathbf{v})^T + \bar{\boldsymbol{\alpha}} \operatorname{div} \mathbf{v} = -\operatorname{curl} \bar{\mathbf{I}}, \quad (6.4)$$

$$\bar{\boldsymbol{\alpha}} = j \bar{\boldsymbol{\alpha}} \mathbf{A}^T, \quad j = |\det \mathbf{A}^{-1}|, \quad (6.5)$$

$$\bar{\mathbf{I}} = \tilde{\mathbf{I}} \mathbf{A}^{-1}, \quad (6.6)$$

$$\mathbf{E} = 1/2(\mathbf{A}^T \mathbf{A} - \bar{\mathbf{I}}), \quad (6.7)$$

the *balance laws* (5.1), (5.2), (5.8), (5.10), and (5.36):

$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0, \quad \dot{\rho} + \tilde{\rho} \operatorname{tr} \bar{\mathbf{I}} = 0 \quad (\text{balance of mass}), \quad (6.8)$$

$$\operatorname{div} \mathbf{T} + \rho \mathbf{f} = \rho \dot{\mathbf{v}} \quad (\text{balance of linear momentum}), \quad (6.9)$$

$$\mathbf{T} = \mathbf{T}^T \quad (\text{balance of angular momentum}). \quad (6.10)$$

$$\rho_0 \theta \dot{\eta} + \rho_0 \frac{\partial \hat{\psi}''}{\partial \bar{\boldsymbol{\alpha}}} \cdot \dot{\bar{\boldsymbol{\alpha}}} - (\mathbf{A}^T \mathbf{A} \bar{\mathbf{T}}) \cdot \bar{\mathbf{I}} + j^{-1} \operatorname{div} \mathbf{q} = \rho_0 r \quad (\text{balance of energy}), \quad (6.11)$$

the *dissipation inequality* (5.34):

$$-\rho_0 \frac{\partial \hat{\psi}''}{\partial \bar{\boldsymbol{\alpha}}} \cdot \dot{\bar{\boldsymbol{\alpha}}} + (\mathbf{A}^T \mathbf{A} \bar{\mathbf{T}}) \cdot \bar{\mathbf{I}} - (j\theta)^{-1} \mathbf{q} \cdot \operatorname{grad} \theta \geq 0, \quad (6.12)$$

the *constitutive equations* (5.38)–(5.40), (5.25), (5.20), and (5.19):

$$\mathbf{T} = j \mathbf{A} \bar{\mathbf{T}} \mathbf{A}^T = \rho \mathbf{A} \frac{\partial \hat{\psi}'}{\partial \mathbf{E}} \mathbf{A}^T, \quad (6.13)$$

$$\eta = -\frac{\partial \hat{\psi}'}{\partial \theta}. \quad (6.14)$$

$$\psi = \hat{\psi}(\mathbf{E}, \bar{\boldsymbol{\alpha}}, \theta) = \hat{\psi}'(\mathbf{E}, \theta) + \hat{\psi}''(\bar{\boldsymbol{\alpha}}), \quad (6.15)$$

$$\mathbf{q} = \hat{\mathbf{q}}(\mathbf{E}, \bar{\boldsymbol{\alpha}}, \theta, \mathbf{A}^T \operatorname{grad} \theta) \quad (6.16)$$

$$\bar{\mathbf{I}} = \Lambda(\bar{\mathbf{T}}, \bar{\boldsymbol{\alpha}}, \theta) \left( \frac{\partial f}{\partial \bar{\mathbf{T}}} \cdot \dot{\bar{\mathbf{T}}} + \frac{\partial f}{\partial \theta} \dot{\theta} \right) \mathbf{H}(\bar{\mathbf{T}}, \bar{\boldsymbol{\alpha}}, \theta), \quad (6.17)$$

$$\text{for } f = K, \frac{\partial f}{\partial \bar{\mathbf{T}}} \cdot \dot{\bar{\mathbf{T}}} + \frac{\partial f}{\partial \theta} \dot{\theta} > 0 \quad (\text{loading}),$$

$$\bar{\mathbf{I}} = 0, \text{ for } f = K, \frac{\partial f}{\partial \bar{\mathbf{T}}} \cdot \dot{\bar{\mathbf{T}}} + \frac{\partial f}{\partial \theta} \dot{\theta} \leq 0 \quad (\text{neutral loading, unloading}),$$

$$\text{or } f < K \quad (\text{elastic range}), \quad (6.18)$$

the *yield condition* (5.13)

$$f(\tilde{\mathbf{T}}, \tilde{\boldsymbol{\alpha}}, \theta) = K \quad (6.19)$$

and the *work-hardening law*

$$\dot{K} = \mathbf{W}(\tilde{\mathbf{T}}, \tilde{\boldsymbol{\alpha}}, \theta) \cdot \tilde{\mathbf{I}}. \quad (6.20)$$

Finally, we have to add to the above field equations the boundary conditions. For the traction boundary-value problem these have the form

$$\mathbf{T}\mathbf{n} = \mathbf{t}, \text{ for } \mathbf{x} \in \partial\mathcal{B}, \quad (6.21)$$

where  $\mathbf{t}$  is the prescribed surface traction, and  $\mathbf{n}$  is the unit normal to the boundary  $\partial\mathcal{B}$  of the body  $\mathcal{B}$ .

When the explicit form of the constitutive equations is known the above system allows us to determine the elastic-plastic behaviour of the material by using a step-by-step procedure. Let us assume that we know the elastic distortion field  $\mathbf{A}(\mathbf{x}, t)$ , the velocity field  $\mathbf{v}(\mathbf{x}, t)$ , the temperature field  $\theta = \theta(\mathbf{x}, t)$ , the surface loading (6.19), and the dislocation density  $\tilde{\boldsymbol{\alpha}} = \tilde{\boldsymbol{\alpha}}(\mathbf{x}, t)$ , at time  $t$ .

From (6.15) and (6.13) we calculate the stress tensor  $\mathbf{T}$ . We apply then for each particle the constitutive equations (6.17) or (6.18) depending on whether the corresponding point in the stress and temperature space belongs to the loading surface or to the elastic range, and in the first case on whether the loading path is directed outward, inward, or tangential to the loading surface. We determine thus  $\tilde{\mathbf{I}}$ ,  $\bar{\mathbf{I}}$ , and by (6.4) also  $\dot{\boldsymbol{\alpha}}$ . We can write now for a sufficiently small interval of time  $(t, t + \Delta t)$

$$\tilde{\boldsymbol{\alpha}}(X, \tau) \approx \tilde{\boldsymbol{\alpha}}(X, t) + \dot{\boldsymbol{\alpha}}(X, t) (t - \tau), \quad \tau \in (t, t + \Delta t). \quad (6.23)$$

$$\tilde{\mathbf{I}}(X, \tau) \approx \tilde{\mathbf{I}}(X, t). \quad (6.24)$$

As  $\tilde{\boldsymbol{\alpha}}$  and  $\tilde{\mathbf{I}}$  are known we may use the method presented in appendix 2 to determine the elastic distortion  $\mathbf{A}$  and the velocity field  $\mathbf{v}$  in the time interval  $(t, t + \Delta t)$ . When the thermal field is non-uniform and time-dependent this method must be generalized in order to include thermal effects, by using the energy equation (6.11). Then we know again the fields  $\mathbf{A}$ ,  $\mathbf{v}$ ,  $\theta$ ,  $\tilde{\boldsymbol{\alpha}}$  and by (6.20) also the variation of the surface loading during the time interval  $(t, t + \Delta t)$ . Of course the same procedure may be repeated at time  $t + \Delta t$  and so on. This scheme is especially adequate when using computers. However, it would be premature to attempt the solving of certain particular problems before the form of the constitutive equations will be better known.

In a further paper we shall study the relations between the present theory and certain dislocational theories concerning the work-hardening of fcc single crystals in simple tensile experiments (see Seeger [17] and Kronmüller [18]). It is hoped that this comparison will provide indications about the possible form of the constitutive equations for particular material classes.

We close this paper with some remarks concerning the choice of our internal state variables. We know that the plastic deformation is produced by the dislocation motion and that work-hardening is due to the self-stresses generated by dislocations.

In the present theory the dislocation multiplication and motion is macroscopically described by the dislocation flux. On the other hand the self-stress is completely determined by the dislocation density. However, we expect that these quantities will not be sufficient as internal state variables. We may understand this better by the following considerations. By definition the dislocation density gives a certain information about the mean dislocation arrangement around the point considered. If the linear dimensions of the Burgers circuit are comparable with the mean distance between the dislocations, then we obtain a complete information about the self-stress but this will vary rapidly from point to point. Alternatively, if the linear dimensions of the Burgers circuit are comparable with those of the macroscopic volume elements of the continuum theory, then the dislocation density will be very small on account of the zero effect of the dislocation loops and we shall obtain a slowly varying and small self-stress, which gives practically no information about the interaction of the self-stresses produced by the isolated dislocations. In fact, as shown by the dislocation theories of work-hardening, the necessary dimensions of the Burgers circuit for a work-hardening theory depend both on the mean distance between the dislocations and on the mean length of the dislocation pile-ups.

It is, therefore, necessary to introduce in the yield condition (6.19), in the work-hardening law (6.20), and in the constitutive equation for the dislocation flux (6.17), supplementary internal state variables describing the dislocation arrangement inside the macroscopic volume elements and characterizing the self-stresses produced by dislocation groups, such as pile-ups, whose linear dimensions are smaller than those of the macroscopic volume elements (the characteristic length of the continuum theory), but larger than the mean distance between the dislocations.<sup>9</sup>

Another possible refinement of the theory would be to replace the dislocation flux by several more detailed characteristics of the dislocation

<sup>9</sup> Such supplementary internal state variables could be, for instance, the correlation functions of the microscopic dislocation arrangement, as suggested by Prof. Kröner in the panel discussion.

multiplication and kinematics, such as the density of the Frank-Read sources and the dislocation velocities, and to consider separate constitutive equations for each of these quantities.

As shown by the theory of multipolar and micropolar continuum mechanics (see Green and Rivlin [4], and Eringen [24]) there are several ways of systematically introducing new phenomenological quantities in order to describe in more detail the microscopic reality. However, as the mathematical difficulties increase very rapidly with the number of new quantities, it would be preferable to find theoretically and/or experimentally the most significant microscopic quantities and to try to describe them by suitable continuum functions on the macroscopic level.

## VII. Appendix 1. Basic Relations from the Tensor Algebra and Analysis Used in the Present Paper

In writing tensor relations we apply mostly a direct notation introduced by Noll (see e.g. [8], and [21]), which has a certain similarity with Gibbs' notation, but deviates from it in some respects. We shall write the principal results in component form, too, and we shall make also use of this notation for some intermediate calculations involving tensors of third or higher order.

To facilitate the transcription of the results from one notation to another we summarize here the basic equivalences employed in this paper. Let  $\mathbf{A}$  and  $\mathbf{B}$  be second-order tensors,  $\mathbf{L}$  a fourth-order tensor,  $\mathbf{u}$ ,  $\mathbf{v}$ , and  $\mathbf{w}$  vectors,  $\mathbf{1}$  the metric tensor whose contravariant, covariant, and mixed components are  $g^{kl}$ ,  $g_{kl}$ , and  $\delta^k_l$  respectively,  $\epsilon^{rsm} = \epsilon_{rsm}$  the permutation tensor ( $\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = 1$ ,  $\epsilon_{213} = \epsilon_{132} = \epsilon_{321} = -1$ , all other components are zero), and

$$\epsilon^{rsm} \equiv g^{-1/2} \epsilon^{rsm}, \quad \epsilon_{rsm} \equiv g^{1/2} \epsilon_{rsm}, \quad g = \det \|g_{km}\|. \quad (\text{A.1})$$

We have then the following formulae:

*Vector and tensor algebra.*

$$(\mathbf{u} \otimes \mathbf{v})^{km} = u^k v^m, \quad (\text{A.2})$$

$$\mathbf{u} \cdot \mathbf{v} = u^m v_m = g_{km} u^k v^m, \quad (\text{A.3})$$

$$(\mathbf{u} \times \mathbf{v})^k = \epsilon^{klm} u_l v_m, \quad (\text{A.4})$$

$$(\mathbf{A}\mathbf{u})^k = A^{km} u_m, \quad (\mathbf{A}^T \mathbf{u})^k = A^{mk} u_m, \quad (\text{A.5})$$

$$(\mathbf{u} \otimes \mathbf{v}) \mathbf{w} = \mathbf{u} (\mathbf{v} \cdot \mathbf{w}) = v^m w_m \mathbf{u}, \quad (\text{A.6})$$

$$(\mathbf{A} \times \mathbf{u})^{km} = \epsilon^{rsm} A^k r u_s, \quad (\text{A.7})$$

$$\det \mathbf{A} = \det \|A^k_m\|, \quad (\text{A.8})$$

$$\text{tr } \mathbf{A} = A^m{}_m \text{ (trace of } \mathbf{A}), \quad (\text{A.9})$$

$$(\text{cr } \mathbf{A})^k = \epsilon^{krs} A_{rs} \text{ (cross or axial vector of } \mathbf{A}), \quad (\text{A.10})$$

$$(\mathbf{AB})^{km} = A^k{}_p B^{pm} \quad (\text{A.11})$$

$$\mathbf{AA}^{-1} = \mathbf{A}^{-1} \mathbf{A} = \mathbf{1} \text{ (} \mathbf{A}^{-1} \text{ inverse of } \mathbf{A}), \quad (\text{A.12})$$

$$\mathbf{A} \cdot \mathbf{B} = \text{tr}(\mathbf{AB}^T) = A^{km} B_{km}, \quad (\text{A.13})$$

$$|\mathbf{A}| = (\mathbf{A} \cdot \mathbf{A})^{1/2} \text{ (magnitude of } \mathbf{A}), \quad (\text{A.14})$$

$$\mathbf{L}[\mathbf{A}]^{kp} = L^{kp\ell m} A_{\ell m}. \quad (\text{A.15})$$

*Vector and tensor analysis.*

We make use only of the right-hand operators grad, div, and curl (see for instance Jaunzemis [19], p. 88, where, however, Gibbs' notation is employed). We have

$$(\text{grad } \mathbf{u})^k{}_m = u^k{}_m, \quad (\text{A.16})$$

$$\text{div } \mathbf{u} = u^m{}_m, \quad (\text{A.17})$$

$$(\text{curl } \mathbf{u})^m = \epsilon^{rsm} u_{r,s}, \quad (\text{A.18})$$

$$(\text{grad } \mathbf{A})^{kl}{}_m = A^{kl}{}_m, \quad (\text{A.19})$$

$$(\text{div } \mathbf{A})^k = A^{km}{}_m, \quad (\text{A.20})$$

$$(\text{curl } \mathbf{A})^{km} = \epsilon^{rsm} A^k{}_{r,s}. \quad (\text{A.21})$$

Frequent use will be made of Kelvin's transformation

$$\oint_c \mathbf{A} d\mathbf{x} = - \int_s (\text{curl } \mathbf{A}) \mathbf{n} \, ds, \quad (\text{A.22})$$

where  $s$  is a smooth surface bounded by the curve  $c$ .

If  $\mathbf{x} = \chi(\mathbf{X}, t)$  is the position vector of the particle  $X$  at time  $t$ , and if  $\mathbf{v} = \frac{\partial}{\partial t} \chi(X, t)$ , the material derivative of the tensor-valued function  $\varphi(\mathbf{x}, t)$  is defined by

$$\dot{\varphi} \equiv \frac{d\varphi}{dt} = \frac{\partial \varphi}{\partial t} + \varphi_{,m} v^m. \quad (\text{A.23})$$

*$\delta$ -functions associated with lines and surfaces.*

To describe the position and motion of isolated dislocation lines we employ the  $\delta$ -functions associated with lines and surfaces, introduced by Kunin [20]. Let  $\varphi(\mathbf{x})$  be an indefinite differentiable scalar-valued function with finite support,  $S$  a smooth surface,  $L$  a smooth curve, and  $E$  the Euclidean three-dimensional space.

The generalized functions  $\delta(L)$  and  $\delta(S)$  are defined by the relations

$$\int_E \varphi(\mathbf{x}) \delta(L) dV = \int_L \varphi(\mathbf{x}) dL, \quad (\text{A.24})$$

$$\int_E \varphi(\mathbf{x}) \delta(S) dV = \int_S \varphi(\mathbf{x}) dS. \quad (\text{A.25})$$

If  $L$  and  $S$  intersect in one point, whose position vector is  $\mathbf{x}_0$ , we have

$$\delta(L) \delta(S) = \delta(\mathbf{x} - \mathbf{x}_0), \quad (\text{A.26})$$

$$\int_S \delta(L) dS = \int_L \delta(S) dL = 1. \quad (\text{A.27})$$

Let us now orient  $L$  and  $S$  by choosing the positive unit vector  $\mathbf{l}$ , tangent to  $L$ , and the positive unit normal  $\mathbf{n}$  to  $S$ . The generalized vector functions  $\delta(\mathbf{L})$  and  $\delta(\mathbf{S})$  are defined by the relations

$$\int_E \varphi(\mathbf{x}) \delta(\mathbf{L}) dV = \int_L \varphi(\mathbf{x}) \mathbf{l} dL = \int_L \varphi(\mathbf{x}) d\mathbf{x}. \quad (\text{A.28})$$

$$\int_E \varphi(\mathbf{x}) \delta(\mathbf{S}) dV = \int_S \varphi(\mathbf{x}) \mathbf{n} dS = \int_S \varphi(\mathbf{x}) d\mathbf{S}, \quad (\text{A.29})$$

which are still applicable if in the both sides of the equations the tensor function  $\varphi(\mathbf{x})$  is related to the vectorial  $\delta$ -function by the same vector or tensor product. If  $L$  and  $S$  intersect in one point  $\mathbf{x}_0$ , we have

$$\delta(\mathbf{L}) \delta(\mathbf{S}) = \begin{cases} +\delta(\mathbf{x} - \mathbf{x}_0), & \text{if } \mathbf{n} \cdot \mathbf{l} > 0 \text{ at } \mathbf{x}_0, \\ -\delta(\mathbf{x} - \mathbf{x}_0), & \text{if } \mathbf{n} \cdot \mathbf{l} < 0 \text{ at } \mathbf{x}_0. \end{cases} \quad (\text{A.30})$$

Let now  $f(\mathbf{x}_L)$  and  $f(\mathbf{x}_S)$  be continuous functions defined on  $L$  and  $S$ , respectively. The generalized functions  $f(\mathbf{x}_L) \delta(\mathbf{L})$  and  $f(\mathbf{x}_S) \delta(\mathbf{S})$  are defined by the relations

$$\int_E \varphi(\mathbf{x}) f(\mathbf{x}_L) \delta(\mathbf{L}) dV = \int_L \varphi(\mathbf{x}) f(\mathbf{x}) d\mathbf{x}, \quad (\text{A.31})$$

$$\int_E \varphi(\mathbf{x}) f(\mathbf{x}_S) \delta(\mathbf{S}) dV = \int_S \varphi(\mathbf{x}) f(\mathbf{x}) d\mathbf{S}. \quad (\text{A.32})$$

The formulae (A.24)–(A.32) remain valid if  $\varphi(\mathbf{x})$  and  $f(\mathbf{x})$  are tensor-valued functions provided that the same product is used in both sides of the equations.

We consider finally the case of a planar surface  $S_t$ , bounded at time  $t$  by the closed line  $L_t$ , whose points are moving with the velocity  $\mathbf{V}(\mathbf{x}_{L_t}, t)$  contained in the plane of  $S_t$ , and directed to the exterior of  $S_t$ . Let us choose the positive unit vector tangent to  $L_t$ ,  $\mathbf{l}(\mathbf{x}_{L_t})$ , and the positive unit normal to  $S_t$ ,  $\mathbf{n}$ , so that  $\mathbf{V} \times \mathbf{l}$  and  $\mathbf{n}$  have the same direction. We shall

prove that

$$\frac{d}{dt} \delta(\mathbf{S}_t) = \mathbf{V}(\mathbf{x}_{L_t}) \times \delta(\mathbf{L}_t). \quad (\text{A.33})$$

From (A.24) follows

$$\int_E \varphi(\mathbf{x}) \frac{d}{dt} \delta(\mathbf{S}_t) dV = \frac{d}{dt} \int_E \varphi(\mathbf{x}) \delta(\mathbf{S}_t) dV = \frac{d}{dt} \int_{S_t} \varphi(\mathbf{x}) d\mathbf{S}, \quad (\text{A.34})$$

because in the first integral  $\mathbf{x}$  does not depend on  $t$ . On the contrary, in the last integral  $\mathbf{x}$  is the position vector of a point on  $S_t$ , hence depends on  $t$ . Let  $\mathbf{V}(\mathbf{x}, t)$  be a continuous field which vanishes in an arbitrary point in the interior of  $S_t$  and whose value on  $L_t$  is  $\mathbf{V}(\mathbf{x}_{L_t}, t)$ . Considering that  $S_t$  is material with respect to the “velocity” field  $\mathbf{V}(\mathbf{x}, t)$  and applying the formula for the rate of a surface integral taken on a material surface (Truesdell and Toupin [9], p. 346) yields

$$\frac{d}{dt} \int_{S_t} \varphi(\mathbf{x}) d\mathbf{S} = \int_{S_t} \{ \dot{\varphi} + \varphi \operatorname{div} \mathbf{V} - \varphi (\operatorname{grad} \mathbf{V})^T \cdot \mathbf{n} \} dS. \quad (\text{A.35})$$

But  $\partial \varphi / \partial t = 0$ , and  $\mathbf{V} \cdot \mathbf{n} = 0$ , hence the component form of the last equation may be written successively

$$\begin{aligned} \frac{d}{dt} \int_{S_t} \varphi(\mathbf{x}) n_k dS &= \int_{S_t} \{ (\varphi_{,m} V^m + \varphi V^m_{,m}) n_k - \varphi V^m_{,k} n_m \} dS, \\ &= \int_{S_t} \{ (\varphi V^m)_{,m} n_k - (\varphi V^m)_{,k} n_m \} dS, \\ &= \int_{S_t} \epsilon_{ptr} \epsilon_{pmk} (\varphi V^m)_{,l} n_r dS \\ &= - \int_{L_t} \epsilon_{pmk} \varphi(\mathbf{x}) V^m(\mathbf{x}) dx^p, \end{aligned}$$

wherefrom it follows

$$\frac{d}{dt} \int_{S_t} \varphi(\mathbf{x}) d\mathbf{S} = \int_E \varphi(\mathbf{x}) [\mathbf{V}(\mathbf{x}_{L_t}) \times \delta(\mathbf{L}_t)] dV. \quad (\text{A.36})$$

Finally, by comparing (A.33) with (A.35) we deduce (A.32).

### VIII. Appendix 2

As already mentioned in section 1, when the dislocation density  $\bar{\alpha}$  and the dislocation flux  $\bar{I}$  are known, the system of kinematic equations (1.10),

(1.26), (1.27), and (1.28) allows the determination of the self-stresses produced by the moving dislocations, when completed by the equations of motion, the elastic constitutive equations, and the boundary conditions. We shall demonstrate this assertion for the linearized system of equations. The solving of the non-linear problem may be reduced to that of a series of linear problems by using an algorithm which slightly generalizes the scheme proposed by Teodosiu and Seeger [7] for uniformly moving dislocations.

Let us assume that  $\bar{\alpha}$  and  $\bar{\mathbf{I}}$  are known and satisfy the linearized compatibility conditions (2.8) and (2.9). For the sake of simplicity we consider an infinite elastic medium  $E$ , free of body forces and surface tractions. The equations of motion and the linear elastic constitutive equations are now

$$\operatorname{div} \mathbf{T} = \rho \frac{\partial \mathbf{v}}{\partial t}, \quad \mathbf{T} = \mathbf{T}^T, \quad (\text{A.37})$$

$$\mathbf{T} = \mathbf{L}_2[\tilde{\mathbf{E}}], \quad (\text{A.38})$$

where  $\mathbf{T}$  is the stress tensor,  $\rho$  is the mass density in the current configuration ( $k$ ), which in the linear approximation is constant if the body is homogeneous in the natural state,  $\mathbf{L}_2$  is the fourth-order tensor of the second-order elasticities, and  $\tilde{\mathbf{E}} \equiv 1/2(\boldsymbol{\beta} + \boldsymbol{\beta}^T)$  is the infinitesimal strain tensor. Our boundary condition will be the vanishing of the self-stress at infinity, that is

$$|\mathbf{T}| \rightarrow 0, \text{ as } |\mathbf{x}| \rightarrow \infty. \quad (\text{A.39})$$

By substituting (A.38) into (A.37), and taking into account the symmetry of the tensor  $\mathbf{L}_2$  we deduce

$$\operatorname{div} \mathbf{L}_2[\dot{\boldsymbol{\beta}}] = \rho \frac{\partial \mathbf{v}}{\partial t}. \quad (\text{A.40})$$

We write now the field equations (A.40), (2.8), and (2.7) in component form, assuming that  $x^k$  are the Cartesian co-ordinates  $z^k$ , so that the components of  $\mathbf{L}_2$  are constants. We obtain

$$\frac{1}{2} L_{klmn} \beta_{mn, l} = \rho \frac{\partial v_k}{\partial t}, \quad (\text{A.41})$$

$$v_{k, r} = I_{kr} + \frac{\partial \beta_{kr}}{\partial t}, \quad (\text{A.42})$$

$$\epsilon_{pst} \beta_{mp, s} = \alpha_{mt}, \quad (\text{A.43})$$

where  $(\cdot)_{,r}$  means now simply  $\frac{\partial}{\partial z^r}(\cdot)$ . To separate the unknowns  $\mathbf{v}$  and  $\boldsymbol{\beta}$ , we differentiate first (A.41) with respect to  $z^r$  and eliminate  $\mathbf{v}$  between the equation obtained and (2.18). We have then

$$\frac{L_{klmn}}{2}\beta_{mn,lr} - \rho \frac{\partial^2 \beta_{kr}}{\partial t^2} = \rho \frac{\partial I_{kr}}{\partial t} \quad (\text{A.44})$$

But, from (2.19) we derive

$$\beta_{mr,n} - \beta_{mn,r} = \in_{rnt} \alpha_{mt}, \quad (\text{A.45})$$

and introducing this result into (A.44) yields

$$\frac{L_{klmn}}{2}\beta_{mr,nt} - \frac{L_{klmn}}{2}\in_{rnt} \alpha_{mt,l} - \rho \frac{\partial I_{kr}}{\partial t} = \rho \frac{\partial^2 \beta_{kr}}{\partial t^2}. \quad (\text{A.46})$$

Furthermore, we differentiate (A.41) with respect to  $t$ . and eliminate  $\boldsymbol{\beta}$  between the equation resulted and (A.42). so obtaining

$$\frac{L_{klmn}}{2}v_{m,nt} - \frac{L_{klmn}}{2}I_{mn,l} = \rho \frac{\partial^2 v_k}{\partial t^2}. \quad (\text{A.47})$$

If the dynamic Green's tensor function  $\mathbf{G}(\mathbf{x} - \mathbf{x}', t - t')$  that is the solution of the equation

$$\frac{L_{klmn}}{2}G_{mp,nt}(\mathbf{x} - \mathbf{x}', t - t') + \delta_{kp}\delta(\mathbf{x} - \mathbf{x}')\delta(t - t')$$

$$= \rho \frac{\partial^2 G_{kp}}{\partial t^2}(\mathbf{x} - \mathbf{x}', t - t') \quad (\text{A.48})$$

with the boundary condition (A.39) is known for the material considered, then the solutions of eqs (A.46) and (A.47) are given by

$$\begin{aligned} \beta_{mr}(\mathbf{x}, t) = & - \int_{-\infty}^{\infty} \int_E \left\{ \frac{L_{plqn}}{2} \in_{rnu} \alpha_{qu,l'}(\mathbf{x}', t') \right. \\ & \left. + \rho \frac{\partial}{\partial t'} I_{pr}(\mathbf{x}', t') \right\} G_{mp}(\mathbf{x} - \mathbf{x}', t - t') dV' dt', \end{aligned} \quad (\text{A.49})$$

$$v_m(\mathbf{x}, t) = - \int_{-\infty}^{\infty} \int_E \frac{L_{plqn}}{2} I_{qn,l'}(\mathbf{x}', t') G_{mp}(\mathbf{x} - \mathbf{x}', t - t') dV' dt', \quad (\text{A.50})$$

where  $(\cdot)_{, \nu} = \frac{\partial}{\partial z^{\nu}} (\cdot)$ . Integrating by parts and taking into consideration that  $G(\mathbf{x} - \mathbf{x}', t - t') \rightarrow 0$  as  $|\mathbf{x}'| \rightarrow \infty$ , for all finite  $\mathbf{x}$ , we have alternatively

$$\begin{aligned} \beta_{mr}(\mathbf{x}, t) = & - \int_{-\infty}^{\infty} \int_E \left\{ L_{p l q n} \in_{r n u} \alpha_{q u}(\mathbf{x}', t') G_{m p, l}(\mathbf{x} - \mathbf{x}', t - t') \right. \\ & \left. + \rho I_{p r}(\mathbf{x}', t') \frac{\partial G_{m p}}{\partial t}(\mathbf{x} - \mathbf{x}', t - t') \right\} dV' dt', \end{aligned} \quad (\text{A.51})$$

$$v_m(\mathbf{x}, t) = - \int_{-\infty}^{\infty} \int_E L_{p l q n} I_{q n}(\mathbf{x}', t') G_{m p, l}(\mathbf{x} - \mathbf{x}', t') dV' dt'. \quad (\text{A.52})$$

Finally, by using the component form of (A.38),

$$T_{kl} = \sum_{m,n} L_{k l m n} \beta_{m n}, \quad (\text{A.53})$$

and the expression (A.51) for  $\beta$  we obtain the self-stress  $\mathbf{T}$ .

The formulae (A.51) and (A.52) were deduced for the first time by Mura [6] by making use of the displacement field produced by an isolated dislocation line and employing a limiting process. The present derivation was included for completeness and because it uses only continuum concepts.

The expressions of the velocity field and of the elastic distortion field produced by the motion of a singular dislocation line may be at once derived from (A.51) and (A.52) by employing the  $\delta$ -functions introduced by Kunin and presented in appendix 1. Indeed, if we replace in these formulae (see sec. 3)

$$\alpha_{q u}(\mathbf{x}, t) = b_q l_u(\mathbf{x}_{L_t}) \delta(L_t), \quad (\text{A.54})$$

$$I_{p r}(\mathbf{x}, t) = b_p \in_{r s u} V_s(\mathbf{x}_{L_t}, t) l_u(\mathbf{x}_{L_t}) \delta(L_t), \quad (\text{A.55})$$

we infer

$$\begin{aligned} \beta_{mr}(\mathbf{x}, t) = & - \int_{-\infty}^{\infty} \int_{L_t} \left\{ L_{p l q n} \in_{r n u} b_q G_{m p, l}(\mathbf{x} - \mathbf{x}', t - t') \right. \\ & \left. + \rho b_p \in_{r s u} V_s(\mathbf{x}', t') \frac{\partial G_{m p}}{\partial t}(\mathbf{x} - \mathbf{x}', t - t') \right\} dL'_u dt', \end{aligned} \quad (\text{A.56})$$

$$v_m(\mathbf{x}, t) = - \int_{-\infty}^{\infty} \int_{L_{t'}} \frac{1}{2} L_{plqn} b_q \in_{nsu} V_s(\mathbf{x}', t') G_{mp, l}(\mathbf{x} - \mathbf{x}', t - t') dL'_u dt'. \quad (\text{A.57})$$

### IX. Appendix 3. Equivalences Between the Notations Used in the Present Paper and Some Other Notations Employed in the Literature

We give in the following table the equivalences between the notations used in the present paper for the linearized theory (secs. 2-4) and some other notations employed in the literature.

TABLE 1

Notations in the present paper	Notations in the references:				
	[6]	[14]	[15]	[10]	[16]
$\beta_{kl}^G$	$U_{k, l}$	—	$U_{lk}$	$\beta_{lk}^G$	$\beta_{lk}^G$
$\beta_{kl}^P$	$\beta_{lk}^*$	—	$u_{lk}^{pl}$	$\beta_{lk}^P$	$\beta_{lk}^P$
$\beta_{kl}$	$\beta_{lk}$	$u_{lk}$	$u_{lk}$	$\beta_{lk}$	$\beta_{lk}$
$v_k$	$\dot{U}_k$	$v_k$	$v_k$	—	$\dot{s}_k^G$
$I_{kl} = \dot{\beta}_{kl}^P$	$- \in_{mn} V_{mnk}$	$- I_{lk}$	$- j_{lk}$	$- b \epsilon_{mn} N_{mnk}$	$\dot{\beta}_{lk}^P$
$\tilde{\alpha}_{kl} = \tilde{\alpha}_{kl} = \alpha_{kl}$	$- \alpha_{lk}$	$D_{lk}$	$\alpha_{lk}$	$- \alpha_{lk}$	$- \alpha_{lk}$
$L_{lkmn}$	$C_{ktnm}$	—	$\lambda_{ktnm}$	$C_{ktnm}$	$C_{ktnm}$
$\tilde{E}_{kl}$	—	$\varepsilon_{kl}$	$\varepsilon_{kl}$	$\varepsilon_{kl}$	$\varepsilon_{kl}$
$\tilde{R}_{kl}$	—	—	—	$\omega_{lk}$	$\omega_{lk}$
$T_{kl}$	$\sigma_{kl}$	—	$\sigma_{lk}$	$\sigma_{lk}$	$\sigma_{kl}$
$\bar{b}_k = b_k$	$- b_k$	$b_k$	$b_k$	$- b_k$	—

As regards the *non-linear* dislocation kinematics, we give the principal equivalences with Günther's notations [5]. These are

$$h^k{}_k \sim A^k{}_k, h^k{}_k \sim \overset{-1}{A}{}^k{}_k, \quad (\text{A.58})$$

$$g_{kl} \sim \overset{-1}{A}{}_{mk} \overset{-1}{A}{}^{ml}, \quad (\text{A.59})$$

$$T_{ml}{}^k \sim A^k{}_p \overset{-1}{A}{}^{pl}{}_{[l}, \quad (\text{A.60})$$

$$T_{mlk} \equiv g_{ks} T_{ml}{}^s \sim \overset{-1}{A}{}_{pk} \overset{-1}{A}{}^{pl}{}_{[l}, \quad (\text{A.61})$$

$$2c_T T_{kl}^0 \sim \overset{-1}{A}{}_{ml} \bar{I}^m{}_{k}. \quad (\text{A.62})$$

By using these relations, it is possible to prove, after some lengthy manipulations, that Günther's kinematic equations ([5], system (43)) are equivalent with our equations (6.1)–(6.4). The relations to the previous work by Amari [13] and Holländer [22] follow from Günther's discussion ([5], sec. II).

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# NON-LINEAR DYNAMIC PROBLEMS FOR ANISOTROPIC ELASTIC BODIES IN THE CONTINUUM THEORY OF DISLOCATIONS

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The non-linear continuum theory of dislocations has been used to solve a number of problems for isotropic materials, including the determination of stresses produced by dislocations, the scattering of elastic waves by straight dislocations and kinks, and the small-angle scattering of x-rays by dislocation lines and rings. For the application of these results it is necessary to know the elastic constants of third or higher order entering the constitutive equations. Third-order elastic constants have recently become available for a large class of single crystals with an accuracy that exceeds considerably the earlier polycrystalline data. It appears therefore desirable to develop a formulation of the theory that may be applied to anisotropic materials.

The present work aims at developing approximate methods for solving non-linear problems such as the determination of the strains produced by stationary or uniformly moving dislocations in anisotropic media and of their effects on a superimposed infinitesimal motion.

The non-linear problems are solved by reduction to a series of linear problems using expansions in terms of small parameters. Three such parameters appear naturally: the magnitude of the distortion produced by dislocations, the magnitude of the deformation gradient of the superimposed motion, and the ratio between the dislocation and sound velocities. To obtain definite approximation algorithms, hypotheses concerning the relative order of magnitude of these three parameters are introduced.

Key words: Anisotropic elasticity; dislocation dynamics; dislocation; elasticity; non-linear elasticity.

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The non-linear continuum theory of dislocations has been used to solve a number of problems for *isotropic* media, including the determination of stresses produced by dislocations, the scattering of elastic waves by

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straight dislocations and kinks, and the small-angle scattering of x rays by dislocation lines and rings [1-6]. For the application of these results it is necessary to know the elastic constants of third or higher order entering the constitutive equations. Third-order elastic constants have recently become available for a large class of single crystals with an accuracy that exceeds considerably that of the earlier polycrystalline data. It appears therefore desirable to develop a formulation of the theory that may be applied to *anisotropic* media.

The present work aims at developing approximate methods for solving non-linear problems of the following kinds: the determination of the strains produced by stationary or uniformly moving dislocations in anisotropic media (secs. III and IV) and of their effects on a superimposed infinitesimal motion (sec. V).

The non-linear problems are solved by reduction to a series of linear problems, using expansions in terms of small parameters. Three such parameters appear naturally: the magnitude of the distortion produced by dislocations, the deformation gradient of the superimposed motion, and the ratio between the dislocation and sound velocities. To obtain definite approximation algorithms, hypotheses concerning the relative order of magnitude of these three parameters have to be introduced.

The approximate methods to be presented have a large field of interest. Their application to various concrete problems will form the subject of further papers.

We shall apply mostly the so-called direct notation (for details see [7]). However, we shall write the principal results in component form, too, and we shall also make use of this notation when considering particular crystal classes or whenever it simplifies the calculations.

To facilitate the transcription of the results from one notation to another we summarize here the basic equivalences. If  $\mathbf{A}$ ,  $\mathbf{B}$  are second-order tensors,  $\mathbf{L}$  is a tensor of order  $n$ , and  $\mathbf{u}$  is a vector, then

$$(\mathbf{A}\mathbf{u})^k = A^{km}u_m, \quad (\mathbf{A}^T\mathbf{u})^k = A^{mk}u_m, \quad (\mathbf{A} \times \mathbf{u})^{km} = \epsilon^{rsm}A^k_ru_s,$$

$$(\mathbf{AB})^{km} = A^k{}_p B^{pm}, \quad \det \mathbf{A} = \det ||A^{km}||, \quad \text{tr } \mathbf{A} = A^m{}_m \text{ (trace of } \mathbf{A}),$$

$$(\text{cr } \mathbf{A})^k = \epsilon^{krs}A_{rs} \text{ (cross or axial vector of } \mathbf{A}),$$

$$|\mathbf{A}| = (A^{km}A_{km})^{1/2} \text{ (magnitude of } \mathbf{A}),$$

$$\mathbf{L}[\mathbf{A}]^{k \dots p} = L^{k \dots p l m} A_{l m}, \quad n > 2,$$

$$\mathbf{L}[\mathbf{A}, \mathbf{B}]^{k \dots q} = L^{k \dots q l m r s} A_{l m} B_{r s}, \quad n > 4,$$

where  $\epsilon^{rsm} = g^{-1/2} \epsilon^{rsm}$ ,  $\epsilon_{rsm} = g^{1/2} \epsilon_{rsm}$ ,  $g = \det \|g_{km}\|$ ,  $g_{km}$  is the metric tensor, and  $\epsilon^{rsm} = \epsilon_{rsm}$  is the permutation symbol ( $\epsilon_{123} = \epsilon_{312} = \epsilon_{231} = 1$ ,  $\epsilon_{213} = \epsilon_{321} = \epsilon_{132} = -1$ , all other components are zero).

We make use only of the *right-hand* operators grad, div, and curl, whose component forms are

$$\begin{aligned} (\text{grad } \mathbf{u})^k{}_m &= u^k{}_{,m}, & (\text{grad } \mathbf{A})^{kl}{}_m &= A^{kl}{}_{,m}, \\ \text{div } \mathbf{u} &= u^m{}_{,m}, & (\text{div } \mathbf{A})^k &= A^{km}{}_{,m}, \\ (\text{curl } \mathbf{u})^m &= \epsilon^{rsm} u_{r,s}, & (\text{curl } \mathbf{A})^{km} &= \epsilon^{rsm} A^k{}_{r,s}. \end{aligned}$$

## I. Basic Equations

The body  $\mathcal{B}$  is considered in a *current configuration* ( $k$ ) at time  $t$ .  $\mathbf{x}$  denotes the position vector and  $x^k$  the coordinates of a material particle  $X$  in this configuration.

Let

$$\mathbf{x} = \chi(X, t), \quad x^k = \chi^k(X, t), \quad (1.1)$$

describe the motion performed by the body, and

$$\mathbf{v} \equiv \dot{\mathbf{x}} \equiv \frac{\partial}{\partial t} \chi(X, t), \quad v^k \equiv \frac{\partial}{\partial t} \chi^k(X, t), \quad (1.2)$$

the particle velocity field.

We assume that the body contains dislocations. Therefore, a *global natural configuration*, that is, a stress-free configuration of the whole body, does not exist. Let  $N(X)$  denote the set of particles in a neighbourhood of the particle  $X$ . To determine the elastic deformation undergone by  $N(X)$  at time  $t$ , we may, at least in principle, cut out of the body this neighbourhood and allow it to relax. We denote by  $(\kappa)$  the *local natural configuration* obtained in this way.

We refer  $(\kappa)$  to a local frame of rectangular Cartesian co-ordinates  $\xi^\kappa$ , fixed with respect to the material. It is possible to describe now the deformation of  $N(X)$  from the local natural configuration  $(\kappa)$  to the global current configuration  $(k)$  by equations of the form<sup>1</sup>

$$x^k = x^k(\xi^\kappa),$$

where  $x^k$  and  $\xi^\kappa$  are the co-ordinates of the same particle belonging to  $N(X)$  in the configurations  $(k)$  and  $(\kappa)$ . Let

$$A^k{}_\kappa \equiv \frac{\partial x^k}{\partial \xi^\kappa} \quad (1.3)$$

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<sup>1</sup>In the presence of dislocations, such a representation is possible only locally.

denote the associated deformation gradient. We assume that, for sufficiently small neighbourhoods  $N(X)$ , the so-defined value of  $\mathbf{A}$  at  $\mathbf{x}$  and  $t$  does not depend on the choice of the neighbourhood  $N(X)$ . By repeating the same procedure for all particles and times, we define the field  $\mathbf{A}(\mathbf{x}, t)$ . We assume that  $\mathbf{A}$  is continuously differentiable and admits the inverse  $\mathbf{A}^{-1}$ , i.e.,

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{1},$$

where  $\mathbf{1}$  is the unit (metric) tensor.

As we are interested to construct a theory for anisotropic bodies, we suppose that the material has a discrete symmetry group. To simplify the formulation of the constitutive equations, we choose the local frames so that they have the same orientation with respect to the axes of material symmetry (for single crystals with respect to the crystallographic axes).

Because the local frames are fixed with respect to the material, the gradient (1.3) does not depend on the rotation of  $N(X)$ . To simplify the shifting of the tensor components from  $(k)$  to  $(\kappa)$  or inversely we may, therefore, suppose<sup>2</sup> that the local frames are rotated together with the corresponding neighbourhoods so that their axes become parallel to a time-independent rectangular Cartesian frame with axes  $z^\kappa$  (for a two-dimensional representation see fig. 1). Consequently, the shifting of the tensor components from  $(k)$  to  $(\kappa)$  and inversely may be done by using the formulae

$$L_{\cdot\cdot\cdot\kappa\cdot\cdot\cdot} g_k^{\kappa} = L_{\cdot\cdot\cdot k\cdot\cdot\cdot}, \quad L_{\cdot\cdot\cdot k\cdot\cdot\cdot} g_{\kappa}^k = L_{\cdot\cdot\cdot\kappa\cdot\cdot\cdot},$$

<sup>2</sup>For a treatment not making use of this possible simplification see [8], Appendix.

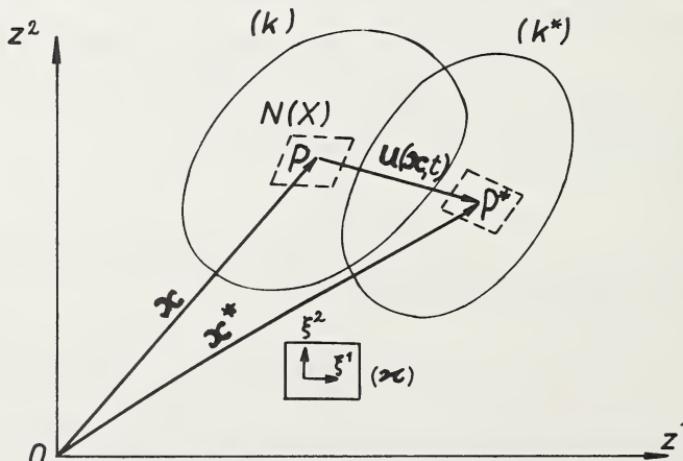


FIGURE 1. Two-dimensional representation of the superimposed motion.

where the shifters  $g_k^\kappa$  and  $g_\kappa^k$  are defined by

$$g_k^\kappa \equiv \frac{\partial z^\kappa}{\partial x^k}, \quad g_\kappa^k \equiv \frac{\partial x^k}{\partial z^\kappa}.$$

Finally, we assume that the material possesses an elastic strain energy density and is uniform, that is the strain energy density  $W$  measured per unit undeformed volume depends on the elastic distortion  $\mathbf{A}$ , but does not depend explicitly on  $X$ .

We summarize now the basic equations. For details the reader is referred to [9].

In the *static* case the field equations and the boundary conditions are:

$$\operatorname{div} \mathbf{T} + \rho \mathbf{b} = 0, \quad T^{kl}_{,l} + \rho b^k = 0, \quad (1.4)$$

$$\mathbf{T} = \mathbf{T}^T, \quad T^{kl} = T^{lk}, \quad (1.5)$$

$$\mathbf{T} = j\mathbf{A} \frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} \mathbf{A}^T, \quad T^{kl} = jA^k{}_\kappa A^l{}_\lambda \frac{\partial W(\mathbf{E})}{\partial E_{\kappa\lambda}}, \quad (1.6)$$

$$\operatorname{curl} \mathbf{A}^{-1} = -\bar{\boldsymbol{\alpha}}, \quad \epsilon^{rsm} \bar{A}^{\kappa}{}_{r,s} = -\bar{\alpha}^{\kappa m}, \quad (1.7)$$

for  $\mathbf{x} \in \mathcal{B}$ , and

$$\mathbf{T}\mathbf{n} = \mathbf{t}, \quad T^{kl} n_l = t^k, \quad (1.8)$$

for  $\mathbf{x} \in \partial \mathcal{B}$ , where  $\mathbf{T}$  is the stress tensor,

$$j = \rho / \tilde{\rho} = |\det \mathbf{A}^{-1}| = |\det \|\bar{A}^k{}_{m}\|| \quad (1.9)$$

is the ratio of the mass densities in the current and the natural configurations,

$$\mathbf{E} = (1/2)(\mathbf{A}\mathbf{A}^T - \mathbf{1}), \quad E_{\kappa\lambda} = (1/2)(g_{kl}A^k{}_\kappa A^l{}_\lambda - \delta_{\kappa\lambda}) \quad (1.10)$$

is the strain tensor,  $\mathbf{b}$  is the body force,  $\mathbf{t}$  is the surface traction,  $\bar{\boldsymbol{\alpha}}$  is the true dislocation density, and  $\partial \mathcal{B}$  is the boundary of  $\mathcal{B}$ , whose unit normal is  $\mathbf{n}$ .

Along with the true dislocation density  $\bar{\boldsymbol{\alpha}}$ , we consider the local dislocation density  $\boldsymbol{\alpha}$ , and Noll's dislocation density  $\tilde{\boldsymbol{\alpha}}$  [10]. These densities are linked by the relations

$$\boldsymbol{\alpha} = \mathbf{A}\bar{\boldsymbol{\alpha}} = j\mathbf{A}\bar{\boldsymbol{\alpha}}\mathbf{A}^T, \quad \alpha^{\kappa m} = A^k{}_\kappa \bar{\alpha}^{\kappa m} = jA^k{}_\kappa A^m{}_\mu \tilde{\alpha}^{\kappa\mu}. \quad (1.11)$$

The density  $\tilde{\alpha}$  has the remarkable property that it is invariant under a superimposed *elastic* motion, in contradistinction to  $\alpha$  and  $\tilde{\alpha}$  (see [9]).

We consider now the case of a *uniformly moving dislocation density* in an infinite medium, and in the absence of body forces.<sup>3</sup> If the dislocations move with a constant velocity  $\mathbf{V}$ , we have

$$\tilde{\alpha}(\mathbf{x}, t) = \tilde{\alpha}_0(\mathbf{x} - \mathbf{V}t), \quad (1.12)$$

where  $\tilde{\alpha}_0(x)$  is Noll's dislocation density at time  $t=0$ . The field equations are in this case

$$\operatorname{div} \mathbf{T} + \rho \mathbf{b} = \rho \dot{\mathbf{v}}, \quad T^{kl},_l + \rho b^k = \rho \dot{v}^k, \quad (1.13)$$

$$\operatorname{grad} \mathbf{v} = \alpha \times (\mathbf{v} - \mathbf{V}) + \dot{\mathbf{A}} \mathbf{A}^{-1},$$

$$v^k,_r = \epsilon_{tsr} \alpha^{kt} (v^s - V^s) + \dot{A}^k{}_\kappa A^{\kappa r}, \quad (1.14)$$

$$\mathbf{T} = j \mathbf{A} \frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} \mathbf{A}^T, \quad T^{kl} = j A^k{}_\kappa A^l{}_\lambda \frac{\partial W(\mathbf{E})}{\partial E_{\kappa\lambda}}, \quad (1.15)$$

$$\operatorname{curl} \mathbf{A}^{-1} = -\tilde{\alpha} = -j \tilde{\alpha}_0(\mathbf{x} - \mathbf{V}t) \mathbf{A}^T,$$

$$\epsilon^{rsm} \dot{A}^k{}_{r,s} = -\tilde{\alpha}^{\kappa m} = -j \tilde{\alpha}_0^{\kappa\mu}(\mathbf{x} - \mathbf{V}t) A^m{}_\mu \quad (1.16)$$

for  $\mathbf{x} \in E$ , where  $E$  is the Euclidean three-dimensional space.

By making use of the relation

$$\operatorname{div} (j \mathbf{A}^T) = js, \quad \epsilon_{\lambda\mu\nu} (j A^l{}_\lambda),_l = js_\lambda, \quad (1.17)$$

where

$$s \equiv \operatorname{cr} \tilde{\alpha}, \quad s_\lambda \equiv \epsilon_{\lambda\mu\nu} \tilde{\alpha}^{\mu\nu}, \quad (1.18)$$

the equation of motion (1.12) may be also written as

$$\tilde{\operatorname{div}} \tilde{\mathbf{T}} + \tilde{\mathbf{T}} s + \tilde{\rho} \mathbf{b} = \tilde{\rho} \dot{\mathbf{v}}, \quad \tilde{T}^{k\lambda},_\lambda + \tilde{T}^{k\lambda} s_\lambda + \tilde{\rho} b^k = \tilde{\rho} \dot{v}^k. \quad (1.19)$$

Here  $\tilde{\operatorname{div}}$  denotes the divergence with respect to the (local) Cartesian co-ordinates and  $;\lambda$  denotes the total covariant derivative. For fields that depend only on  $\mathbf{x}$  and for local Cartesian co-ordinates we have ([8], Appendix)

$$(\quad)_{;\lambda} \equiv (\quad)_{,l} A^l{}_\lambda, \quad (1.20)$$

$\tilde{\mathbf{T}}$  represents the first Piola-Kirchoff stress tensor given by

$$\mathbf{T} = j \tilde{\mathbf{T}} \mathbf{A}^T, \quad T^{kl} = j \tilde{T}^{k\lambda} A^l{}_\lambda. \quad (1.21)$$

<sup>3</sup>For a finite body and in the presence of body forces, the hypothesis that the dislocations move with a constant velocity would not be realistic.

The form (1.19) of the equation of motion was derived for the first time by Noll [10]. A derivation in component form of the relations (1.17) and (1.19) is given in Appendix 1.

Finally we give another form of the boundary conditions (1.8) in terms of the first Piola-Kirchoff stress tensor  $\bar{\mathbf{T}}$ . Let  $\mathbf{n} ds$  be an oriented material surface element in the current configuration. By releasing a material neighbourhood of the surface element, the magnitude and the orientation of the vector  $\mathbf{n} ds$  will change to  $\tilde{\mathbf{n}} d\tilde{s}$ , say, and we have:

$$\tilde{\mathbf{n}} d\tilde{s} = j \mathbf{A}^T \mathbf{n} ds, \quad \tilde{n}_\lambda d\tilde{s} = j A^l_\lambda n_l ds. \quad (1.22)$$

Substituting (1.22) into (1.8) gives

$$\bar{\mathbf{T}} \tilde{\mathbf{n}} = \bar{\mathbf{t}}, \quad \bar{T}^{k\lambda} n_\lambda = \bar{t}^k, \quad (1.23)$$

where

$$\bar{\mathbf{t}} \equiv \mathbf{t} ds/d\tilde{s}, \quad \bar{t}^k \equiv t^k ds/d\tilde{s}. \quad (1.24)$$

## II. The Solution of the Linearized System for an Infinite Medium

To linearize the system of field equations, we write

$$\mathbf{A} = \mathbf{1} + \boldsymbol{\beta} \quad (2.1)$$

and assume that  $\boldsymbol{\alpha}$ ,  $\boldsymbol{\beta}$ ,  $\mathbf{b}$ , and  $\mathbf{v}$  are “small.” By neglecting the products of these quantities we get from (1.4) and (1.9)–(1.11)

$$\mathbf{A}^{-1} \approx \mathbf{1} - \boldsymbol{\beta}, \quad j \approx 1 - \text{tr } \boldsymbol{\beta}, \quad (2.2)$$

$$\mathbf{E} \approx (1/2)(\boldsymbol{\beta} + \boldsymbol{\beta}^T), \quad \boldsymbol{\alpha} \approx \bar{\boldsymbol{\alpha}} \approx \tilde{\boldsymbol{\alpha}}. \quad (2.3)$$

We assume also that  $\partial W(\mathbf{E})/\partial \mathbf{E}$  may be developed into a power series with respect to  $\mathbf{E}$ , whose coefficients are the elasticities of different orders

$$\frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} = \mathbf{L}_2[\mathbf{E}] + \frac{1}{2} \mathbf{L}_3[\mathbf{E}, \mathbf{E}] + \dots$$

As  $\mathbf{E}$  is symmetric we may suppose  $\mathbf{L}_2[\mathbf{A}] = \mathbf{L}_2[\mathbf{A}^T]$  for every second-order tensor  $\mathbf{A}$ . Consequently, the last two equations give

$$\frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} \approx \mathbf{L}_2[\boldsymbol{\beta}].$$

Substituting this relation and (2.2) into (1.6) yields

$$\mathbf{T} \approx \mathbf{L}_2[\boldsymbol{\beta}]. \quad (2.4)$$

Furthermore, we have

$$\rho \mathbf{b} = j \tilde{\rho} \mathbf{b} \approx \tilde{\rho} \mathbf{b}, \quad (2.5)$$

$$\dot{\mathbf{v}} = \frac{\partial \mathbf{v}}{\partial t} + (\text{grad } \mathbf{v}) \mathbf{v} \approx \frac{\partial \mathbf{v}}{\partial t}. \quad (2.6)$$

We consider the case of an infinite elastic medium  $E$  and assume

$$|\mathbf{T}| \rightarrow 0, \text{ as } |\mathbf{x}| \rightarrow \infty. \quad (2.7)$$

In the *static* case, we introduce (2.2), (2.4), and (2.5) into (1.4) and (1.7), so obtaining

$$\text{div } \mathbf{L}_2[\boldsymbol{\beta}] + \tilde{\rho} \mathbf{b} = 0, \quad (2.8)$$

$$\text{curl } \boldsymbol{\beta} = \boldsymbol{\alpha}. \quad (2.9)$$

The component form of this system, in Cartesian co-ordinates, is

$$\frac{L_{k l m n}}{2} \beta_{m n, l} + \tilde{\rho} b_k = 0, \quad (2.10)$$

$$\in_{p s t} \beta_{m p, s} = \alpha_{m t}, \quad (2.11)$$

where  $,l$  denotes now simply the partial derivative with respect to  $x_l$ . From (2.11) we have

$$\beta_{m r, n} - \beta_{m n, r} = \in_{r n t} \alpha_{m t}. \quad (2.12)$$

By differentiating (2.10) with respect to  $x_r$  and taking into account the last relation we obtain

$$\frac{L_{k l m n}}{2} \beta_{m r, n l} + \tilde{\rho} b_{k, r} - \frac{L_{k l m n}}{2} \in_{r n t} \alpha_{m t, l} = 0. \quad (2.13)$$

If the static Green's tensor function  $\mathbf{G}(\mathbf{x} - \mathbf{x}')$ , that is the solution of the equation

$$\frac{L_{k l m n}}{2} G_{m p, n l}(\mathbf{x} - \mathbf{x}') + \delta_{k p} \delta(\mathbf{x} - \mathbf{x}') = 0, \quad (2.14)$$

with the boundary condition (2.7), is known for the material considered, then the solution of (2.13) is given by

$$\beta_{m r}(\mathbf{x}) = \int_E \{ \tilde{\rho} b_{p, r'}(\mathbf{x}') + \frac{L_{p l q n}}{2} \in_{n r t} \alpha_{q t, l'}(\mathbf{x}') \} G_{m p}(\mathbf{x} - \mathbf{x}') dV', \quad (2.15)$$

where  $,l'$  denotes the partial derivative with respect to  $x'_l$ . Integrating in (2.15) by parts and taking into consideration that  $G_{kr}(\mathbf{x} - \mathbf{x}') \rightarrow 0$  as  $|\mathbf{x}'| \rightarrow \infty$  for all finite  $\mathbf{x}$ , we may write (2.15) also as

$$\begin{aligned} \beta_{mr}(\mathbf{x}) = & \int_E \{ \tilde{\rho} b_p(\mathbf{x}') G_{mp,r}(\mathbf{x} - \mathbf{x}') \\ & + \frac{L_{ptqn}}{2} \in_{nrt} \alpha_{qt}(\mathbf{x}') G_{mp,t}(\mathbf{x} - \mathbf{x}') \} dV'. \end{aligned}$$

The solution of the system (2.10), (2.11) in the presence of body forces by means of Green's function was given for the first time by Willis[11].

In the case of a *uniformly moving dislocation density*, we introduce (2.2)<sub>1</sub>, (2.5), and (2.6) into (1.13), (1.15), and (1.16), and assume  $\mathbf{b} = 0$ . In this way we obtain

$$\operatorname{div} \mathbf{L}_2[\boldsymbol{\beta}] = \tilde{\rho} \partial \mathbf{v} / \partial t, \quad (2.17)$$

$$\operatorname{grad} \mathbf{v} = -\boldsymbol{\alpha} \times \mathbf{V} + \partial \boldsymbol{\beta} / \partial t, \quad (2.18)$$

$$\operatorname{curl} \boldsymbol{\beta} = \boldsymbol{\alpha}, \quad \boldsymbol{\alpha}(\mathbf{x}, t) = \boldsymbol{\alpha}_0(\mathbf{x} - \mathbf{V}t). \quad (2.19)$$

The component form of this system, in Cartesian co-ordinates,<sup>4</sup> is

$$\frac{L_{klmn}}{2} \beta_{mn,l} = \tilde{\rho} \partial v_k / \partial t, \quad (2.20)$$

$$v_{k,r} = -\in_{ntr} \alpha_{kt} V_n + \partial \beta_{kr} / \partial t, \quad (2.21)$$

$$\in_{pst} \beta_{mp,s} = \alpha_{mt}, \quad \alpha_{mt}(\mathbf{x}, t) = \alpha_{mt}^0(\mathbf{x} - \mathbf{V}t). \quad (2.22)$$

In order to separate the unknowns  $\mathbf{v}$  and  $\boldsymbol{\beta}$ , we differentiate first (2.20) with respect to  $x_r$  and eliminate  $\mathbf{v}$  between the equation obtained and (2.21). We have then

$$\frac{L_{klmn}}{2} \beta_{mn,lr} - \tilde{\rho} \partial^2 \beta_{kr} / \partial t^2 = -\tilde{\rho} \in_{ntr} V_n \partial \alpha_{kt}^0 / \partial t.$$

In view of (2.12) this equation becomes

$$\frac{L_{klmn}}{2} \beta_{mr,rl} - \tilde{\rho} \partial^2 \beta_{kr} / \partial t^2 = -\frac{L_{klmn}}{2} \in_{nrt} \alpha_{mt,t}^0 - \tilde{\rho} \in_{ntr} V_n \partial \alpha_{kt}^0 / \partial t. \quad (2.23)$$

Furthermore, we differentiate (2.20) with respect to  $t$ , and eliminate  $\boldsymbol{\beta}$  between the equation resulted and (2.21), so obtaining

$$\frac{L_{klmn}}{2} v_{m,nt} - \tilde{\rho} \partial^2 v_k / \partial t^2 = -\frac{\bar{L}_{klmn}}{2} \in_{nts} \alpha_{mt,l}^0 V_s. \quad (2.24)$$

<sup>4</sup> When using the component form of tensor equations we write for convenience non-tensorial subscripts, e.g., 2, 0, P, under the kernel index or as superscripts, and non-tensorial superscripts, e.g., -1, above the kernel index.

As the right-hand sides of eqs (2.23) and (2.24) depend only on  $\mathbf{x} - \mathbf{V}t$ , there will be solutions  $\beta(\mathbf{x}, t)$ ,  $\mathbf{v}(\mathbf{x}, t)$  that depend also only on the combination  $\mathbf{x} - \mathbf{V}t$ . We may simplify these equations by introducing the new variable

$$\mathbf{y} = \mathbf{x} - \mathbf{V}t \quad (2.25)$$

and, observing that for an arbitrary scalar or tensor function  $\Psi(\mathbf{x} - \mathbf{V}t)$

$$\Psi_{,l} = \partial\Psi/\partial y_l, \quad \partial\Psi/\partial t = -V_l \partial\Psi/\partial y_l. \quad (2.26)$$

It then follows

$$\begin{aligned} \left( L_{klmn} - \tilde{\rho} V_l V_n \delta_{km} \right) \frac{\partial^2 \beta_{mr}}{\partial y_l \partial y_n} \\ + \left( L_{klmn} - \tilde{\rho} V_l V_n \delta_{km} \right) \in_{nrt} \frac{\partial \alpha_{mt}^0}{\partial y_l} = 0, \end{aligned} \quad (2.27)$$

$$\left( L_{klmn} - \tilde{\rho} V_l V_n \delta_{km} \right) \frac{\partial^2 v_k}{\partial y_l \partial y_n} + L_{klmn} \in_{snt} \frac{\partial \alpha_{mt}^0}{\partial y_l} V_s = 0. \quad (2.28)$$

Assume we know the static Green's function  $\bar{G}(\mathbf{y} - \mathbf{y}')$  for the infinite medium with the "apparent" elastic constants  $L_{klmn} - \tilde{\rho} V_l V_n \delta_{km}$ , i.e., the solution of the equation

$$\left( L_{klmn} - \tilde{\rho} V_l V_n \delta_{km} \right) \frac{\partial^2 \bar{G}_{mp}}{\partial y_n \partial y_l} (\mathbf{y} - \mathbf{y}') + \delta_{kp} \delta(\mathbf{y} - \mathbf{y}') = 0. \quad (2.29)$$

We may then write the solutions of eqs (2.27) and (2.28) as

$$\beta_{mr}(\mathbf{y}) = \int_E \left( L_{plqn} - \tilde{\rho} V_l V_n \delta_{pq} \right) \in_{nrt} \frac{\partial \alpha_{qt}^0}{\partial y_l'} (\mathbf{y}') \bar{G}_{mp}(\mathbf{y} - \mathbf{y}') dV', \quad (2.30)$$

$$v_m(\mathbf{y}) = \int_E L_{plqn} \in_{snt} V_s \frac{\partial \alpha_{qt}^0}{\partial y_l'} (\mathbf{y}') \bar{G}_{mp}(\mathbf{y} - \mathbf{y}') dV'. \quad (2.31)$$

Integrating by parts and taking into consideration that  $\bar{G}(\mathbf{y} - \mathbf{y}') \rightarrow 0$  as  $|\mathbf{y}'| \rightarrow 0$  for all finite  $\mathbf{y}$ , we have also

$$\beta_{mr}(\mathbf{y}) = \int_E \left( L_{plqn} - \tilde{\rho} V_l V_n \delta_{pq} \right) \in_{nrt} \alpha_{qt}^0(\mathbf{y}') \frac{\partial \bar{G}_{mp}}{\partial y_l} (\mathbf{y} - \mathbf{y}') dV', \quad (2.32)$$

$$v_m(\mathbf{y}) = \int_E L_{plqn} \in_{snt} V_s \alpha_{qt}^0(\mathbf{y}') \frac{\partial \bar{G}_{mp}}{\partial y_l} (\mathbf{y} - \mathbf{y}') dV'. \quad (2.33)$$

The solution of eq (2.29) was recently obtained for an isotropic medium by Beltz, Davis, and Malén [12]. If  $|\mathbf{V}|$  is small in comparison with the smallest sound velocity of the medium,  $c_{\min}$ , the Green's functions may be obtained from the usual static Green functions by developing in (2.29) the apparent elastic constants in a power series with respect to  $|\mathbf{V}|/c$ , where  $c$  is an appropriately chosen sound velocity, as has been done by Kosevich [13] and Kosevich and Natsik [14].

### III. The Solution of the Non-Linear Problem in the Static Case

We begin the solving of non-linear problems by summarizing and generalizing Willis' scheme [12] for the determination of the stresses generated by a known time-independent dislocation density in an anisotropic elastic body  $\mathcal{B}$ , free of body forces and surface tractions.<sup>5</sup> As mentioned in section I, the basic static field equations for  $\mathbf{b} = \mathbf{t} = 0$  are

$$\operatorname{div} \mathbf{T} = 0, \quad (3.1)$$

$$\mathbf{T} = j\mathbf{A} \frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} \mathbf{A}^T, \quad (3.2)$$

$$\mathbf{E} = (1/2)(\mathbf{A}^T \mathbf{A} - \mathbf{I}), \quad (3.3)$$

$$j = |\det \mathbf{A}^{-1}|, \quad \mathbf{A} \mathbf{A}^{-1} = \mathbf{I}, \quad (3.4)$$

$$\operatorname{curl} \mathbf{A}^{-1} = -\bar{\boldsymbol{\alpha}} = -\mathbf{A}^{-1} \boldsymbol{\alpha}, \quad (3.5)$$

$$\operatorname{div} \bar{\boldsymbol{\alpha}} = \operatorname{div} (\mathbf{A}^{-1} \boldsymbol{\alpha}) = 0, \quad (3.6)$$

for  $\mathbf{x} \in \mathcal{B}$ , and

$$\mathbf{T} \mathbf{n} = 0, \text{ for } \mathbf{x} \in \partial \mathcal{B}. \quad (3.7)$$

In order to obtain a definite algorithm for the solving of this traction boundary-value problem we introduce now the following hypotheses:

**HYPOTHESIS H<sub>1</sub>.** The true dislocation density is known, depends analytically on a small parameter  $\epsilon$ ,  $0 < \epsilon \ll 1$ , and vanishes when  $\epsilon = 0$ , that is

$$\bar{\boldsymbol{\alpha}} = \sum_{n=1}^{\infty} \epsilon^n \bar{\boldsymbol{\alpha}}_n. \quad (3.8)$$

Each term of the expansion (3.8) satisfies the compatibility condition (3.6), that is

$$\operatorname{div} \bar{\boldsymbol{\alpha}}_n = 0, \quad n = 1, 2, \dots \quad (3.9)$$

<sup>5</sup>This scheme adapts in fact to the continuum theory of dislocations an approximate method originally proposed in the non-linear theory of elasticity by Signorini (see e.g. [7], Sect. 6.3).

The difference in magnitude between the terms of the expansion (3.8) may be used, for example, to distinguish the dislocation densities produced by different glide systems. In practical calculations only the first one or two terms of the expansion will be retained.

If, instead of the true dislocation density  $\bar{\alpha}$ , the local dislocation density  $\alpha$  is given, we assume similarly that

$$\alpha = \sum_{n=1}^{\infty} \epsilon^n \alpha_n, \quad (3.10)$$

but the compatibility condition (3.9) takes a more intricate form resulting from (3.6) by equating to zero the divergence of the coefficients in the expansion of  $\mathbf{A}^{-1}\alpha$ .

HYPOTHESIS H<sub>2</sub>. There exists a solution  $\mathbf{A}$  of the boundary-value problem which depends analytically on  $\epsilon$  and reduces to  $\mathbf{1}$  when  $\epsilon=0$ , that is

$$\mathbf{A} = \mathbf{1} + \boldsymbol{\beta}, \quad \boldsymbol{\beta} = \sum_{n=1}^{\infty} \epsilon^n \boldsymbol{\beta}_n.$$

We assume that  $|\boldsymbol{\beta}| \ll 1$ , so that  $\epsilon$  is naturally related to the magnitude of  $\boldsymbol{\beta}$ .

HYPOTHESIS H<sub>3</sub>. The strain energy density  $W$  may be developed into a power series with respect to the strain tensor  $\mathbf{E}$ . The coefficients of this series are the elasticities of different orders. More exactly, we assume that

$$\frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} = \mathbf{L}_2[\mathbf{E}] + (1/2)\mathbf{L}_3[\mathbf{E}, \mathbf{E}] + (1/6)\mathbf{L}_4[\mathbf{E}, \mathbf{E}, \mathbf{E}] + \dots, \quad (3.11)$$

where  $\mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_{k-1}]$ ,  $k=2, 3, \dots$ , are multilinear tensor functions having the following properties of symmetry:

$$\begin{aligned} \mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_l, \dots, \mathbf{A}_m, \dots, \mathbf{A}_{k-1}] \\ = \mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_m, \dots, \mathbf{A}_l, \dots, \mathbf{A}_{k-1}], \end{aligned} \quad (3.12)$$

$$\begin{aligned} \mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_l, \dots, \mathbf{A}_{k-1}] &= \mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_l^T, \dots, \mathbf{A}_{k-1}] \\ &= \mathbf{L}_k[\mathbf{A}_1, \dots, (1/2)(\mathbf{A}_l + \mathbf{A}_l^T), \dots, \mathbf{A}_{k-1}], \end{aligned} \quad (3.13)$$

$$\mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_{k-1}] \mathbf{B} = \mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_{k-1}] \mathbf{B}^T, \quad (3.14)$$

and the property of linearity with respect to each argument:

$$\begin{aligned} \mathbf{L}_k[\mathbf{A}_1, \dots, p\mathbf{A}_l' + q\mathbf{A}_l'', \dots, \mathbf{A}_{k-1}] &= p\mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_l', \dots, \mathbf{A}_{k-1}] \\ &+ q\mathbf{L}_k[\mathbf{A}_1, \dots, \mathbf{A}_l'', \dots, \mathbf{A}_{k-1}], \end{aligned} \quad (3.15)$$

where  $p$  and  $q$  are arbitrary scalars.  $\mathbf{L}_k$  is the tensor of the elasticities of the  $k$ th order. The component form of (3.11) is

$$\frac{\partial W}{\partial E_{\kappa\lambda}} = \frac{1}{2} L_2^{\kappa\lambda\mu\nu} E_{\mu\nu} + (1/2) L_3^{\kappa\lambda\mu\nu\sigma\tau} E_{\mu\nu} E_{\sigma\tau} + (1/6) L_4^{\kappa\lambda\mu\nu\sigma\tau\rho\varphi} E_{\mu\nu} E_{\sigma\tau} E_{\rho\varphi} + \dots \quad (3.16)$$

Substitution of (3.10) into (3.3) and (3.4) shows that  $\mathbf{E}$ ,  $j$ , and  $\mathbf{A}^{-1}$  depend analytically on  $\epsilon$ , and gives for the first terms of the expansions:

$$\begin{aligned} \mathbf{E} = & (1/2) \epsilon (\boldsymbol{\beta}_1 + \boldsymbol{\beta}_1^T) + (1/2) \epsilon^2 (\boldsymbol{\beta}_2 + \boldsymbol{\beta}_2^T + \boldsymbol{\beta}_1^T \boldsymbol{\beta}_1) \\ & + (1/2) \epsilon^3 (\boldsymbol{\beta}_3 + \boldsymbol{\beta}_3^T + \boldsymbol{\beta}_1^T \boldsymbol{\beta}_2 + \boldsymbol{\beta}_2^T \boldsymbol{\beta}_1) + \dots \end{aligned} \quad (3.17)$$

$$j = 1 - \epsilon \text{tr} \boldsymbol{\beta}_1 + \epsilon^2 \{ (1/2) (\text{tr} \boldsymbol{\beta}_1)^2 + (1/2) \text{tr} \boldsymbol{\beta}_1^2 - \text{tr} \boldsymbol{\beta}_2 \} + \dots \quad (3.18)$$

$$\mathbf{A}^{-1} = \mathbf{I} - \epsilon \boldsymbol{\beta}_1 - \epsilon^2 (\boldsymbol{\beta}_2 - \boldsymbol{\beta}_1^2) - \epsilon^3 (\boldsymbol{\beta}_3 - \boldsymbol{\beta}_1 \boldsymbol{\beta}_2 - \boldsymbol{\beta}_2 \boldsymbol{\beta}_1 + \boldsymbol{\beta}_1^3) + \dots \quad (3.19)$$

By introducing (3.17)–(3.19) into (3.2) and taking into account (3.11) and the properties (3.12)–(3.15), we see that the stress tensor  $\mathbf{T}$  depends analytically on  $\epsilon$ , namely

$$\mathbf{T} = \epsilon \mathbf{T}_1 + \epsilon^2 \mathbf{T}_2 + \epsilon^3 \mathbf{T}_3 + \dots \quad (3.20)$$

$$\begin{aligned} \mathbf{T}_1 &= \mathbf{L}_2[\boldsymbol{\beta}_1], \\ \mathbf{T}_2 &= \mathbf{L}_2[\boldsymbol{\beta}_2] + \mathfrak{T}_2(\boldsymbol{\beta}_1), \\ \mathbf{T}_3 &= \mathbf{L}_2[\boldsymbol{\beta}_3] + \mathfrak{T}_3(\boldsymbol{\beta}_1, \boldsymbol{\beta}_2), \end{aligned} \quad (3.21)$$

and in general

$$\mathbf{T}_n = \mathbf{L}_2[\boldsymbol{\beta}_n] + \mathfrak{T}_n(\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_{n-1}), \quad (3.22)$$

where  $\mathfrak{T}_n$  is a known tensor function of its variables. In particular

$$\begin{aligned} \mathfrak{T}_2(\boldsymbol{\beta}_1) &= -(\text{tr} \boldsymbol{\beta}_1) \mathbf{T}_1 + \boldsymbol{\beta}_1 \mathbf{T}_1 + \mathbf{T}_1 \boldsymbol{\beta}_1^T + (1/2) \mathbf{L}_2[\boldsymbol{\beta}_1^T \boldsymbol{\beta}_1] + (1/2) \mathbf{L}_3[\boldsymbol{\beta}_1, \boldsymbol{\beta}_1], \\ & \quad (3.23) \end{aligned}$$

$$\begin{aligned} \mathfrak{T}_3(\boldsymbol{\beta}_1, \boldsymbol{\beta}_2) &= \{ 1/2 \text{tr} \boldsymbol{\beta}_1^2 - 1/2 (\text{tr} \boldsymbol{\beta}_1)^2 - \text{tr} \boldsymbol{\beta}_2 \} \mathbf{T}_1 + \{ (\text{tr} \boldsymbol{\beta}_1) \boldsymbol{\beta}_1 - \boldsymbol{\beta}_1^2 + \boldsymbol{\beta}_2 \} \mathbf{T}_1 \\ & + \mathbf{T}_1 \{ (\text{tr} \boldsymbol{\beta}_1) \boldsymbol{\beta}_1^T - (\boldsymbol{\beta}_1^T)^2 + \boldsymbol{\beta}_2^T \} - \boldsymbol{\beta}_1 \mathbf{T}_1 \boldsymbol{\beta}_1^T - (\text{tr} \boldsymbol{\beta}_1) \mathbf{T}_2 + \boldsymbol{\beta}_1 \mathbf{T}_2 + \mathbf{T}_2 \boldsymbol{\beta}_1^T \\ & + \mathbf{L}_2[\boldsymbol{\beta}_1^T \boldsymbol{\beta}_1] + \mathbf{L}_3[\boldsymbol{\beta}_1, \boldsymbol{\beta}_2 + (1/2) \boldsymbol{\beta}_1^T \boldsymbol{\beta}_1] + (1/6) \mathbf{L}_4[\boldsymbol{\beta}_1, \boldsymbol{\beta}_1, \boldsymbol{\beta}_1]. \end{aligned} \quad (3.24)$$

Substituting of the series (3.8) or (3.16), (3.19), and (3.20) into (3.1), (3.4), and (3.7), and then equating equal powers of  $\epsilon$  yields the following

successive systems of differential equations and associated boundary conditions ( $n = 1, 2, \dots$ )

$$\begin{aligned} \operatorname{div} \mathbf{L}_2[\boldsymbol{\beta}_n] + \operatorname{div} \mathfrak{T}_n(\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_{n-1}) &= 0, \\ \operatorname{curl} \boldsymbol{\beta}_n &= \mathfrak{A}_n(\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_{n-1}; \boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_{n-1}), \\ \mathbf{L}_2[\boldsymbol{\beta}_n] \mathbf{n} &= -\mathfrak{T}_n(\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_{n-1}) \mathbf{n}, \end{aligned} \quad (3.25)$$

where  $\mathfrak{A}_n$  is a known tensor function of its variables. The boundary-value problem obtained in the  $n$ th stage is obviously linear with respect to  $\boldsymbol{\beta}_n$ . For an infinite medium this problem may be solved by means of Green's tensor functions, as indicated in the preceding section. For a finite body, the boundary-value problem reduces to a usual traction boundary-value problem in the infinitesimal theory of elasticity if we can find<sup>6</sup> a particular solution  $\hat{\boldsymbol{\beta}}_n$  of eq (3.25)<sub>2</sub>. We have then

$$\boldsymbol{\beta}_n = \hat{\boldsymbol{\beta}}_n + \operatorname{grad} \mathbf{U}_n, \quad (3.26)$$

where  $\mathbf{U}_n$  is an arbitrary vector field. Substitution of (3.26) into (3.25) gives an usual linear boundary-value problem for the associated "displacement" field  $\mathbf{U}_n$ .

We write now explicitly the systems (3.25) for  $n = 1, 2, 3$ .

*First step*

$$\begin{aligned} \operatorname{div} \mathbf{L}_2[\boldsymbol{\beta}_1] &= 0, \\ \mathbf{L}_2[\boldsymbol{\beta}_1] \mathbf{n} &= 0, \\ \operatorname{curl} \boldsymbol{\beta}_1 &= \bar{\boldsymbol{\alpha}}_1 = \boldsymbol{\alpha}_1. \end{aligned}$$

*Second step*

$$\begin{aligned} \operatorname{div} \mathbf{L}_2[\boldsymbol{\beta}_2] + \operatorname{div} \mathfrak{T}_2(\boldsymbol{\beta}_1) &= 0, \\ \mathbf{L}_2[\boldsymbol{\beta}_2] \mathbf{n} &= -\mathfrak{T}_2(\boldsymbol{\beta}_1) \mathbf{n}, \\ \operatorname{curl} \boldsymbol{\beta}_2 &= \operatorname{curl} \boldsymbol{\beta}_1^2 + \bar{\boldsymbol{\alpha}}_2 = \operatorname{curl} \boldsymbol{\beta}_1^2 + \boldsymbol{\alpha}_2 - \boldsymbol{\beta}_1 \boldsymbol{\alpha}_1. \end{aligned}$$

<sup>6</sup>This could be done, for instance, by extending  $\bar{\boldsymbol{\alpha}}_n$  continuously differentiable through the boundary  $\partial\mathcal{B}$  to the whole space, and by using Green's functions for infinite media.

*Third step*

$$\operatorname{div} \mathbf{L}_2[\boldsymbol{\beta}_3] + \operatorname{div} \mathfrak{T}_3(\boldsymbol{\beta}_1, \boldsymbol{\beta}_2) = 0,$$

$$\mathbf{L}_2[\boldsymbol{\beta}_3]\mathbf{n} = -\mathfrak{T}_3(\boldsymbol{\beta}_1, \boldsymbol{\beta}_2)\mathbf{n},$$

$$\begin{aligned} \operatorname{curl} \boldsymbol{\beta}_3 &= \operatorname{curl} (\boldsymbol{\beta}_1 \boldsymbol{\beta}_2 + \boldsymbol{\beta}_2 \boldsymbol{\beta}_1 - \boldsymbol{\beta}_1^3) + \bar{\alpha}_3 \\ &= \operatorname{curl} (\boldsymbol{\beta}_1 \boldsymbol{\beta}_2 + \boldsymbol{\beta}_2 \boldsymbol{\beta}_1 - \boldsymbol{\beta}_1^3) + \alpha_3 - \boldsymbol{\beta}_1 \alpha_2 - (\boldsymbol{\beta}_2 - \boldsymbol{\beta}_1^2) \alpha_1. \end{aligned}$$

In the above systems,  $\mathfrak{T}_2(\boldsymbol{\beta}_1)$  and  $\mathfrak{T}_3(\boldsymbol{\beta}_1, \boldsymbol{\beta}_2)$  must be replaced by their expressions (3.23) and (3.24). At present, only elasticities of second and third order have been determined experimentally, in general for single crystals belonging to the cubic system or to one of the hexagonal subsystems with higher symmetry. Consequently, we are interested to write down explicitly the equations of the first two stages of approximation for these crystal classes. Inspection of the relation (3.23) shows that it is sufficient to know the components of the tensor-valued functions  $\mathbf{L}_2[\mathbf{A}]$ ,  $\mathbf{L}_3[\mathbf{A}, \mathbf{B}]$ . Since these functions appear frequently in the present paper, we give in Appendix 2 their components in Cartesian co-ordinates for cubic crystals and for hexagonal crystals with higher symmetry, that is for the crystallographic subsystems 6, 7, 10, and 11, in the classification given by Dana and Hurlbut [15], which is nowadays generally employed in continuum mechanics.

For isotropic materials we have for general curvilinear co-ordinates

$$\mathbf{L}_2[\mathbf{A}] = \frac{1}{2} g^{kl} A_{mn} + 2\mu A^{(kl)}, \quad (3.27)$$

$$\mathbf{L}_3[\mathbf{A}, \mathbf{B}] = \nu_1 g^{kl} A_{mn} B_{n}^{m} + 2\nu_2 (g^{kl} A_{(mn)} B^{(mn)} + A_{m}^{m} B^{(kl)}), \quad (3.28)$$

where  $g^{kl}$  are the contravariant components of the metric tensor,  $\lambda$  and  $\mu$  are Lamé's constants, and  $\nu_1$ ,  $\nu_2$ ,  $\nu_3$  are the elastic constants of the third order introduced by Toupin and Bernstein [16].

#### IV. The Solution of the Non-Linear Problem for Uniformly Moving Dislocations

We consider now a uniformly moving dislocation density in an infinite elastic medium free of body forces. As mentioned in section I, the basic field equations are in this case:

$$\operatorname{div} \mathbf{T} = \rho \dot{\mathbf{v}}, \quad (4.1)$$

$$\text{grad } \mathbf{v} = \boldsymbol{\alpha} \times (\mathbf{v} - \mathbf{V}) + \dot{\mathbf{A}} \mathbf{A}^{-1}, \quad (4.2)$$

$$\mathbf{T} = j\mathbf{A} \frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} \mathbf{A}^T, \quad (4.3)$$

$$\mathbf{E} = (1/2)(\mathbf{A}^T \mathbf{A} - \mathbf{1}), \quad (4.4)$$

$$j = |\det \mathbf{A}^{-1}| = \rho/\tilde{\rho}, \quad \mathbf{A} \mathbf{A}^{-1} = \mathbf{1}, \quad (4.5)$$

$$\text{curl } \mathbf{A}^{-1} = -\tilde{\boldsymbol{\alpha}}(\mathbf{x}, t) = -j\tilde{\boldsymbol{\alpha}}(\mathbf{x}, t) \mathbf{A}^T = -j\tilde{\boldsymbol{\alpha}}_0(\mathbf{x} - \mathbf{V}t) \mathbf{A}^T, \quad (4.6)$$

$$\text{div } \tilde{\boldsymbol{\alpha}} = \text{div } (j\tilde{\boldsymbol{\alpha}} \mathbf{A}^T) = 0. \quad (4.7)$$

The last but one relation expresses the fact that the dislocations are moving with a *constant* velocity  $\mathbf{V}$ , so that (1.12) holds. For the local and the true dislocation densities we cannot write relations similar to (1.12) because they do depend on the elastic distortion.

We attempt to set up an algorithm for the determination of the solution, similar to that presented in section III for the static case. To this end we keep the hypothesis  $H_3$  in the form adopted for the static case, but modify  $H_1$  and  $H_2$  so as to allow for dynamic effects:

**HYPOTHESIS  $H'_1$ .** Noll's dislocation density is known at time  $t=0$  as  $\tilde{\boldsymbol{\alpha}}_0(\mathbf{x})$ , and moves with a constant velocity  $\mathbf{V}$ , so that

$$\tilde{\boldsymbol{\alpha}}(\mathbf{x}, t) = \tilde{\boldsymbol{\alpha}}_0(\mathbf{x} - \mathbf{V}t). \quad (4.8)$$

$\tilde{\boldsymbol{\alpha}}_0(\mathbf{x})$  depends analytically on a parameter  $\epsilon$  and vanishes when  $\epsilon=0$ , that is

$$\tilde{\boldsymbol{\alpha}}_0(\mathbf{x} - \mathbf{V}t) = \sum_{n=1}^{\infty} \epsilon^n \tilde{\boldsymbol{\alpha}}_n(\mathbf{x} - \mathbf{V}t). \quad (4.9)$$

Each term of the expansion of  $\tilde{\boldsymbol{\alpha}} = j\tilde{\boldsymbol{\alpha}}_0 \mathbf{A}^T$  satisfies the compatibility condition (4.7).

**HYPOTHESIS  $H'_2$ .** There exists a solution  $\mathbf{A}(\mathbf{x} - \mathbf{V}t)$ ,  $\mathbf{v}(\mathbf{x} - \mathbf{V}t)$  of the problem which depends analytically on  $\epsilon$  and reduces to  $\mathbf{1}$  respectively  $\mathbf{0}$  when  $\epsilon=0$ , that is

$$\mathbf{A} = \mathbf{1} + \boldsymbol{\beta}, \quad \boldsymbol{\beta} = \sum_{n=1}^{\infty} \epsilon^n \boldsymbol{\beta}_n, \quad (4.10)$$

$$\mathbf{v} = \sum_{n=1}^{\infty} \epsilon^n \mathbf{v}_n. \quad (4.11)$$

By making use of (4.9), (4.10), and (3.18) we get

$$\bar{\alpha} = j\bar{\alpha}_0 \mathbf{A}^T = \epsilon \bar{\alpha}_1 + \epsilon^2 \{ \bar{\alpha}_2 - (\text{tr} \boldsymbol{\beta}_1) \bar{\alpha}_1 + \bar{\alpha}_1 \boldsymbol{\beta}_1^T \} + \dots, \quad (4.12)$$

$$\alpha = \mathbf{A} \bar{\alpha} = \epsilon \bar{\alpha}_1 + \epsilon^2 \{ \bar{\alpha}_2 - (\text{tr} \boldsymbol{\beta}_1) \bar{\alpha}_1 + \boldsymbol{\beta}_1 \bar{\alpha}_1 + \bar{\alpha}_1 \boldsymbol{\beta}_1^T \} + \dots \quad (4.13)$$

Furthermore, as

$$\dot{\mathbf{v}} = \partial \mathbf{v} / \partial t + (\text{grad } \mathbf{v}) \mathbf{v}, \quad (4.14)$$

$$\dot{\mathbf{A}} = \dot{\boldsymbol{\beta}} = \partial \boldsymbol{\beta} / \partial t + (\text{grad } \boldsymbol{\beta}) \mathbf{v}, \quad (4.15)$$

$$\rho = j\tilde{\rho}, \quad (4.16)$$

we get from (4.10)<sub>2</sub>, (4.11), (3.18), and (3.19):

$$\rho \mathbf{v} = \epsilon \tilde{\rho} \frac{\partial \mathbf{v}_1}{\partial t} + \epsilon^2 \tilde{\rho} \left\{ \frac{\partial \mathbf{v}_2}{\partial t} + (\text{grad } \mathbf{v}_1) \mathbf{v}_1 - (\text{tr} \boldsymbol{\beta}_1) \frac{\partial \mathbf{v}_1}{\partial t} \right\} + \dots, \quad (4.17)$$

$$\dot{\mathbf{A}} \mathbf{A}^{-1} = \epsilon \frac{\partial \boldsymbol{\beta}_1}{\partial t} + \epsilon^2 \left\{ \frac{\partial \boldsymbol{\beta}_2}{\partial t} + (\text{grad } \boldsymbol{\beta}_1) \mathbf{v}_1 - \frac{\partial \boldsymbol{\beta}_1}{\partial t} \boldsymbol{\beta}_1 \right\} + \dots \quad (4.18)$$

Since the constitutive equations (3.2) have the same form as in the static case, we may write

$$\mathbf{T} = \epsilon \mathbf{T}_1 + \epsilon^2 \mathbf{T}_2 + \dots, \quad (4.19)$$

where

$$\mathbf{T}_1 = \mathbf{L}_2[\boldsymbol{\beta}_1], \quad (4.20)$$

$$\mathbf{T}_n = \mathbf{L}_2[\boldsymbol{\beta}_n] + \mathfrak{T}_n(\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_{n-1}), \quad n \geq 2. \quad (4.21)$$

Finally, substituting (4.12), (4.13), and (4.17)–(4.21) into eqs (4.1), (4.2), and (4.6), and equating equal powers of  $\epsilon$  yields a series of *linear* systems of differential equations for the determination of the unknown pairs  $\boldsymbol{\beta}_n, \mathbf{v}_n$ . For the first two stages of approximation we have:

*First step*

$$\text{div } \mathbf{L}_2[\boldsymbol{\beta}_1] = \tilde{\rho} \partial \mathbf{v}_1 / \partial t,$$

$$\text{grad } \mathbf{v}_1 = -\bar{\alpha}_1 \times \mathbf{V} + \partial \boldsymbol{\beta}_1 / \partial t,$$

$$\text{curl } \boldsymbol{\beta}_1 = \bar{\alpha}_1.$$

*Second step*

$$\begin{aligned} \operatorname{div} \mathbf{L}_2[\boldsymbol{\beta}_2] + \operatorname{div} \mathfrak{T}_2(\boldsymbol{\beta}_1) &= \tilde{\rho} \partial \mathbf{v}_2 / \partial t + \tilde{\rho} \{ (\operatorname{grad} \mathbf{v}_1) \mathbf{v}_1 - (\operatorname{tr} \boldsymbol{\beta}_1) \partial \mathbf{v}_1 / \partial t \}, \\ \operatorname{grad} \mathbf{v}_2 &= -\tilde{\boldsymbol{\alpha}}_2 \times \mathbf{V} + \partial \boldsymbol{\beta}_2 / \partial t + \tilde{\boldsymbol{\alpha}}_1 \times \mathbf{v}_1 + \{ (\operatorname{tr} \boldsymbol{\beta}_1) \tilde{\boldsymbol{\alpha}}_1 - \boldsymbol{\beta}_1 \tilde{\boldsymbol{\alpha}}_1 - \tilde{\boldsymbol{\alpha}}_1 \boldsymbol{\beta}_1^T \} \times \mathbf{V}, \\ \operatorname{curl} \boldsymbol{\beta}_2 &= \operatorname{curl} \boldsymbol{\beta}_1^2 - (\operatorname{tr} \boldsymbol{\beta}_1) \tilde{\boldsymbol{\alpha}}_1 + \tilde{\boldsymbol{\alpha}}_1 \boldsymbol{\beta}_1^T. \end{aligned}$$

where  $\mathfrak{T}_2(\boldsymbol{\beta}_1)$  is given by (3.23). These systems are obviously of the same type as the linear system (2.17)–(2.19) and may hence be solved by using modified Green's tensor functions, as shown in section II. To write the explicit form of the first two systems for a certain anisotropic material, we need the expression of  $\mathfrak{T}_2(\boldsymbol{\beta}_1)$  and consequently again the components of the tensor functions  $\mathbf{L}_2[\mathbf{A}]$  and  $\mathbf{L}_3[\mathbf{A}, \mathbf{B}]$ , which are given in Appendix 2.

## V. Infinitesimal Motion Superimposed upon a Strain Produced by Dislocations

We consider now an infinitesimal displacement (fig. 1)

$$\mathbf{u} = \mathbf{u}(\mathbf{x}, t), \quad (5.1)$$

superimposed upon a strain produced by time-independent or uniformly moving dislocations and, possibly, in the first case, by external forces (body forces and surface tractions). We denote the resultant configuration by  $(k^*)$ , the position vector of the particle  $X$  in this configuration by  $\mathbf{x}^*(X, t)$ , and attach stars to all quantities relative to the configuration  $(k^*)$ . We assume that the superimposed motion is “elastic,” i.e., that it leaves invariant Noll’s dislocation density  $\tilde{\boldsymbol{\alpha}}$  and for uniformly moving dislocations also the velocity  $\mathbf{V}$ .

We denote by

$$\mathbf{H} \equiv \operatorname{grad} \mathbf{u} \quad (5.2)$$

the gradient of the superimposed displacement with respect to the position  $\mathbf{x}$  in the configuration  $(k)$ . We have then

$$\mathbf{A}^* = (\mathbf{1} + \mathbf{H})\mathbf{A}. \quad (5.3)$$

The equations (1.14) and (1.16), expressing the conservation of the Burgers vector and of its flux, remain invariant under the superimposed motion. To render evident the changes undergone by the equations of motion and the boundary conditions, it is convenient to employ the forms (1.19), (1.23)

$$\left. \begin{aligned} \tilde{\operatorname{div}} \bar{\mathbf{T}} + \bar{\mathbf{T}} \mathbf{s} + \tilde{\rho} \mathbf{b} &= \tilde{\rho} \dot{\mathbf{v}}, & \mathbf{x} \in \mathcal{B}, \\ \bar{\mathbf{T}} \tilde{\mathbf{n}} &= \bar{\mathbf{t}}, & \mathbf{x} \in \partial \mathcal{B}, \end{aligned} \right\} \quad (5.4)$$

and to make use of the fact that  $\mathbf{s}$  remains invariant (as  $\tilde{\alpha}$  does) under the superimposed motion. Denoting by  $\mathbf{b}^*$  and  $\bar{\mathbf{t}}^*$  the body force and the surface traction associated with the resulting motion and admitting that they may be different from  $\mathbf{b}$  and  $\mathbf{t}$ , we obtain at  $\mathbf{x}^*$ :

$$\left. \begin{aligned} \tilde{\operatorname{div}} \bar{\mathbf{T}}^* + \bar{\mathbf{T}}^* \mathbf{s} + \tilde{\rho} \mathbf{b}^* &= \tilde{\rho} \dot{\mathbf{v}}^*, & \mathbf{x}^* \in \mathcal{B}, \\ \bar{\mathbf{T}}^* \tilde{\mathbf{n}} &= \bar{\mathbf{t}}^*, & \mathbf{x}^* \in \partial \mathcal{B}. \end{aligned} \right\} \quad (5.5)$$

By subtracting (5.4) from (5.5) we obtain

$$\left. \begin{aligned} j \tilde{\operatorname{div}} (\bar{\mathbf{T}}^* - \bar{\mathbf{T}}) + j(\bar{\mathbf{T}}^* - \bar{\mathbf{T}}) \mathbf{s} + \rho(\mathbf{b}^* - \mathbf{b}) &= \rho \ddot{\mathbf{u}}, & \mathbf{x} \in \mathcal{B}, \\ (\bar{\mathbf{T}}^* - \bar{\mathbf{T}}) \tilde{\mathbf{n}} &= \bar{\mathbf{t}}^* - \bar{\mathbf{t}}, & \mathbf{x} \in \partial \mathcal{B}. \end{aligned} \right\} \quad (5.6)$$

Taking into account that, as shown in Appendix 2,

$$j \tilde{\operatorname{div}} \bar{\mathbf{T}} + j \bar{\mathbf{T}} \mathbf{s} = \operatorname{div} (j \bar{\mathbf{T}} \mathbf{A}^T), \quad (5.7)$$

and in view of (1.22) and (1.24), we deduce finally the equations of motion and the boundary conditions for the superimposed displacement field

$$\left. \begin{aligned} \operatorname{div} \{j(\bar{\mathbf{T}}^* - \bar{\mathbf{T}}) \mathbf{A}^T\} + \rho(\mathbf{b}^* - \mathbf{b}) &= \rho \ddot{\mathbf{u}}, & \mathbf{x} \in \mathcal{B}, \\ \{j(\bar{\mathbf{T}}^* - \bar{\mathbf{T}}) \mathbf{A}^T\} \mathbf{n} &= \mathbf{t}^* - \mathbf{t}, & \mathbf{x} \in \partial \mathcal{B}, \end{aligned} \right\} \quad (5.8)$$

where now  $\mathbf{t}^*$  is the surface traction associated with the configuration  $(k^*)$ , measured per unit area in the configuration  $(k)$ .

From (1.15) and (1.21) we have

$$\mathbf{T} = \mathbf{A} \frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} \quad (5.9)$$

and, therefore,

$$j(\bar{\mathbf{T}}^* - \bar{\mathbf{T}}) \mathbf{A}^T = j \left\{ \mathbf{A}^* \frac{\partial W(\mathbf{E}^*)}{\partial \mathbf{E}^*} - \mathbf{A} \frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} \right\} \mathbf{A}^T. \quad (5.10)$$

It is noteworthy that while the equations (5.8) do depend on the distortion  $\mathbf{A}$ , they assume the same form whether  $\mathbf{A}$  is produced by moving dislocations or by dislocations at rest. Consequently, the equations determining the superimposed elastic displacement depend only on the strain

in the configuration ( $k$ ) and on the variation of the body forces and surface tractions.

To solve the boundary-value problem (5.8) for the superimposed displacement we employ again an iteration scheme. For the sake of simplicity we suppose that the medium is infinite and free of body forces and that the stress tensor produced by dislocations vanishes at infinity. Such a problem appears for example when studying the propagation of plane waves in a stressed medium.

Assume that the magnitude  $|\mathbf{H}|$  of  $\mathbf{H}$  is small. We look for a solution of the equation of motion

$$\operatorname{div} \{j(\bar{\mathbf{T}}^* - \bar{\mathbf{T}})\mathbf{A}^T\} = \rho \ddot{\mathbf{u}}, \quad (5.11)$$

of the form

$$\mathbf{u} = \nu \mathbf{u}_1 + \nu^2 \mathbf{u}_2 + \dots, \quad (5.12)$$

where  $\nu$  is a small parameter. We denote

$$\mathbf{H}_1 = \operatorname{grad} \mathbf{u}_1, \quad \mathbf{H}_2 = \operatorname{grad} \mathbf{u}_2, \dots \quad (5.13)$$

and remember that all operators are taken with respect to the particle positions in the configuration ( $k$ ).

Introducing (5.12) into (5.2) and (5.3) gives

$$\begin{aligned} \mathbf{A}^* &= (\mathbf{1} + \nu \mathbf{H}_1 + \nu^2 \mathbf{H}_2 + \dots) \mathbf{A}, \\ \mathbf{A}^{*T} &= \mathbf{A}^T (\mathbf{1} + \nu \mathbf{H}_1^T + \nu^2 \mathbf{H}_2^T + \dots), \end{aligned} \quad (5.14)$$

hence

$$\begin{aligned} \mathbf{E}^* &= (1/2) (\mathbf{A}^{*T} \mathbf{A}^* - \mathbf{1}) \\ &= \mathbf{E} + (\nu/2) \mathbf{A}^T (\mathbf{H}_1 + \mathbf{H}_1^T) \mathbf{A} + (\nu^2/2) \mathbf{A}^T (\mathbf{H}_2 + \mathbf{H}_2^T + \mathbf{H}_1^T \mathbf{H}_1) \mathbf{A} + \dots \end{aligned} \quad (5.15)$$

We develop now the gradient of the strain energy density into a Taylor series

$$\begin{aligned} \frac{\partial W(\mathbf{E}^*)}{\partial \mathbf{E}^*} &= \frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} + \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{E}^* - \mathbf{E}] \\ &\quad + \frac{1}{2} \frac{\partial^3 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E} \partial \mathbf{E}} [\mathbf{E}^* - \mathbf{E}, \mathbf{E}^* - \mathbf{E}] + \dots \end{aligned} \quad (5.16)$$

By taking into account (5.15), the last formula becomes

$$\begin{aligned} \frac{\partial W(\mathbf{E}^*)}{\partial \mathbf{E}^*} = & \frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} + \nu \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_1 \mathbf{A}] + \nu^2 \left\{ \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T (\mathbf{H}_2 \right. \\ & \left. + \frac{1}{2} \mathbf{H}_1^T \mathbf{H}_1) \mathbf{A}] + \frac{1}{2} \frac{\partial^3 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_1 \mathbf{A}, \mathbf{A}^T \mathbf{H}_1 \mathbf{A}] \right\} + \dots \end{aligned}$$

Substituting this result into (5.10) and considering (5.14) and (1.6) yields

$$\begin{aligned} j(\bar{\mathbf{T}}^* - \bar{\mathbf{T}})\mathbf{A}^T = & \nu \left\{ j\mathbf{A} \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_1 \mathbf{A}] \mathbf{A}^T + \mathbf{H}_1 \mathbf{T} \right\} \\ & + \nu^2 \left\{ j\mathbf{A} \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_1 \mathbf{A}] \mathbf{A}^T + \mathbf{H}_2 \mathbf{T} + \mathfrak{H}(\mathbf{A}, \mathbf{H}_1) \right\} + \dots, \quad (5.17) \end{aligned}$$

where

$$\begin{aligned} \mathfrak{H}(\mathbf{A}, \mathbf{H}_1) = & \frac{1}{2} j\mathbf{A} \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_1^T \mathbf{H}_1 \mathbf{A}] \mathbf{A}^T + j\mathbf{H}_1 \mathbf{A} \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_1 \mathbf{A}] \mathbf{A}^T \\ & + \frac{1}{2} j\mathbf{A} \frac{\partial^3 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_1 \mathbf{A}, \mathbf{A}^T \mathbf{H}_1 \mathbf{A}] \mathbf{A}^T. \quad (5.18) \end{aligned}$$

Finally, introducing (5.17) into (5.11) and equating the coefficients of  $\nu, \nu^2, \dots$  we get the equations for the determination of  $\mathbf{H}_1, \mathbf{H}_2, \dots$ , namely

$$\operatorname{div} \left\{ j\mathbf{A} \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_1 \mathbf{A}] \mathbf{A}^T + \mathbf{H}_1 \mathbf{T} \right\} = \rho \ddot{\mathbf{u}}_1, \quad (5.19)$$

$$\operatorname{div} \left\{ j\mathbf{A} \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} [\mathbf{A}^T \mathbf{H}_2 \mathbf{A}] \mathbf{A}^T + \mathbf{H}_2 \mathbf{T} \right\} + \operatorname{div} \mathfrak{H}(\mathbf{A}, \mathbf{H}_1) = \rho \ddot{\mathbf{u}}_2. \quad (5.20)$$

Denoting as previously

$$\frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} = \mathbf{L}_2, \quad \frac{\partial^3 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E} \partial \mathbf{E}} = \mathbf{L}_3, \dots, \quad (5.21)$$

where  $\mathbf{L}_2, \mathbf{L}_3, \dots$  are the elasticities of different orders, we have

$$\frac{\partial W(\mathbf{E})}{\partial \mathbf{E}} = \mathbf{L}_2[\mathbf{E}] + \frac{1}{2} \mathbf{L}_3[\mathbf{E}, \mathbf{E}] + \dots, \quad (5.22)$$

which makes explicit eqs (5.18)–(5.20).

So far we have not made any assumption concerning the magnitude of the strains produced by dislocations. We suppose now that the distortion  $\mathbf{A}$  is also obtained as a power series

$$\mathbf{A} = \mathbf{1} + \epsilon \boldsymbol{\beta}_1 + \epsilon^2 \boldsymbol{\beta}_2 + \dots \quad (5.23)$$

by means of the iteration schemes presented in sections III and IV.

If we want for instance to satisfy the equation of motion for the superimposed displacement up to  $0(\nu^2)$  we have to solve (5.19), (5.20) for  $\mathbf{H}_1$  and  $\mathbf{H}_2$ . By hypothesis  $\epsilon \ll 1$ ,  $\epsilon \nu^2 \ll \nu^2$ , therefore, if we replace in (5.20)

$$\mathbf{A} = \mathbf{1}, j=1, \mathbf{T} = \mathbf{E} = 0, \quad (5.24)$$

the corresponding error in the equation of motion (5.11) will be of the order  $\epsilon \nu^2$ , i.e., much smaller than  $\nu^2$ . Consequently we may write (5.20) in the simpler form

$$\text{div} \left\{ \mathbf{L}_2[\mathbf{H}_2] + \mathfrak{H}(\mathbf{1}, \mathbf{H}_1) \right\} = \rho \ddot{\mathbf{u}}_2, \quad (5.25)$$

where

$$\mathfrak{H}(\mathbf{1}, \mathbf{H}_1) = \frac{1}{2} \mathbf{L}_2[\mathbf{H}_1^T \mathbf{H}_1] + \mathbf{H}_1 \mathbf{L}_2[\mathbf{H}_1] + \frac{1}{2} \mathbf{L}_3[\mathbf{H}_1, \mathbf{H}_1], \quad (5.26)$$

as it is easily seen from (5.18), (5.21), and (5.24).

In order to simplify (5.19) by means of (5.23) we need a supplementary hypothesis concerning the relative magnitude of the small parameters. We distinguish two cases.

$$\text{Case 1. } \epsilon \ll \nu \ll 1. \quad (5.27)$$

In this case we have  $\nu \epsilon \ll \nu^2$  and, therefore, we may use the same approximation (5.24) for eq (5.19), which becomes

$$\text{div } \mathbf{L}_2[\mathbf{H}_1] = \rho \ddot{\mathbf{u}}_1. \quad (5.28)$$

Equations (5.28) and (5.25) determine  $\mathbf{u}_1$  and  $\mathbf{u}_2$ , respectively. If  $\mathbf{u}$  is a plane wave, this system of equations describes the lowest-order anharmonic effects due to the non-linearity of the equations of motion. Under the hypothesis (5.27) the influence of the strains produced by dislocations is negligible up to the order  $\nu^2$ .

$$\text{Case 2. } \epsilon^n \approx \nu \ll 1, n \text{ integer.} \quad (5.29)$$

In this case we have  $\nu \epsilon^n \approx \nu^2$  and, therefore, we must replace  $\mathbf{A}$  in (5.19) by

$$\mathbf{A} = \mathbf{1} + \epsilon \boldsymbol{\beta}_1 + \dots + \epsilon^n \boldsymbol{\beta}_n. \quad (5.30)$$

To outline the supplementary intervening effects let us consider the simplest case  $\epsilon \approx \nu$ , i.e.,  $n=1$ .

We have then, successively, by neglecting all terms of an order higher than one in  $\epsilon$ ,

$$\mathbf{A} = \mathbf{1} + \epsilon \boldsymbol{\beta}_1, \quad \mathbf{E} = \frac{1}{2} \epsilon (\boldsymbol{\beta}_1 + \boldsymbol{\beta}_1^T),$$

$$\mathbf{T} = \epsilon \mathbf{T}_1 = \epsilon \mathbf{L}_2 [\boldsymbol{\beta}_1], \quad j = 1 - \epsilon \text{tr} \boldsymbol{\beta}_1, \quad \frac{\partial^2 W(\mathbf{E})}{\partial \mathbf{E} \partial \mathbf{E}} = \mathbf{L}_2 + \epsilon \mathbf{L}_3 [\boldsymbol{\beta}_1].$$

Introducing the above relations into (5.19) gives

$$\text{div } \mathbf{L}_2 [\mathbf{H}_1] + \epsilon \text{ div } \mathfrak{B} (\boldsymbol{\beta}_1, \mathbf{H}_1) = \rho \ddot{\mathbf{u}}_1, \quad (5.31)$$

where

$$\begin{aligned} \mathfrak{B} (\boldsymbol{\beta}_1, \mathbf{H}_1) \equiv & \{ -(\text{tr} \boldsymbol{\beta}_1) \mathbf{1} + \boldsymbol{\beta}_1 + \boldsymbol{\beta}_1^T \} \mathbf{L}_2 [\mathbf{H}_1] + \mathbf{L}_2 [\boldsymbol{\beta}_1^T \mathbf{H}_1 + \mathbf{H}_1 \boldsymbol{\beta}_1] \\ & + \mathbf{H}_1 \mathbf{L}_2 [\boldsymbol{\beta}_1] + \mathbf{L}_3 [\mathbf{H}_1, \boldsymbol{\beta}_1]. \end{aligned} \quad (5.32)$$

Equations (5.31) and (5.25) allow the determination of  $\mathbf{u}_1$  and  $\mathbf{u}_2$ . If  $\mathbf{u}$  is a plane wave, eq (5.31) describes the anharmonicity due to the strains produced by dislocations and (5.25) the anharmonicity due to the non-linearity of the equations of motion.

The importance of the particular case  $n=1$  just considered results also from the following. If  $\nu \ll \epsilon \ll 1$ , which corresponds to larger values of  $n$  in (5.29), we may neglect completely the equation (5.20) and retain only the first term in (5.12). In this case, by putting  $\mathbf{A} = \mathbf{1} + \epsilon \boldsymbol{\beta}_1$  into (5.19) we describe the lowest anharmonic effects due to the strains produced by dislocations. It is noteworthy that these effects depend on the third-order elastic constants but involve only the linear approximation to the strains produced by dislocations.

Using a similar scheme it is also possible to describe the anharmonic effects in the case of the propagation of two plane waves, as has been done for isotropic materials by Bross, Gruner, and Kirschenmann [17].

For further indications about the possible physical applications of the methods developed in this work, the reader is referred to the paper by Seeger [3].

## VI. Appendix 1

By applying the rule for the differentiation of a determinant we obtain from (1.9)

$$j_{,\lambda} = j A^m_{\mu} A^{\mu}_{m,\lambda}, \quad (A.1)$$

hence

$$(j A'_{\lambda})_{,\lambda} = j_{,\lambda} A'_{\lambda} + j A'_{\lambda,\lambda} = j (A'_{\lambda} A^m_{\mu} A^{\mu}_{m,\lambda} + A'_{\lambda,\lambda}).$$

Differentiating  $\mathbf{A}\mathbf{A}^{-1} = \mathbf{I}$

$$A^l_{\lambda, l} = -A^l_{\lambda} A^m_{\mu} A^{-1}_{l, m},$$

hence we have

$$\begin{aligned} (jA^l_{\lambda})_{, l} &= 2jA^l_{\lambda} A^m_{\mu} A^{-1}_{l, m}, \\ &= j\epsilon_{\lambda\mu\nu}\epsilon^{\sigma\tau\nu}A^l_{\sigma} A^m_{\tau} A^{-1}_{m, l}. \end{aligned}$$

From (1.9) we deduce

$$j\epsilon^{\sigma\tau\nu} = \epsilon_{lmp} A^{-1}_{\sigma l} A^{-1}_{\tau m} A^{\nu p}$$

and, therefore,

$$(jA^l_{\lambda})_{, l} = \epsilon_{\lambda\mu\nu}\epsilon^{lmp} A^{-1}_{\nu p} A^{-1}_{m, l}.$$

Finally, taking into consideration (1.7), (1.11), and (1.18), we infer

$$\begin{aligned} (jA^l_{\lambda})_{, l} &= \epsilon_{\lambda\mu\nu}\bar{\alpha}^{\mu\nu} A^{-1}_{\nu p} \\ &= j\epsilon_{\lambda\mu\nu}\bar{\alpha}^{\mu\nu} \equiv js_{\lambda}, \end{aligned} \quad (\text{A.2})$$

which proves (1.17).

To demonstrate (1.19) we substitute first (1.21) into (1.13), so obtaining

$$(j\bar{T}^{k\lambda} A^l_{\lambda})_{, l} + \rho b^k = \rho \dot{v}^k.$$

Taking into account (1.17), this equation becomes

$$j\bar{T}^{k\lambda} A^l_{\lambda} + j\bar{T}^{k\lambda} s_{\lambda} + \rho b^k = \rho \dot{v}^k,$$

which in view of (1.20) and (1.9) may be also written

$$\bar{T}^{k\lambda}_{;\lambda} + \bar{T}^{k\lambda} s_{\lambda} + \rho b^k = \rho \dot{v}^k. \quad (\text{A.3})$$

## VII. Appendix 2

As we have several times remarked in this paper, in order to write down explicitly the equations determining second-order effects in anisotropic materials, we need the components of the tensor functions  $\mathbf{L}_2[\mathbf{A}]$  and  $\mathbf{L}_3[\mathbf{A}, \mathbf{B}]$  for different crystal classes. These expressions assume a simpler form if we take into account the symmetry properties (3.12)–

(3.14) and make use of Voigt's notation of the pairs of indices, namely:  $11 \sim 1, 22 \sim 2, 33 \sim 3, 23 \sim 4, 13 \sim 5, 12 \sim 6$ .

If we denote, as proposed by Brugger [18],  $L_{\substack{k \\ 2}} l m n$  by  $c_{KM}$ , and  $L_{\substack{k l m n s t \\ 3}}$  by  $C_{KMS}$ , where the subscripts  $K, M, \dots$  take the values  $1, 2, \dots, 6$  in accordance with the above-mentioned equivalence, we may write in Cartesian components, making use of the summation convention:

$$L_{\substack{k l m n \\ 2}} A_{mn} = c_{KM} A_M = c_{K1} A_1 + c_{K2} A_2 + \dots + c_{K6} A_6, \quad (A.4)$$

$$\begin{aligned} L_{\substack{k l m n s t \\ 3}} A_{mn} B_{st} &= C_{KMS} A_M B_S = C_{K11} A_1 B_1 + C_{K12} (A_1 B_2 + A_2 B_1) + \dots \\ &+ C_{K16} (A_1 B_6 + A_6 B_1) + \dots + C_{K45} (A_4 B_5 + A_5 B_4) + \dots + C_{K66} A_6 B_6, \end{aligned} \quad (A.5)$$

where  $c_{KM}, C_{KMS}$  are fully symmetric Cartesian tensors, and

$$A_1 = A_{11}, A_2 = A_{22}, A_3 = A_{33}, A_4 = A_{23} + A_{32} = 2A_{(23)},$$

$$A_5 = A_{13} + A_{31} = 2A_{(13)}, A_6 = A_{12} + A_{21} = 2A_{(12)}. \quad (A.6)$$

However, when, as in our case, the tensor arguments **A** and **B** may be products of other tensors, it is very difficult to maintain the convention (A.6) for the arguments without hiding the interesting components of their factors. Therefore, while adopting Voigt's notation for the elastic constants  $c_{KM}$  and  $C_{KMS}$ , which is more and more employed in the literature, we make use of the customary notation with two subscripts for the tensor arguments **A** and **B**. We have then from (A.4) and (A.5), taking into consideration (A.6),

$$\begin{aligned} L_{\substack{k l m n \\ 2}} A_{mn} &= c_{K1} A_{11} + c_{K2} A_{22} + c_{K3} A_{33} \\ &+ 2c_{K4} A_{(23)} + 2c_{K5} A_{(13)} + 2c_{K6} A_{(12)}. \end{aligned} \quad (A.7)$$

$$\begin{aligned} L_{\substack{k l m n s t \\ 3}} A_{mn} B_{st} &= C_{K11} A_{11} B_{11} + C_{K12} A_{11} B_{22} + \dots \\ &+ 2C_{K16} (A_{11} B_{(12)} + B_{11} A_{(12)}) + \dots + 4C_{K45} (A_{(23)} B_{(13)} + A_{(13)} B_{(23)}) + \dots \\ &+ 4C_{K66} A_{(12)} B_{(12)}. \end{aligned} \quad (A.8)$$

We write now explicitly the relations (A.7) and (A.8) for the following crystal classes:

Cubic system, subsystem 6: tetratoidal and diploidal.

Cubic system, subsystem 7: hexrahedral, gyroidal, and hexoctahedral.

Hexagonal system, subsystem 10: trigonal-dipyramidal,  
hexagonal-pyramidal, and  
hexagonal-dipyramidal.

Hexagonal system, subsystem 11: ditrigonal-dipyramidal,  
dihexagonal-pyramidal,  
hexagonal-trapezohedral, and  
dihexagonal-dipyramidal.

We have taken the non-zero elastic constants of third order for various classes from two papers by Fumi [19], [20]. For details concerning the choice of the rectangular Cartesian axes with respect to the crystallographic axes, we refer to the papers by Hearmon [21] and Smith and Rivlin [22].

For experimental values of the third-order elasticities, the reader is referred to the papers by Hiki and Granato [23], Swartz [24], Gerlich [25], and Thomas, Jr. [26], which contain further references to experimental work and make use consistently of Brugger's notation of the elasticities.<sup>7</sup>

### *Components of $\mathbf{L}_2$ [A]*

*Cubic system, subsystems 6 and 7* (3 second-order elastic constants)

$$\frac{L_{11mn}A_{mn}}{2} = c_{11}A_{11} + c_{12}(A_{22} + A_{33}),$$

$$\frac{L_{22mn}A_{mn}}{2} = c_{12}(A_{11} + A_{33}) + c_{11}A_{22},$$

$$\frac{L_{33mn}A_{mn}}{2} = c_{12}(A_{11} + A_{22}) + c_{11}A_{33},$$

$$\frac{L_{23mn}A_{mn}}{2} = 2c_{44}A_{(23)},$$

$$\frac{L_{13mn}A_{mn}}{2} = 2c_{44}A_{(13)},$$

$$\frac{L_{12mn}A_{mn}}{2} = 2c_{44}A_{(12)}.$$

*Hexagonal system, subsystems 10 and 11* (5 second-order elastic constants)

$$\frac{L_{11mn}A_{mn}}{2} = c_{11}A_{11} + c_{12}A_{22} + c_{13}A_{33},$$

$$\frac{L_{22mn}A_{mn}}{2} = c_{12}A_{11} + c_{11}A_{22} + c_{13}A_{33},$$

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<sup>7</sup> The compilation of experimental values of the second- and third-order elasticities given by Truell, Elbaum, and Chick [28, App. D] appears to be in disagreement with the definition of the elasticities adopted by these authors on pp. 5 and 43 of the same book, which deviate from the Brugger notation.

$$L_{23mn}A_{mn} = c_{13}(A_{11} + A_{22}) + c_{33}A_{33},$$

$$L_{23mn}A_{mn} = 2c_{44}A_{(23)},$$

$$L_{13mn}A_{mn} = 2c_{44}A_{(13)},$$

$$L_{12mn}A_{mn} = (c_{11} - c_{12})A_{(12)}.$$

### Components of $\mathbf{L}_3[\mathbf{A}, \mathbf{B}]$

Cubic system, subsystem 6 (8 third-order elastic constants)

$$L_{11mnst}A_{mn}B_{st} = C_{111}A_{11}B_{11} + C_{112}(A_{11}B_{22} + A_{22}B_{11} + A_{33}B_{33}) \\ + C_{113}(A_{11}B_{33} + A_{22}B_{22} + A_{33}B_{11}) + C_{123}(A_{22}B_{33} + A_{33}B_{22}) \\ + 4C_{144}A_{(23)}B_{(23)} + 4C_{155}A_{(13)}B_{(13)} + 4C_{166}A_{(12)}B_{(12)}$$

$$L_{22mnst}A_{mn}B_{st} = C_{111}A_{22}B_{22} + C_{112}(A_{11}B_{11} + A_{22}B_{33} + A_{33}B_{22}) \\ + C_{113}(A_{11}B_{22} + A_{22}B_{11} + A_{33}B_{33}) + C_{123}(A_{11}B_{33} + A_{33}B_{11}) \\ + 4C_{144}A_{(13)}B_{(13)} + 4C_{155}A_{(12)}B_{(12)} + 4C_{166}A_{(23)}B_{(23)}$$

$$L_{33mnst}A_{mn}B_{st} = C_{111}A_{33}B_{33} + C_{112}(A_{11}B_{33} + A_{22}B_{22} + A_{33}B_{11}) \\ + C_{113}(A_{11}B_{11} + A_{22}B_{33} + A_{33}B_{22}) + C_{123}(A_{11}B_{22} + A_{22}B_{11}) \\ + 4C_{144}A_{(12)}B_{(12)} + 4C_{155}A_{(23)}B_{(23)} + 4C_{166}A_{(13)}B_{(13)}$$

$$L_{23mnst}A_{mn}B_{st} = 2C_{144}(A_{11}B_{(23)} + A_{(23)}B_{11}) + 2C_{155}(A_{33}B_{(23)} + A_{(23)}B_{33}) \\ + 2C_{166}(A_{22}B_{(23)} + A_{(23)}B_{22}) + 4C_{456}(A_{(13)}B_{(12)} + A_{(12)}B_{(13)})$$

$$L_{13mnst}A_{mn}B_{st} = 2C_{144}(A_{22}B_{(13)} + A_{(13)}B_{22}) + 2C_{155}(A_{11}B_{(13)} + A_{(13)}B_{11}) \\ + 2C_{166}(A_{33}B_{(13)} + A_{(13)}B_{33}) + 4C_{456}(A_{(23)}B_{(12)} + A_{(12)}B_{(23)})$$

$$L_{12mnst}A_{mn}B_{st} = 2C_{144}(A_{33}B_{(12)} + A_{(12)}B_{33}) + 2C_{155}(A_{22}B_{(12)} + A_{(12)}B_{22}) \\ + 2C_{166}(A_{11}B_{(12)} + A_{(12)}B_{11}) + 4C_{456}(A_{(23)}B_{(13)} + A_{(13)}B_{(23)})$$

Cubic system, subsystem 7 (6 third-order elastic constants)

Put in the preceding relations:  $C_{113} = C_{112}$ ,  $C_{166} = C_{155}$ .

Hexagonal system, subsystem 10 (12 third-order elastic constants)

$$L_{11mnst}A_{mn}B_{st} = C_{111}(A_{11}B_{11} + A_{22}B_{22} - 2A_{(12)}B_{(12)}) \\ + C_{112}(A_{11}B_{22} + A_{22}B_{11} + A_{22}B_{22} - A_{(12)}B_{(12)}) + C_{113}(A_{11}B_{33} + A_{33}B_{11}) \\ + 2C_{116}\{(A_{11} - A_{22})B_{(12)} + A_{(12)}(B_{11} - B_{22})\} + C_{123}(A_{22}B_{33} + A_{33}B_{22})$$

$$+C_{133}A_{33}B_{33}+C_{144}A_{(23)}B_{(23)}+4C_{145}(A_{(23)}B_{(13)}+A_{(13)}B_{(23)}) \\ +4C_{155}A_{(13)}B_{(13)}+C_{222}(3A_{(12)}B_{(12)}-A_{22}B_{22})$$

$$L_{22mnst}A_{mn}B_{st} = C_{111}(A_{11}B_{22}+A_{22}B_{11}+2A_{(12)}B_{(12)})+C_{112}(A_{11}B_{11} \\ +A_{11}B_{22}+A_{22}B_{11}-A_{(12)}B_{(12)})+C_{113}(A_{22}B_{33}+A_{33}B_{22}) \\ +2C_{116}\{(A_{22}-A_{11})B_{(12)}+A_{(12)}(B_{22}-B_{11})\}+C_{123}(A_{11}B_{33} \\ +A_{33}B_{11})+C_{133}A_{33}B_{33}+4C_{144}A_{(13)}B_{(13)}-4C_{145}(A_{(23)}B_{(13)} \\ +A_{(13)}B_{(23)})+4C_{155}A_{(23)}B_{(23)}+C_{222}(A_{22}B_{22}-A_{11}B_{22}-A_{22}B_{11} \\ -A_{(12)}B_{(12)})$$

$$L_{33mnst}A_{mn}B_{st} = C_{113}(A_{11}B_{11}+A_{22}B_{22}+2A_{(12)}B_{(12)})+C_{123}(A_{11}B_{22} \\ +A_{22}B_{11}-2A_{(12)}B_{(12)})+C_{133}\{(A_{11}+A_{22})B_{33}+A_{33}(B_{11}+B_{22})\} \\ +C_{333}A_{33}B_{33}+4C_{344}(A_{(23)}B_{(23)}+A_{(13)}B_{(13)})$$

$$L_{23mnst}A_{mn}B_{st} = 2C_{144}(A_{11}B_{(23)}+A_{(23)}B_{11}-A_{(13)}B_{(12)}-A_{(12)}B_{(13)}) \\ +2C_{145}\{(A_{11}-A_{22})B_{13}+A_{(13)}(B_{11}-B_{22})+2A_{(23)}B_{(12)}+2A_{(12)}B_{(23)}\} \\ +2C_{155}(A_{22}B_{(23)}+A_{(23)}B_{22}+A_{(13)}B_{(12)}+A_{(12)}B_{(13)}) \\ +2C_{344}(A_{33}B_{(23)}+A_{(23)}B_{33})$$

$$L_{13mnst}A_{mn}B_{st} = 2C_{144}(A_{22}B_{(13)}+A_{(13)}B_{22}-A_{(23)}B_{(12)}-A_{(12)}B_{(23)}) \\ +2C_{145}\{(A_{11}-A_{22})B_{(23)}+A_{(23)}(B_{11}-B_{22})-2A_{(13)}B_{(12)} \\ -2A_{(12)}B_{(13)}\}+2C_{155}(A_{11}B_{(13)}+A_{(13)}B_{11}+A_{(23)}B_{(12)}+A_{(12)}B_{(23)}) \\ +2C_{344}(A_{33}B_{(13)}+A_{(13)}B_{33})$$

$$L_{12mnst}A_{mn}B_{st} = C_{111}\{(A_{22}-A_{11})B_{(12)}+A_{(12)}(B_{22}-B_{11})\} \\ -(1/2)C_{112}\{(A_{11}+A_{22})B_{(12)}+A_{(12)}(B_{11}+B_{22})\} \\ +(C_{113}-C_{123})(A_{33}B_{(12)}+A_{(12)}B_{33})+C_{116}\{(A_{11}-A_{22})(B_{11}-B_{22}) \\ -4A_{(12)}B_{(12)}\}+4C_{145}(A_{(23)}B_{(23)}-A_{(13)}B_{(13)}) \\ +2(C_{155}-C_{144})(A_{(23)}B_{(13)}+A_{(13)}B_{(23)}) \\ +(1/2)C_{222}\{(3A_{11}-A_{22})B_{(12)}+A_{(12)}(3B_{11}-B_{22})\}.$$

*Hexagonal system, subsystem 11 (10 third-order elastic constants)*

Put in the preceding relations:  $C_{116}=C_{145}=0$ .

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# ON THE THERMODYNAMICS OF INHOMOGENEOUS BODIES

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This paper concerns the thermodynamics of inhomogeneous elastic bodies. I adopt the constitutive equations for thermoelastic materials given by Coleman & Noll (1963) and develop a theory for bodies made up of such materials. The general scheme of this theory is based on my paper on Generalized Simple Bodies (1969). The main result is the explicit field equations for the deformation and the temperature on a thermoelastic body.

Key words: Continuum mechanics; dislocations; constitutive relations; inhomogeneous elastic bodies.

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## I. Introduction

A purely mechanical theory of inhomogeneous bodies was formulated recently by Noll [1] and Wang [2]. In that theory, two basic assumptions were used, namely *material uniformity* and *smoothness*. This paper generalizes that mechanical theory in two respects. First, we introduce thermodynamical variables and treat the corresponding thermodynamical field equations. Second, we replace the assumption of material uniformity by the weaker assumption of *symmetry uniformity*. That is, we require the material points of a body to have the same material symmetry rather than the same material response. Evidently, material uniformity is sufficient for symmetry uniformity, but the converse is not true in general.

The symmetry of a material is characterized by the symmetry group of the constitutive relations defining that material. In continuum mechanics, the classification of materials is based on material symmetry. We call a maximal collection of materials having the same symmetry group a *material type*, e.g., fluids, isotropic solids, transversely isotropic solids, etc. The assumption of symmetry uniformity means simply that the material points of a body be all of the same material type.

While the symmetry uniformity is a condition that limits the response of the material points of a body to within a fixed material type, the smoothness condition is a condition on the distribution of the response of the material points on the body. In the reference [2], we have introduced a

general smoothness condition for a materially uniform body. This paper generalizes that condition in such a way that the smoothness condition can be applied to bodies with uniform symmetry.

We review briefly the constitutive relations for a thermoelastic material in section II. This special class of materials is chosen mainly for the sake of simplicity. The concept of material symmetry, of course, can be defined for far more general classes of materials, but we do not consider them in this paper. In section III, we explore the geometric structure of a smooth thermoelastic body with uniform symmetry. Then in section IV we derive the equation of motion and the equation of heat transfer in terms of the state variables for such bodies.

## II. Constitutive Relations and Their Symmetry Conditions

For definiteness, we assume that a fixed rectangular Cartesian coordinate system has been chosen on the physical space. Then a *configuration* of a body  $\mathcal{B}$  is a diffeomorphism

$$\kappa : \mathcal{B} \rightarrow \mathcal{R}^3. \quad (2.1)$$

We can regard such a configuration simply as a global coordinate system on  $\mathcal{B}$ . Let  $p$  be a point of  $\mathcal{B}$ . Then a *local configuration* of  $p$  is an isomorphism of the tangent space  $\mathcal{B}_p$  with  $\mathcal{R}^3$ , say

$$\delta_p : \mathcal{B}_p \rightarrow \mathcal{R}^3. \quad (2.2)$$

As usual, each configuration  $\kappa$  gives rise to a local configuration at  $p$ , namely

$$\kappa_{*p} : \mathcal{B}_p \rightarrow \mathcal{R}^3, \quad (2.3)$$

called the *induced local configuration* of  $\kappa$  at  $p$ .

In the purely mechanical theory,  $p$  is called an *elastic point* if the stress tensor at  $\kappa(p)$  in any configuration  $\kappa$  is given by a constitutive relation of the form

$$\mathbf{T}(\kappa(p)) = \mathbf{G}(\kappa_{*p}). \quad (2.4)$$

This equation says that the local configuration  $\kappa_{*p}$  is the only state variable utilized in the model. For an elastic point  $p$ , the symmetry group  $\mathcal{S}_p$  is the group of all automorphisms

$$\mathbf{A} : \mathcal{B}_p \rightarrow \mathcal{B}_p \quad (2.5)$$

such that

$$\mathbf{G}(\delta_p \circ \mathbf{A}) = \mathbf{G}(\delta_p), \quad \forall \delta_p. \quad (2.6)$$

$\mathcal{S}_p$  is necessarily a subgroup of the unimodular group of  $\mathcal{B}_p$ , since physically the stress tensor cannot remain unchanged when the body is compressed or dilatated under an arbitrary power  $\mathbf{A}^n$  or  $\mathbf{A}^{-n}$  of  $\mathbf{A}$ .

Choosing a fixed local reference configuration  $\boldsymbol{\mu}_p$ , we can express the constitutive equation (2.4) in the form

$$\mathbf{T} = \mathbf{H}(\mathbf{F}, \boldsymbol{\mu}_p), \quad (2.7)$$

where  $\mathbf{F}$  is the deformation gradient from  $\boldsymbol{\mu}_p$  to any  $\boldsymbol{\delta}_p$ , *viz.*,

$$\mathbf{F} = \boldsymbol{\delta}_p \circ \boldsymbol{\mu}_p^{-1}, \quad (2.8)$$

and where  $\mathbf{H}$  is given by

$$\mathbf{H}(\mathbf{F}, \boldsymbol{\mu}_p) = \mathbf{G}(\mathbf{F} \circ \boldsymbol{\mu}_p) \quad (2.9)$$

The symmetry group  $\mathcal{S}_p(\boldsymbol{\mu}_p)$  of  $\mathbf{H}$  is the group of all automorphisms

$$\mathbf{P} : \mathcal{R}^3 \rightarrow \mathcal{R}^3 \quad (2.10)$$

such that

$$\mathbf{H}(\mathbf{F}\mathbf{P}, \boldsymbol{\mu}_p) = \mathbf{H}(\mathbf{F}, \boldsymbol{\mu}_p), \quad \nabla \mathbf{F}. \quad (2.11)$$

From (2.9),  $\mathcal{S}_p(\boldsymbol{\mu}_p)$  is given by

$$\mathcal{S}_p(\boldsymbol{\mu}_p) = \boldsymbol{\mu}_p \circ \mathcal{S}_p \circ \boldsymbol{\mu}_p^{-1}. \quad (2.12)$$

The function  $\mathbf{H}(\mathbf{F}, \boldsymbol{\mu}_p)$  and its symmetry group  $\mathcal{S}_p(\boldsymbol{\mu}_p)$ , of course, depend on the local reference configuration  $\boldsymbol{\mu}_p$ . From (2.9) and (2.12), the following transformation rules hold:

$$\mathbf{H}(\mathbf{F}, \bar{\boldsymbol{\mu}}_p) = \mathbf{H}(\mathbf{F}\mathbf{P}, \boldsymbol{\mu}_p), \quad (2.13)$$

and

$$\mathcal{S}_p(\bar{\boldsymbol{\mu}}_p) = \mathbf{P} \mathcal{S}_p(\boldsymbol{\mu}_p) \mathbf{P}^{-1}, \quad (2.14)$$

where  $\mathbf{P}$  is the deformation gradient from  $\boldsymbol{\mu}_p$  to  $\bar{\boldsymbol{\mu}}_p$ , *viz.*,

$$\mathbf{P} = \bar{\boldsymbol{\mu}}_p \circ \boldsymbol{\mu}_p^{-1}. \quad (2.15)$$

The transformation rule (2.14) implies that the symmetry groups relative to all  $\boldsymbol{\mu}_p$  form a conjugate class of subgroups in the unimodular group of  $\mathcal{R}^3$ .

Next, we consider the constitutive relations that define a *thermoelastic point*  $p$ . Let  $p \in \mathcal{B}$  as before. Then in any configuration  $\kappa$  of  $\mathcal{B}$  we introduce two new state variables, namely the local *temperature*  $\theta(p)$  and the local *temperature gradient*  $\mathbf{g}(p)$ , the former being a positive real variable, while the latter being a vector in the physical space, here represented by  $\mathcal{R}^3$ . We introduce three new state functions also, namely, the internal energy function  $\epsilon$ , the entropy  $\eta$ , and the heat flux vector  $\mathbf{q}$ , the first two being scalars, while the last one being a vector. The resulting constitutive relations are

$$\mathbf{T} = \mathbf{G}(\delta_p, \theta, \mathbf{g}), \quad (2.16)$$

$$\epsilon = \bar{e}(\delta_p, \theta, \mathbf{g}), \quad (2.17)$$

$$\eta = \bar{h}(\delta_p, \theta, \mathbf{g}), \quad (2.18)$$

and

$$\mathbf{q} = \bar{\mathbf{I}}(\delta_p, \theta, \mathbf{g}). \quad (2.19)$$

Introducing a local reference configuration  $\mu_p$  as before, we can express these constitutive relations as

$$\mathbf{T} = \mathbf{H}(\mathbf{F}, \theta, \mathbf{g}, \mu_p), \quad (2.20)$$

$$\epsilon = e(\mathbf{F}, \theta, \mathbf{g}, \mu_p), \quad (2.21)$$

$$\eta = h(\mathbf{F}, \theta, \mathbf{g}, \mu_p), \quad (2.22)$$

and

$$\mathbf{q} = \mathbf{I}(\mathbf{F}, \theta, \mathbf{g}, \mu_p). \quad (2.23)$$

In 1963, Coleman and Noll [3] proved that under some reasonable assumptions this set of constitutive relations is consistent with the second law of thermodynamics if and only if the following two conditions are satisfied:

(i) The function  $\mathbf{I}$  satisfies the inequality

$$\mathbf{I}(\mathbf{F}, \theta, \mathbf{g}, \mu_p) \cdot \mathbf{g} \leq 0 \quad (2.24)$$

for all  $(\mathbf{F}, \theta, \mathbf{g})$ .

(ii) The functions  $\mathbf{H}$ ,  $e$ , and  $h$  do not depend on the variable  $\mathbf{g}$ . Further, there exists a function  $\sigma(\mathbf{F}, \theta, \mu_p)$  called the *free energy*, such that

$$\mathbf{H}(\mathbf{F}, \theta, \mu_p) = \rho \mathbf{F} \sigma_{\mathbf{F}}(\mathbf{F}, \theta, \mu_p)^T, \quad (2.25)$$

$$e(\mathbf{F}, \theta, \mu_p) = \sigma(\mathbf{F}, \theta, \mu_p) + \theta \sigma_{\theta}(\mathbf{F}, \theta, \mu_p), \quad (2.26)$$

and

$$h(\mathbf{F}, \theta, \mu_p) = \sigma_{\theta}(\mathbf{F}, \theta, \mu_p). \quad (2.27)$$

Here  $\sigma_{\mathbf{F}}$  and  $\sigma_{\theta}$  denote the partial derivatives of  $\sigma$  with respect to  $\mathbf{F}$  and  $\theta$ , respectively.

Henceforth, we use the constitutive relations (2.20)–(2.23) only to the extent that they satisfy the conditions (2.24)–(2.27). In particular, if we define the symmetry group  $\mathcal{G}_p^*(\mu_p)$  of  $\sigma$  in the usual way that  $\mathbf{P} \in \mathcal{G}_p^*(\mu_p)$  if and only if

$$\sigma(\mathbf{F}\mathbf{P}, \theta, \mu_p) = \sigma(\mathbf{F}, \theta, \mu_p), \quad \forall \mathbf{F}, \theta, \quad (2.28)$$

then  $\mathcal{G}_p^*(\mu_p)$  is contained in the symmetry group of  $e$  and  $h$ . The symmetry group  $\mathcal{G}_p(\mu_p)$  of  $\mathbf{H}$  need not be equal to  $\mathcal{G}_p^*(\mu_p)$  either. From a theorem of Truesdell [4], the relation (2.25) implies that  $\mathbf{P} \in \mathcal{G}_p(\mu_p)$  if and only if

$$\sigma(\mathbf{F}\mathbf{P}, \theta, \mu_p) = \sigma(\mathbf{F}, \theta, \mu_p) + \sigma(\mathbf{P}, \theta, \mu_p) - \sigma(\mathbf{I}, \theta, \mu_p). \quad (2.29)$$

Using the principle of material frame-indifference, Truesdell [4] proved further that  $\mathcal{G}_p^*(\mu_p)$  coincides with  $\mathcal{G}_p(\mu_p)$  if  $p$  is a solid point. On the other hand,  $\mathcal{G}_p^*(\mu_p)$  is generally a proper subgroup of  $\mathcal{G}_p(\mu_p)$  if  $p$  is a fluid crystal point (cf. Wang [5], [6], [7]).

Coleman and Noll's theorem does not limit the symmetry group of  $\mathbf{I}$  in any fixed way with respect to either  $\mathcal{G}_p^*(\mu_p)$  or  $\mathcal{G}_p(\mu_p)$ . But for simplicity, we assume that  $\mathcal{G}_p(\mu_p)$  is also the symmetry group of  $\mathbf{I}$ . Of course,  $\mathcal{G}_p^*(\mu_p)$  and  $\mathcal{G}_p(\mu_p)$  are necessarily closed Lie subgroups of the unimodular group of  $\mathcal{R}^3$ , since the free energy function  $\sigma$  is assumed to be a smooth function.

Under a change of local reference configuration from  $\mu_p$  to  $\bar{\mu}_p$ , the functions  $\mathbf{H}$ ,  $e$ ,  $h$ ,  $\mathbf{I}$ , and  $\sigma$  satisfy the same transformation rule as before, e.g.,

$$\sigma(\mathbf{F}, \theta, \bar{\mu}_p) = \sigma(\mathbf{F}\mathbf{P}, \theta, \mu_p) \quad (2.30)$$

etc., where  $\mathbf{P}$  is given by (2.15). Further,  $\mathcal{G}_p(\mu_p)$  satisfies (2.14), and likewise

$$\mathcal{G}_p^*(\bar{\mu}_p) = \mathbf{P} \mathcal{G}_p^*(\mu_p) \mathbf{P}^{-1}. \quad (2.31)$$

To prove (2.31), we may introduce the abstract symmetry group  $\mathcal{G}_p^*$  of  $\bar{\sigma}$  as the group of automorphisms  $\mathbf{A}$  of  $\mathcal{B}_p$  such that

$$\bar{\sigma}(\delta_p \cdot \mathbf{A}, \theta) = \bar{\sigma}(\delta_p, \theta), \quad \forall \delta_p, \theta. \quad (2.32)$$

Then as before

$$\mathcal{G}_p^*(\mu_p) = \mu_p \circ \mathcal{G}_p^* \circ \mu_p^{-1}, \quad (2.33)$$

which in turn implies (2.31).

### III. The Concept of a Smooth Thermoelastic Body With Uniform Symmetry

In the preceding section, we proved that the relative symmetry groups  $\mathcal{G}_p(\boldsymbol{\mu}_p)$  of  $p$  form a conjugate class of subgroups of the unimodular group of  $\mathcal{R}^3$ . Suppose that the conjugate classes of the relative symmetry groups of the points of a thermoelastic body  $\mathcal{B}$  coincide with one another. Then we say that  $\mathcal{B}$  is a *thermoelastic body with uniform symmetry*.

In terms of the abstract symmetry groups, the condition of symmetry uniformity means that for any two points  $p$  and  $q$  in  $\mathcal{B}$  there exists a linear isomorphism

$$\mathbf{A}(p, q) : \mathcal{B}_p \rightarrow \mathcal{B}_q, \quad (3.1)$$

called a *symmetry isomorphism of  $p$  with  $q$* , such that

$$\mathcal{G}_q = \mathbf{A}(p, q) \circ \mathcal{G}_p \circ \mathbf{A}(p, q)^{-1}. \quad (3.2)$$

Indeed, if  $\boldsymbol{\mu}_p$  and  $\boldsymbol{\mu}_q$  are any two local reference configurations of  $p$  and  $q$  such that

$$\mathcal{G}_p(\boldsymbol{\mu}_p) = \mathcal{G}_q(\boldsymbol{\mu}_q), \quad (3.3)$$

then a particular symmetry isomorphism  $\mathbf{A}(p, q)$  is given by

$$\mathbf{A}(p, q) = \boldsymbol{\mu}_q^{-1} \circ \boldsymbol{\mu}_p. \quad (3.4)$$

Conversely, if  $\mathbf{A}(p, q)$  is a given symmetry isomorphism, and if  $\boldsymbol{\mu}_p$  and  $\boldsymbol{\mu}_q$  are local reference configurations satisfying the condition (3.4), then the relative symmetry groups  $\mathcal{G}_p(\boldsymbol{\mu}_p)$  and  $\mathcal{G}_q(\boldsymbol{\mu}_q)$  coincide.

An isomorphism  $\mathbf{I}(p, q)$  from  $\mathcal{B}_p$  to  $\mathcal{B}_q$  is called a *material isomorphism of  $p$  with  $q$*  if

$$\mathbf{G}(\boldsymbol{\delta}_q, \theta) = \mathbf{G}(\boldsymbol{\delta}_q \circ \mathbf{I}(p, q), \theta), \quad \forall \boldsymbol{\delta}_q, \theta. \quad (3.5)$$

If such an isomorphism  $\mathbf{I}(p, q)$  exists, then  $p$  and  $q$  are called *materially isomorphic*. In this case,

$$\mathbf{H}(\mathbf{F}, \theta, \boldsymbol{\mu}_p) = \mathbf{H}(\mathbf{F}, \theta, \boldsymbol{\mu}_q), \quad \forall \mathbf{F}, \theta, \quad (3.6)$$

if  $\boldsymbol{\mu}_p$  and  $\boldsymbol{\mu}_q$  are related by

$$\mathbf{I}(p, q) = \boldsymbol{\mu}_q^{-1} \circ \boldsymbol{\mu}_p. \quad (3.7)$$

Hence the condition of material isomorphism means indeed that the response of  $p$  and  $q$  be the same. A direct consequence of the condition (3.6) is the condition (3.3). Thus every material isomorphism is a symmetry isomorphism, but the converse is not true in general.

Next, we set forth a smoothness condition on a thermoelastic body with uniform symmetry. For this purpose, we follow closely the procedure developed in the reference [2]. We define a *symmetry chart* as a pair  $(\mathcal{U}, \boldsymbol{\mu})$  consisting of a subbody  $\mathcal{U}$  of  $\mathcal{B}$  and a smooth field  $\boldsymbol{\mu}$  of local reference configurations on  $\mathcal{U}$ , such that the symmetry groups relative to  $\boldsymbol{\mu}$  are independent of the points of  $\mathcal{U}$ . For such a symmetry chart, we put

$$\mathcal{S}(\boldsymbol{\mu}) = \mathcal{S}_p(\boldsymbol{\mu}_p), \quad \forall p \in \mathcal{U}, \quad (3.8)$$

called the *symmetry group of  $\mathcal{U}$  relative to  $\boldsymbol{\mu}$* . NOTE: Since  $\boldsymbol{\mu}$  is required to be a smooth field, it generally fails to have any smooth global extension on the whole body  $\mathcal{B}$ . (Many counter examples were given in the reference [2].) Thus the existence of a symmetry chart is strictly a local condition.

We call two symmetry charts  $(\mathcal{U}, \boldsymbol{\mu})$  and  $(\bar{\mathcal{U}}, \bar{\boldsymbol{\mu}})$  *compatible* if the response functions relative  $\boldsymbol{\mu}$  and  $\bar{\boldsymbol{\mu}}$  coincide on the overlap  $\mathcal{U} \cap \bar{\mathcal{U}}$ , *viz.*

$$\mathbf{H}(\mathbf{F}, \theta, \boldsymbol{\mu}_p) = \mathbf{H}(\mathbf{F}, \theta, \bar{\boldsymbol{\mu}}_p), \quad \forall \mathbf{F}, \theta, \quad (3.9)$$

for all  $p \in \mathcal{U} \cap \bar{\mathcal{U}}$ . Equivalently, this condition means

$$\boldsymbol{\mu}_p^{-1} \circ \bar{\boldsymbol{\mu}}_p \in \mathcal{S}_p, \quad \forall p \in \mathcal{U} \cap \bar{\mathcal{U}}. \quad (3.10)$$

Of course, (3.9) implies directly

$$\mathcal{S}(\boldsymbol{\mu}) = \mathcal{S}(\bar{\boldsymbol{\mu}}), \quad (3.11)$$

but the converse is again not true in general.

For the two compatible symmetry charts  $(\mathcal{U}, \boldsymbol{\mu})$  and  $(\bar{\mathcal{U}}, \bar{\boldsymbol{\mu}})$ , the field

$$\mathbf{G}_{\boldsymbol{\mu}\bar{\boldsymbol{\mu}}}(p) = \boldsymbol{\mu}_p \circ \bar{\boldsymbol{\mu}}_p^{-1}, \quad p \in \mathcal{U} \cap \bar{\mathcal{U}}, \quad (3.12)$$

is called the *coordinate transformation* from  $\boldsymbol{\mu}$  to  $\bar{\boldsymbol{\mu}}$ , since it characterizes the transition from the field  $\boldsymbol{\mu}$  to the field  $\bar{\boldsymbol{\mu}}$  on the overlap  $\mathcal{U} \cap \bar{\mathcal{U}}$ . In particular, if  $\mathbf{G}_{\boldsymbol{\mu}\bar{\boldsymbol{\mu}}}$  is the identity transformation at all points in  $\mathcal{U} \cap \bar{\mathcal{U}}$ , then  $\boldsymbol{\mu}$  and  $\bar{\boldsymbol{\mu}}$  agree on the overlap of their domains. In this case,  $\bar{\boldsymbol{\mu}}$  can be regarded as a smooth extension of  $\boldsymbol{\mu}$  to the subbody  $\mathcal{U} \cup \bar{\mathcal{U}}$ . On the other hand, if  $\mathbf{G}_{\boldsymbol{\mu}\bar{\boldsymbol{\mu}}}$  is not equal to the identity transformation, then  $\boldsymbol{\mu}$  and  $\bar{\boldsymbol{\mu}}$  are different fields. But in any case, the condition of compatibility requires that the field of relative response functions on  $\mathcal{U}$  have a smooth extension to a field on  $\mathcal{U} \cup \bar{\mathcal{U}}$ .

We define a *symmetry atlas*  $\mathbf{A}$  to be a maximal covering of  $\mathcal{B}$  consisting of mutually compatible symmetry charts, say

$$\mathbf{A} = \{(\mathcal{U}_\alpha, \mu_\alpha), \alpha \in \mathbf{I}\}, \quad (3.13)$$

where  $\mathbf{I}$  is an index set. The reader will verify easily that the following three conditions are satisfied:

(i) There exists a smooth distribution of relative response functions  $\mathbf{H}_\mathbf{A}(\mathbf{F}, \theta, p)$  on  $\mathcal{B}$  with

$$\mathbf{H}_\mathbf{A}(\mathbf{F}, \theta, p) = \mathbf{H}(\mathbf{F}, \theta, \mu_\alpha p), \forall p \in \mathcal{U}_\alpha, \alpha \in \mathbf{I}. \quad (3.14)$$

We call  $\mathbf{H}_\mathbf{A}$  the *distribution of response functions relative to  $\mathbf{A}$* .

(ii) The distribution  $\mathbf{H}_\mathbf{A}$  has a uniform relative symmetry group  $\mathcal{G}(\mathbf{A})$ , namely

$$\mathcal{G}(\mathbf{A}) = \mathcal{G}_\alpha(\mu_\alpha), \forall \alpha \in \mathbf{I}. \quad (3.15)$$

We call  $\mathcal{G}(\mathbf{A})$  the *symmetry group of  $\mathcal{B}$  relative to  $\mathbf{A}$* .

(iii) The coordinate transformation

$$\mathbf{G}_{\alpha\beta} \equiv \mu_\alpha \cdot \mu_\beta^{-1}, \alpha, \beta \in \mathbf{I} \quad (3.16)$$

from  $\mu_\alpha$  to  $\mu_\beta$  is a smooth  $\mathcal{G}(\mathbf{A})$ -valued field on  $\mathcal{U}_\alpha \cap \mathcal{U}_\beta$ , for all  $\alpha, \beta \in \mathbf{I}$ . Further, from (3.16), the collection  $\{\mathbf{G}_{\alpha\beta}, \alpha, \beta \in \mathbf{I}\}$  satisfies the characteristic conditions of the coordinate transformations of a fibre bundle, namely

$$\mathbf{G}_{\alpha\alpha}(p) = \mathbf{1}, \forall p \in \mathcal{U}_\alpha, \quad (3.17)$$

$$\mathbf{G}_{\alpha\beta}(p) = \mathbf{G}_{\beta\alpha}(p)^{-1}, \forall p \in \mathcal{U}_\alpha \cap \mathcal{U}_\beta, \quad (3.18)$$

and

$$\mathbf{G}_{\alpha\beta}(p) \mathbf{G}_{\beta\gamma}(p) = \mathbf{G}_{\alpha\gamma}(p), \forall p \in \mathcal{U}_\alpha \cap \mathcal{U}_\beta \cap \mathcal{U}_\gamma, \quad (3.19)$$

for all  $\alpha, \beta, \gamma \in \mathbf{I}$ .

Naturally, we say that  $\mathcal{B}$  is *smooth* if it can be equipped with a symmetry material atlas  $\mathbf{A}$ . As explained before, a smooth materially uniform body treated in the reference [2] is smooth body with uniform symmetry. In particular, a material atlas of a materially uniform body is a symmetry atlas, but the converse is not true in general, of course. A necessary and sufficient condition for a symmetry atlas  $\mathbf{A}$  to be a material atlas is that the distribution of relative response functions  $\mathbf{H}_\mathbf{A}$  be a fixed function independent of the material points of  $\mathcal{B}$ .

Like a material atlas, a symmetry atlas  $\mathbf{A}$  is characterized by the distribution of the relative response functions  $\mathbf{H}_\mathbf{A}$ , *viz.*,

$$\mathbf{A} = \bar{\mathbf{A}} \Leftrightarrow \mathbf{H}_\mathbf{A} = \mathbf{H}_{\bar{\mathbf{A}}}. \quad (3.20)$$

Further, the general linear group of  $\mathcal{R}^3$  is a left transformation group on the symmetry atlases. Namely, for any non-singular tensor  $\mathbf{P}$  over  $\mathcal{R}^3$ , we define

$$\mathbf{P} \circ \mathbf{A} = \{(\mathcal{U}_\alpha, \mathbf{P} \circ \boldsymbol{\mu}_\alpha), \alpha \in \mathcal{I}\}. \quad (3.21)$$

The  $\mathbf{P} \circ \mathbf{A}$  is a symmetry atlas of  $\mathcal{B}$ , and the transformation rules for  $\mathbf{H}_A$  and  $\mathcal{S}(\mathbf{A})$  under the operation  $\mathbf{P}$  are

$$\mathbf{H}_{\mathbf{P} \circ \mathbf{A}}(\mathbf{F}, \theta, p) = \mathbf{H}_A(\mathbf{F}\mathbf{P}, \theta, p), \forall \mathbf{F}, \theta, p, \quad (3.22)$$

and

$$\mathcal{S}(\mathbf{P} \circ \mathbf{A}) = \mathbf{P} \mathcal{S}(\mathbf{A}) \mathbf{P}^{-1}. \quad (3.23)$$

In particular,  $\mathcal{S}(\mathbf{A})$  can be characterized by the condition

$$\mathbf{P} \in \mathcal{S}(\mathbf{A}) \Leftrightarrow \mathbf{P} \circ \mathbf{A} = \mathbf{A}. \quad (3.24)$$

However, unlike the material atlases, the symmetry atlases are not transitive under the general linear group of  $\mathcal{R}^3$ .

Aside from the distribution of the relative response functions, a symmetry atlas is formally the same as a material atlas. Hence the geometric structure characterized by a symmetry atlas is also the same as that characterized by a material atlas. In reference [2], we have analyzed that geometric structure in detail. An important geometric object in that structure is a structural connection, called a *material connection* with respect to  $\mathcal{S}(\mathbf{A})$  as the structure group. For a smooth body with uniform symmetry, such a structural connection may be called a *symmetry connection*, since its induced parallel transports are all symmetry isomorphisms among the points of  $\mathcal{B}$ .

In reference [2], we have proved the following necessary and sufficient condition for a structural connection with respect to a bundle atlas  $\mathbf{A}$ : Let  $(x^i)$  be a coordinate system on  $\mathcal{B}$ , and let  $\Gamma_{jk}^i$  be the connection symbols of a connection  $\mathcal{H}$  relative to  $(x^i)$ . Then  $\mathcal{H}$  is a structural connection with respect to  $\mathbf{A}$  if and only if the fields of matrices

$$\left[ F_j^{-1i} \left( \frac{\partial F_k^i}{\partial x^m} + \Gamma_{lm}^j F_k^i \right) \right], m = 1, 2, 3 \quad (3.25)$$

are contained in the Lie algebra of  $\mathcal{S}(\mathbf{A})$ . Here  $F_j^i$  denotes the components of the deformation gradient  $\mathbf{F}$  from  $\boldsymbol{\mu}$  to  $(x^i)$  for any chart  $(\mathcal{U}, \boldsymbol{\mu})$  in  $\mathbf{A}$ . As we shall see in the next section, the condition (3.25) enables us to express the field equations of  $\mathcal{B}$  in global forms.

#### IV. The Field Equations of a Smooth Thermoelastic Body With Uniform Symmetry

We follow the procedure developed in the reference [2] for the derivation

of the field equations in terms of the state variables of the body  $\mathcal{B}$ . First, we consider the equation of motion.

Let  $\mathbf{A}$  be a fixed symmetry atlas of  $\mathcal{B}$ . For simplicity, we suppress the dependence on  $\mathbf{A}$  from the notations of the relative response functions and their symmetry group. We put

$$H^{ij}_{kl} = H^{ij}_{kl}(\mathbf{F}, \theta, p) \equiv \frac{\partial H_{ij}}{\partial F_{kl}}, \quad (4.1)$$

where the components are referred to the standard basis of  $\mathcal{R}^3$ . The order of the indices is important here, since it is understood that the indices may be raised or lowered with respect to the Euclidean metric of  $\mathcal{R}^3$ . From the condition (ii) of the symmetry atlas  $\mathbf{A}$ ,  $\mathbf{H}$  satisfies the condition

$$\mathbf{H}(\mathbf{FP}, \theta, p) = \mathbf{H}(\mathbf{F}, \theta, p), \forall \mathbf{F}, \theta, p, \quad (4.2)$$

for all  $\mathbf{P} \in \mathcal{P}$ . Then the gradient of  $\mathbf{H}$  satisfies the conditions

$$H^{ij}_{kl}(\mathbf{F}, \theta, p) F^{km} K_m^l = 0, \quad (4.3)$$

and

$$H^{ij}_{km}(\mathbf{FP}, \theta, p) P_l^m = H^{ij}_{kl}(\mathbf{F}, \theta, p), \quad (4.4)$$

for all  $\mathbf{K}$  belonging to the Lie algebra of  $\mathcal{P}$  and all  $\mathbf{P}$  belonging to  $\mathcal{P}$ .

Now let  $\chi$  be a configuration of  $\mathcal{B}$  corresponding to the coordinate system  $(x^i)$ . Then the stress tensor in  $\chi(\mathcal{B})$  can be determined in the following way: First, we choose a symmetry chart  $(\mathcal{U}_\alpha, \mu_\alpha)$  in  $\mathbf{A}$ . For any point  $p$  covered by the chart, the deformation gradient from  $\mu_{\alpha p}$  to  $\chi_{*p}$  is

$$\mathbf{F} = \chi_{*p} \circ \mu_{\alpha p}^{-1}. \quad (4.5)$$

Substituting (4.5) into the response function  $\mathbf{H}$  yields the stress tensor

$$\mathbf{T}(\chi(p)) = \mathbf{H}(\chi_{*p} \circ \mu_{\alpha p}^{-1}, \theta(p), p). \quad (4.6)$$

But this is a local formula, valid only for  $p$  belonging to the subbody  $\mathcal{U}_\alpha$ .

Substituting the formula (4.6) into Cauchy's equation

yields

$$\operatorname{div} \mathbf{T} + \rho \mathbf{b} = \rho \mathbf{a} \quad (4.7)$$

$$H^{ij}_{kl} \frac{\partial F^{kp}}{\partial x^j} + H_{\theta}^{ij} g_j + H^i + \rho b^i = \rho a^i, \quad (4.8)$$

where  $F^{kl}$  denotes the components of  $\mathbf{F}$  relative to  $(x^i)$ , and where

$$H_{\theta}^{ij} = \frac{\partial H^{ij}}{\partial \theta}, \quad (4.9)$$

and

$$H^i = \frac{\partial H^{ij}}{\partial x^j}, \quad (4.10)$$

the arguments of  $H^{ij}_{kl}$ ,  $H^{ij}_\theta$ , and  $H^i$  being  $\mathbf{F}$ ,  $\theta(p)$ , and  $x^i$ . Like  $H^{ij}_{kl}$ , the fields  $H^{ij}_\theta$  and  $H^i$  satisfy the symmetry conditions

$$H^{ij}_\theta(\mathbf{F}, \theta, x^m) = H^{ij}_\theta(\mathbf{F}, \theta, x^m), \quad (4.11)$$

and

$$H^i(\mathbf{F}, \theta, x^m) = H^i(\mathbf{F}, \theta, x^m), \quad (4.12)$$

for all  $\mathbf{P}$  belonging to  $\mathcal{S}$ .

Now from the condition (iii) of the symmetry atlas  $\mathbf{A}$  and the conditions (4.11) and (4.12) just observed, the local fields  $H^{ij}_\theta$  and  $H^i$  in (4.8) are independent of the choice of the symmetry chart. Hence in the field equation (4.8), only the leading term is a local expression. Using the technique developed in [2], we can convert that local expression into a global one, as follows:

We choose a symmetry connection  $\mathcal{H}$  associated with the symmetry atlas  $\mathbf{A}$ . Then the matrices in (3.25) belong to the Lie algebra of  $\mathcal{S}$ . Hence from (4.3), we have

$$H^{ij}_{kl} \left( \frac{\partial F^{kl}}{\partial x^m} + \Gamma^k_{nm} F^{nl} \right) = 0. \quad (4.13)$$

Substituting this equation into (4.8) yields

$$-H^{ij}_{kl} F^{nl} \Gamma^k_{nj} + H^{ij}_\theta g_j + H^i + \rho b^i = \rho a^i. \quad (4.14)$$

Now the leading term is a global expression, since from (4.4) the field

$$\bar{H}^{ij}_{kl} \equiv H^{ij}_{kl}(\mathbf{F}, \theta, x^m) F^{nl} \quad (4.15)$$

is independent of the choice of the symmetry chart  $(\mathcal{U}_\alpha, \mu_\alpha)$ .

In application, the field equation (4.14) is not convenient, since the connection symbols  $\Gamma^i_{jk}$  depend on the coordinate system  $(x^i)$  of  $\mathbf{X}$ , which changes with time in a motion of  $\mathcal{B}$ . To render the time dependence of  $\Gamma^i_{jk}$  explicit, we introduce a fixed reference configuration  $\underline{\mathbf{X}}$  with coordinates  $(X^A)$ , on  $\mathcal{B}$ . Then a motion of  $\mathcal{B}$  can be characterized by the deformation functions

$$x^i = x^i(X^A, t), \quad i = 1, 2, 3, \quad (4.16)$$

which merely correspond to a one-parameter family of change of co-ordinates.

Now let the connection symbols of  $\mathcal{H}$  relative to  $(X^A)$  be  $\bar{\Gamma}_{BC}^A$ , and let the components of the deformation gradient  $\mu$  to  $\kappa$  be  $\bar{F}^{Ai}$  for any symmetry chart  $(\mathcal{U}, \mu)$  in  $\mathbf{A}$ . Then we have the usual transformation rules:

$$\Gamma_{jk}^i = \bar{\Gamma}_{B\bar{C}}^A \frac{\partial x^i}{\partial X^A} \frac{\partial X^B}{\partial x^j} \frac{\partial X^C}{\partial x^k} - \frac{\partial^2 x^i}{\partial X^A \partial X^B} \frac{\partial X^A}{\partial x^j} \frac{\partial X^B}{\partial x^k}, \quad (4.17)$$

and

$$F^{ij} = \frac{\partial x^i}{\partial X^A} \bar{F}^{Aj} \quad (4.18)$$

Substituting these into (4.14) yields

$$\tilde{H}^{ij}{}_k{}^A \left( \frac{\partial^2 x^k}{\partial X^A \partial X^B} - \bar{\Gamma}_{AB}^C \frac{\partial x^k}{\partial X^C} \right) \frac{\partial X^B}{\partial x^j} + H_{\theta}^{ij} g_j + H^i + \rho b^i = \rho \ddot{x}^i, \quad (4.19)$$

where locally

$$\tilde{H}^{ij}{}_k{}^A = H^{ij}{}_{kl}(\mathbf{F}, \theta, x^M) \bar{F}^{Al}. \quad (4.20)$$

The equation (4.19) is a global equation of motion in terms of the state variables of  $\mathcal{B}$ .

We can express the equation of motion also in terms of the Piola-Kirchhoff stress tensor  $\mathbf{T}_\kappa$  relative to the fixed reference configuration  $\kappa$ . By definition,  $\mathbf{T}$  and  $\mathbf{T}_\kappa$  are related by

$$T_{\kappa}^{kA} = JT^{kl} \frac{\partial X^A}{\partial x^l} \quad (4.21)$$

where  $J$  denotes the determinant of the deformation gradient

$$J = \det \left[ \frac{\partial x^i}{\partial X^A} \right]. \quad (4.22)$$

In terms of  $\mathbf{T}_\kappa$ , Cauchy's equation of motion is

$$\text{Div } \mathbf{T}_\kappa + \rho_\kappa \mathbf{b} = \rho_\kappa \mathbf{a}, \quad (4.23)$$

where  $\text{Div}$  denotes the divergence with respect to  $\kappa$ , and  $\rho_\kappa$  denotes the density field in  $\kappa(\mathcal{B})$ .

We define the Piola-Kirchhoff response function  $\mathbf{A}$  relative to  $\mathbf{A}$  by

$$\mathbf{A} = \mathbf{A}(\mathbf{F}, \theta, p) \equiv (\det \mathbf{F}) \mathbf{H}(\mathbf{F}, \theta, p) (\mathbf{F}^{-1})^T, \quad (4.24)$$

where the superscript T denotes the transposition. We can solve (4.24) for  $\mathbf{H}$  obtaining

$$\mathbf{H} = \frac{1}{\det \mathbf{F}} \mathbf{A} \mathbf{F}^T. \quad (4.25)$$

Differentiating this equation with respect to  $\mathbf{F}$ , we get

$$H^{ij}_{kl} = \frac{1}{\det \mathbf{F}} [F_m^j A^{im}_{kl} + (\delta_k^j \delta_{lm} - F_m^j F_{lk}^{-1}) A^{im}] \quad (4.26)$$

where

$$A^{ij}_{kl} = \frac{\partial A^{ij}}{\partial F^{kl}}. \quad (4.27)$$

Now substituting (4.26) into (4.19) yields

$$\tilde{A}^{iA}{}_k{}^B \left( \frac{\partial^2 x^k}{\partial X^A \partial X^B} - \bar{\Gamma}_{BA}^C \frac{\partial x^k}{\partial X^C} \right) - T_{\kappa}^{iA} \bar{C}_{AB}^B + J H_{\theta}^{ij} g_j + J H^i + \rho_{\kappa} b^i = \rho_{\kappa} a^i, \quad (4.28)$$

where locally

$$\tilde{A}^{iA}{}_k{}^B \equiv \frac{1}{\det \bar{\mathbf{F}}} A^{ir}{}_{kl} (\mathbf{F}, \theta, x^m) \bar{F}^A{}_r \bar{F}^{Bl}, \quad (4.29)$$

$$\bar{C}_{BC}^A \equiv \bar{\Gamma}_{BC}^A - \bar{\Gamma}_{CB}^A, \quad (4.30)$$

$$\text{and} \quad T_{\kappa}^{iA} = \frac{1}{\det \bar{\mathbf{F}}} A^{ir} (\mathbf{F}, \theta, x^m) \bar{F}^A{}_r = J H_{\theta}^{ij} (\mathbf{F}, \theta, x^m) \frac{\partial X^A}{\partial x^j} \quad (4.31)$$

Notice that, we can express the terms  $J H_{\theta}^{ij} g_j$  and  $J H^i$  in (4.28) also by

$$J H_{\theta}^{ij} g_j = \frac{\partial T_{\kappa}^{iA}}{\partial \theta} \bar{g}_A, \quad (4.32)$$

$$\text{and} \quad J H^i = \frac{\partial T_{\kappa}^{iA}}{\partial X^A} = \frac{\partial T_{\kappa}^{iA}}{\partial x^m} \frac{\partial x^m}{\partial X^A}, \quad (4.33)$$

$$\text{where} \quad \bar{g}_A = (\text{grad } \theta)_A = g_i \frac{\partial x^i}{\partial X^A}. \quad (4.34)$$

Next, we consider the energy equation of  $\mathcal{B}$ . In terms of the state functions  $\epsilon$ ,  $\mathbf{T}$ , and  $\mathbf{q}$ , the principle of balance of energy takes the field equation

$$\rho \dot{\epsilon} = \text{tr}(\mathbf{T} \text{ grad } \mathbf{v}) + \text{div } \mathbf{q} + \rho r, \quad (4.35)$$

where  $\mathbf{v}$  is the velocity field and  $r$  is the energy supply. For a thermo-

elastic body  $\mathcal{B}$ ,  $\epsilon$  and  $\mathbf{T}$  are determined by the free-energy function  $\sigma$  through the relations (2.26) and (2.27). In particular, we have the identities

$$\rho\dot{\sigma} = \text{tr}(\mathbf{T} \text{ grad } \mathbf{v}) - \rho\eta\dot{\theta}, \quad (4.36)$$

and

$$\rho\dot{\sigma} = \rho\dot{\epsilon} - \rho\eta\dot{\theta} - \rho\theta\dot{\eta}. \quad (4.37)$$

Substituting these identities into (4.35) yields the usual equation of heat transfer:

$$\text{div } \mathbf{q} + \rho r = \rho\theta\dot{\eta}. \quad (4.38)$$

We proceed to express this equation in terms of the state variables.

By assumption, the symmetry group of the heat flux function  $\mathbf{I}$  is the same as that of the response function  $\mathbf{H}$ . Hence relative to the fixed symmetry atlas  $\mathbf{A}$ ,  $\mathbf{I}$  is a smooth global field on  $\mathcal{B}$  with

$$\mathbf{I}(\mathbf{F}, \theta, \mathbf{g}, p) = \mathbf{I}(\mathbf{F}, \theta, \mathbf{g}, \boldsymbol{\mu}_\alpha) \quad (4.39)$$

for any symmetry chart  $(\mathcal{U}_\alpha, \boldsymbol{\mu}_\alpha)$  in  $\mathbf{A}$  covering the point  $p$ . We put

$$l^i_{jk} = l^i_{jk}(\mathbf{F}, \theta, \mathbf{g}, p) = \frac{\partial l^i}{\partial F_{jk}}. \quad (4.40)$$

Then the following two conditions are satisfied:

$$l^i_{jk}(\mathbf{F}, \theta, \mathbf{g}, p) P_m^k = l^i_{jm}(\mathbf{F}, \theta, \mathbf{g}, p) \quad (4.41)$$

for all  $\mathbf{P}$  belonging to  $\mathcal{F}$ , and

$$l^i_{jk}(\mathbf{F}, \theta, \mathbf{g}, p) F^{jm} K^k_m = 0, \quad (4.42)$$

for all  $\mathbf{K}$  belonging to the Lie algebra of  $\mathcal{F}$ .

As before, let  $\chi$  be a configuration of  $\mathcal{B}$  corresponding to the coordinate system  $(x^i)$ . Then the heat flux in  $\chi(\mathcal{B})$  can be determined by the local formula

$$\mathbf{q}(\chi(p)) = \mathbf{I}(\mathbf{F}, \theta, \mathbf{g}, x^m(p)) \quad (4.43)$$

where  $\mathbf{F}$  is given by (4.5). Substituting this local formula into the heat equation (4.38) yields

$$l^i_{jk} \frac{\partial F^{jk}}{\partial x^i} + l^i_\theta g_j + l^i_{\mathbf{g}} \frac{\partial g_j}{\partial x^i} + l + \rho r = \rho\theta\dot{\eta}, \quad (4.44)$$

where

$$l^i_\theta = \frac{\partial l^i}{\partial \theta}, \quad (4.45)$$

$$l^i_{\mathbf{g}} = \frac{\partial l^i}{\partial g_j}, \quad (4.46)$$

and

$$l = \frac{\partial l^i}{\partial x^i}. \quad (4.47)$$

Like (4.8), the equation (4.44) contains a local expression in the leading term.

Introducing the symmetry connection  $\mathcal{H}$  and using the condition (4.42), we can rewrite the equation (4.44) as

$$-l_{jk}^i F^{xk} \Gamma_{ni}^j + l_{\theta}^i g_i + l_{\mathbf{g}}^{ij} \frac{\partial g_j}{\partial x^i} + l + \rho r = \rho \theta \dot{\eta}. \quad (4.48)$$

Then from (4.41) the combination

$$\tilde{l}^i_j n = l^i_{jk} (\mathbf{F}, \theta, \mathbf{g}, x^m) F^{nk} \quad (4.49)$$

is a global field.

Now introducing the deformation functions (4.16) and carrying out the same analysis as before, we obtain the global equation

$$\tilde{l}^i u^A \left( \frac{\partial^2 x^k}{\partial X^A \partial X^B} - \bar{\Gamma}_{AB}^C \frac{\partial x^k}{\partial X^C} \right) \frac{\partial X^B}{\partial x^j} + l_{\theta}^i g_i + l_{\mathbf{g}}^{ij} \frac{\partial g_j}{\partial x^i} + l + \rho r = \rho \theta \dot{\eta}, \quad (4.50)$$

where locally

$$\tilde{l}^i_k A = l^i_{kl} (\mathbf{F}, \theta, \mathbf{g}, x^m) \bar{F}^{Al}. \quad (4.51)$$

Next, we introduce the heat flux vector  $\mathbf{q}_\kappa$  relative to the reference configuration  $\kappa$  by

$$q_\kappa^A = J q^I \frac{\partial X^A}{\partial x^I}. \quad (4.52)$$

Then the heat equation (4.38) takes the alternative form

$$\text{Div } \mathbf{q}_\kappa + \rho_\kappa r = \rho_\kappa \theta \dot{\eta}. \quad (4.53)$$

As before, we define the heat flux function  $\mathbf{s}$  relative to  $\mathbf{A}$  by

$$\mathbf{s} = \mathbf{s} (\mathbf{F}, \theta, \mathbf{g}, p) \equiv (\det \mathbf{F}) \mathbf{F}^{-1} \mathbf{l} (\mathbf{F}, \theta, \mathbf{g}, p). \quad (4.54)$$

Then

$$\mathbf{l} = \frac{1}{\det \mathbf{F}} \mathbf{F} \mathbf{s}. \quad (4.55)$$

Differentiating this equation with respect to  $\mathbf{F}$  yields

$$l^i_{jk} = \frac{1}{\det \mathbf{F}} [F_m^i s^m_{jk} + (\delta_j^i \delta_{km} - F_m^i F_{kj}^{-1}) s^m] \quad (4.56)$$

where

$$s^m_{jk} = \frac{\partial s^m}{\partial F^{jk}} \quad (4.57)$$

Now substituting (4.56) into (4.50), we get

$$\tilde{l}^A_k B \left( \frac{\partial^2 x^k}{\partial X^A \partial X^B} - \bar{\Gamma}_{BA}^C \frac{\partial x^k}{\partial X^C} \right) - q_{\kappa}^A \bar{C}_{AB}^B + Jl_{\theta}^i g_i + Jl_{\bar{g}}^{ij} \frac{\partial \bar{g}_j}{\partial x^i} + Jl + \rho_{\kappa} r = \rho_{\kappa} \theta \dot{\eta} \quad (4.58)$$

where locally

$$\tilde{l}^A_k B = \frac{1}{\det \bar{\mathbf{F}}} l^r_{kl} (\mathbf{F}, \theta, \mathbf{g}, x^m) \bar{F}_r^A \bar{F}^{Bl}. \quad (4.59)$$

Of course the terms  $Jl_{\theta}^i g_i$ ,  $Jl_{\bar{g}}^{ij} \frac{\partial \bar{g}_j}{\partial x^i}$ , and  $Jl$  in (4.58) can be expressed also by

$$Jl_{\theta}^i g_i = \frac{\partial q_{\kappa}^A}{\partial \theta} \bar{g}_A, \quad (4.60)$$

$$Jl_{\bar{g}}^{ij} \frac{\partial \bar{g}_j}{\partial x^i} = \frac{\partial q_{\kappa}^A}{\partial \bar{g}_B} \frac{\partial \bar{g}_B}{\partial X^A}, \quad (4.61)$$

and

$$Jl = \frac{\partial q_{\kappa}^A}{\partial X^A}, \quad (4.62)$$

where  $\bar{g}_A$  is given by (4.34).

So far, we have expressed the state functions on the left-hand side of the heat equation in terms of the state variables. Next we consider the state function on the right-hand side, namely, the function  $\dot{\eta}$ . Using the constitutive relation (2.22) together with the restriction (2.27), we have the local formula

$$\eta(\chi(p)) = h(\mathbf{F}, \theta, \boldsymbol{\mu}_{\alpha p}). \quad (4.63)$$

Now there are two possibilities:

(I)  $\mathcal{J} = \mathcal{J}^*$ . (This case includes all solid bodies.)

In this case the function  $h$  is a smooth global field on  $\mathcal{B}$  with

$$h(\mathbf{F}, \theta, p) = h(\mathbf{F}, \theta, \boldsymbol{\mu}_{\alpha p}) \quad (4.64)$$

for any symmetry chart  $(\mathcal{U}_{\alpha}, \boldsymbol{\mu}_{\alpha})$  in  $\mathbf{A}$  covering the point  $p$ . We put

$$h_{jk} = h_{jk}(\mathbf{F}, \theta, p) \equiv \frac{\partial h}{\partial F^{jk}}, \quad (4.65)$$

and

$$h_\theta = h_\theta(\mathbf{F}, \theta, p) \equiv \frac{\partial h}{\partial \theta}. \quad (4.66)$$

Then we have the identities

and

$$h_{jk}(\mathbf{FP}, \theta, p) P_m^k = h_{jm}(\mathbf{F}, \theta, p), \quad (4.67)$$

$$h_\theta(\mathbf{FP}, \theta, p) = h_\theta(\mathbf{F}, \theta, p), \quad (4.68)$$

for all  $\mathbf{P}$  belonging to  $\mathcal{S}$ .

From (4.63), we have

$$\dot{\eta} = h_{jk} \dot{F}^{jk} + h_\theta \dot{\theta}. \quad (4.69)$$

Of course, the leading term on the right-hand side is a local expression. We can convert that local expression into a global one by using the time derivative of the formula (4.18)

$$\dot{F}^{jk} = \bar{F}^{Ak} \frac{\partial x^l}{\partial X^A} \frac{\partial v^i}{\partial x^l}. \quad (4.70)$$

Substituting (4.70) into (4.69) yields

$$\dot{\eta} = \tilde{h}_j^A \frac{\partial x^l}{\partial X^A} \frac{\partial v^i}{\partial x^l} + h_\theta \dot{\theta}, \quad (4.71)$$

where locally

$$\tilde{h}_j^A = h_{jk}(\mathbf{F}, \theta, p) \bar{F}^{Ak}. \quad (4.72)$$

(II)  $\mathcal{S} \neq \mathcal{S}^*$ . (This case includes fluid crystal bodies only.)

In this case the function  $h$  does not form a smooth global field on  $\mathcal{B}$ . But from (2.27) and (2.29), we have the identity

$$h(\mathbf{FP}, \theta, \mu_p) = h(\mathbf{F}, \theta, \mu_p) + h(\mathbf{P}, \theta, \mu_p) - h(\mathbf{1}, \theta, \mu_p) \quad (4.73)$$

for all  $\mathbf{P}$  belonging to  $\mathcal{S}$ . Differentiating this identity with respect to  $\mathbf{F}$  shows that the gradient of  $h$  is a global field on  $\mathcal{B}$ , viz,

$$h_{jk}(\mathbf{F}, \theta, p) = h_{jk}(\mathbf{F}, \theta, \mu_{\alpha p}) \quad (4.74)$$

for all  $(\mathcal{U}_\alpha, \mu_\alpha)$  in  $\mathbf{A}$  covering  $p$ . Thus as far as the leading term on the right-hand side of (4.69) is concerned, we can proceed in exactly the same way as in the previous case.

The last term of (4.69) remains a global field in this case.

### V. Acknowledgement

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# ELASTIC-PLASTIC PLANE BENDING OF A SINGLE CRYSTAL

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The elastic-plastic bending of a single crystal beam which deforms by single slip on a plane containing the axis of bending and in a direction normal to the axis of bending is analyzed. Both continuum plasticity and dislocation approaches are used to obtain stresses and/or displacements in the elastic and plastic regions. The relation between the applied bending moment and the curvature of the neutral axis is also obtained. The approaches are compared and correspondences between the two theories are discussed.

Key words: Dislocation distributions; mechanical properties; plane blending.

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## I. Introduction

The utility of dislocation theory as a tool to describe the inelastic behavior of macroscopic material bodies has not been exploited until quite recently. Analytical methods for such problems have employed mathematical models for material behavior, which generally excluded any explicit consideration of the role of microstructure in material properties. Studies of dislocation behavior have been concentrated primarily on the properties of individual dislocations and finite arrays, and on the role of dislocations in the deformation of materials under uniform state of stress. In the present work a simple problem of plastic deformation under a nonuniform state of stress—pure bending of a simply supported prismatic beam—is analyzed both by classical continuum methods and by an approach based on continuum dislocation theory.

The problem considered is illustrated in figure 1. A rectangular prismatic beam, simply supported on either end, is bent by applying equal and opposite couples,  $M$ , about the ends. The structural axis of the beam is the  $x_1$  axis and the axis of bending is the  $x_3$  axis. The origin is taken at the centroid of the beam. In the following analyses it is assumed that the couples are slowly increased from zero to their final value, and that the resulting deformations are time-independent.

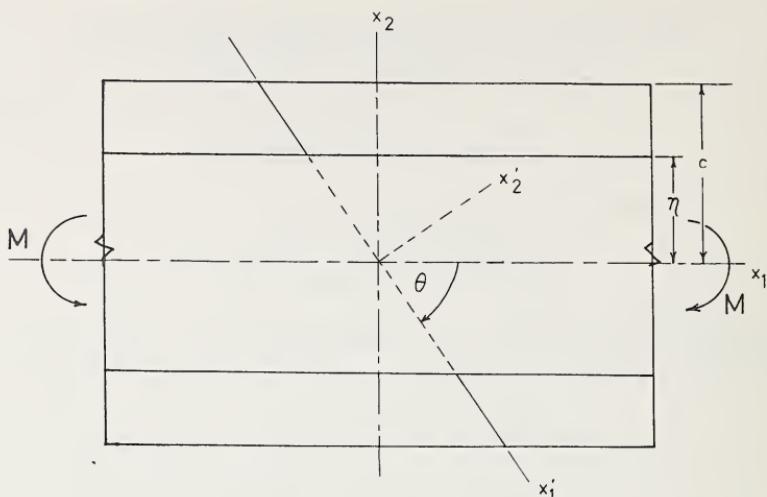


FIGURE 1. Coordinate system.

The beam consists of a single crystal having a single set of slip planes parallel to the axis of bending and inclined at an angle  $\theta$  to the structural axis. The slip direction is normal to the axis of bending. The  $x'_1$  and  $x'_2$  axes are parallel to the slip direction and normal to the slip plane, respectively. After plastic flow has occurred in the beam, the elastic-plastic interface, defined as that surface in the beam where the elastic solution for the stress distribution satisfies the yield condition, is parallel to the neutral surface and located a distance  $\pm\eta$  from it. Plane stress conditions are assumed, and linearized strain components are used throughout; hence, the results do not apply to large deformations.

In the second section continuum plasticity is employed to obtain the displacement and stress fields in the elastic-plastic beam. Both elastic-perfectly plastic and linear work-hardening models are investigated. The third section treats the identical problem from the viewpoint of a continuous distribution of dislocations in the plastic region. The states of dislocation corresponding to particular stress distributions in the plastic region are determined, and it is shown by a direct integration that these dislocation arrangements do have stress components which result in the assumed value of residual stress in the plastically deformed zone. The effect of slip geometry is also examined. The results obtained by both techniques are summarized in the fourth section.

## II. Continuum Plasticity Solution

Let the beam considered be a single crystal of an hexagonal close-packed metal, having a slip direction in the basal plane along  $x'_1$  and the normal to the basal plane along  $x'_2$ .

The stress distribution and displacements throughout the beam are obtained subject to the assumptions that (a) plane cross sections remain plane, (b) plastic flow occurs by single slip in the  $x'_1$  direction, and (c) the material obeys an elastic-perfectly plastic flow law. Elastic anisotropy is also taken into account.

### A. ANISOTROPIC SOLUTION

When  $M$  is sufficiently small, the beam is elastic throughout and the stress distribution is given by the ordinary beam theory. That is, the only nonvanishing stress component is  $\sigma_{11}$ , which varies linearly with  $x_2$  and is constant in the  $x_1$  direction.

*Elastic behavior.* The displacements in this case are obtained by integrating the strains given by the anisotropic form of Hooke's Law. Thus,

$$\sigma_{11} = \sigma = Mx_2/I, \quad (1)$$

and

$$e_{11} = S_{11}\sigma = u_{1,1},$$

$$e_{22} = S_{21}\sigma = u_{2,2},$$

$$2e_{12} = S_{61}\sigma = u_{1,2} + u_{2,1}, \quad (2)$$

where  $I$  is the centroidal moment of inertia of the beam cross section,  $u_1$  and  $u_2$  are the horizontal and vertical displacements, respectively, and  $S_{ij}$  are the elastic compliances of the crystal.<sup>1</sup>

In a coordinate system based on the principal crystallographic axes of an hexagonal crystal, the compliance matrix has the form

$$S'_{ij} = \begin{matrix} S'_{11} & S'_{12} & S'_{13} & 0 & 0 & 0 \\ S'_{12} & S'_{22} & S'_{12} & 0 & 0 & 0 \\ S'_{13} & S'_{12} & S'_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & S'_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S'_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & S'_{44} \end{matrix} \quad (3)$$

where

$$x'_1 \parallel [11\bar{2}0], x'_2 \parallel [0001], \text{ and } x'_3 \parallel [10\bar{1}0].$$

Under coordinate rotation about the  $x'_3$  axis, the relevant coefficients are given by

<sup>1</sup> The usual contracted notation is employed here for single crystal compliances [1].

$$\begin{aligned} S_{11} &= m^4 S'_{11} + n^4 S'_{22} + m^2 n^2 (2S'_{12} + S'_{66}) \\ S_{21} &= m^2 n^2 (S'_{11} + S'_{22} - S'_{66}) + (m^4 + n^4) S'_{12} \\ S_{61} &= m^3 n (-2S'_{11} + 2S'_{12} + S'_{66}) - mn^3 (2S'_{12} + S'_{66}) \end{aligned} \quad (4)$$

where  $m = \cos \theta$  and  $n = \sin \theta$ . The displacements are obtained by integrating eqs (2) subject to the boundary conditions

$$u_1(0, 0) = 0, \quad u_2(L, 0) = 0, \quad u_2(-L, 0) = 0 \quad (5)$$

where  $2L$  is the length of the beam.

Thus, as long as the beam remains elastic

$$u_1 = M [S_{11}x_1 x_2 + S_{61}x_2^2/2]/I \quad (6)$$

$$u_2 = M [S_{21}x_2^2 - S_{11}(x_1^2 - L^2)]/2I, \quad (7)$$

and the centerline displacements are

$$u_1 = 0, \quad u_2 = -MS_{11}(x_1^2 - L^2)/2I. \quad (8)$$

*Elastic-plastic behavior.* The elastic solution described above remains valid as long as plastic flow does not occur. Since plastic deformation occurs by slip on planes normal to  $x_2'$  along directions parallel to  $x_1'$ , the yield condition adopted is that of a critical resolved shear stress,

$$f = [mn(\sigma_{11} - \sigma_{22}) + (m^2 - n^2)\sigma_{12}]^2 = k^2, \quad (9)$$

where  $f$  is the yield function and  $k$  is the critical resolved shear stress in  $x_2'$  plane along the  $x_1'$  direction.

Since  $\sigma_{11} = \sigma$  is the only nonvanishing stress component, the stress at which plastic flow occurs is

$$\pm \sigma = \sigma^* = k/mn, \quad (10)$$

hence,

$$M^* = Ik/cmn = 2kc^2t/3mn. \quad (11)$$

Thus, for  $M > M^*$  plastic flow occurs in the outer fibers of the beam. It can be shown that in the plastically deforming regions ( $x_2^2 > \eta^2$ ) the stress state is a constant, so that  $\sigma_{22}$  and  $\sigma_{12}$  remain zero throughout. The proof follows the same lines as that employed by Prager and Hodge [2].

It follows then, that

$$\sigma_{11} = \begin{cases} \sigma^* & x_2 \geq \eta \\ \sigma^* x_2 / \eta & \eta \geq x_2 \geq -\eta \\ -\sigma^* & x_2 \leq -\eta. \end{cases} \quad (12)$$

We must require that the moment about  $x_3$  of the internal stress distribution be equal to the applied moment  $M$ , so

$$M = t \int_{-c}^c \sigma_{11} x_2 dx_2$$

or

$$\frac{M}{t} = \sigma^* (3c^2 - \eta^2) / 3. \quad (13)$$

The position of the elastic plastic interface is thus determined as a function of the applied moment. The collapse moment  $M^{**}$  is then found by setting  $\eta = 0$  and so

$$M^{**} = 3M^*/2. \quad (14)$$

However, it will be shown later that the corresponding curvature violates the assumptions of small strains. The stress distribution for  $M^* < M < M^{**}$  is thus determined by eq (12) and by inverting eq (13) to obtain

$$(\eta/c)^2 = (3M^* - 2M) / M^*. \quad (15)$$

The displacement solution in the elastic region has the same form as that for the completely elastic solution;  $M/I$  is replaced in the latter by  $\sigma^*/\eta$ , i.e.,

$$u_1 = \sigma^* [S_{11}x_1x_2 + S_{61}x_2^2/2] / \eta \quad (16)$$

$$u_2 = \sigma^* [(S_{21}x_2^2/2) - S_{11}(x_1^2 - L^2)/2] / \eta \quad (17)$$

for  $x_2^2 \leq \eta^2$ . The moment-curvature relation may be obtained from (17) by evaluating the second derivative of the vertical displacement along the centerline. Thus,

$$-K = \sigma^* S_{11} / c [(3M^* - 2M) / M^*]^{1/2} = \sigma^* S_{11} \eta. \quad (18)$$

In the plastically deforming region the displacements are determined by using the plane section hypothesis and the associated flow law corresponding to the yield condition (10). A linear strain variation is assumed throughout the beam, and since the strain gradient is known in the elastic core, it follows that

$$e_{11} = S_{11} \sigma^* x_2 / \eta \quad (19)$$

in the upper plastic zone. The elastic component of strain, determined from Hooke's law, is constant so the plastic strain component is found to be

$$e''_{11} S_{11} \sigma^* (x_2 - \eta) / \eta. \quad (20)$$

Now, the direction of the plastic strain rate vector is determined by the normality condition,

$$e''_{ij} = \Lambda (\partial f / \partial \sigma_{ij}). \quad (21)$$

The plastic strains are all initially zero, so

$$e''_{22} = -e''_{11} \quad (22)$$

$$e''_{12} = \cot 2\theta e''_{11} \quad (23)$$

throughout the plastic region. Adding the elastic and plastic strain components gives the total strain

$$e_{11} = \sigma^* \{ S_{11} x_2 / \eta \} \quad (24)$$

$$e_{22} = \sigma^* \{ S_{21} - [S_{11} (x_2 - \eta) / \eta] \} \quad (25)$$

$$e_{12} = \sigma^* \{ (S_{61}/2) + S_{11} \cot 2\theta [x_2 - \eta] / \eta \}. \quad (26)$$

These equations may be integrated subject to continuity conditions across the elastic-plastic interface to obtain the displacements in the plastic region,

$$u_1 = \sigma^* [2S_{11}(x_1 x_2 + (x_2 - \eta)^2 \cot 2\theta) + S_{61}(x_2 - (x_2 - \eta)^2)] / 2\eta \quad (27)$$

$$u_2 = \sigma^* [S_{21}(x_2 - (x_2 - \eta)^2) - S_{11}((x_2 - \eta)^2 + x_1^2 - L^2)] / 2\eta. \quad (28)$$

## B. ISOTROPIC SOLUTION

If the material is assumed to be elastically isotropic, then

$$S_{11} = 1/E, S_{12} = -\nu/E, S_{16} = 0$$

and so

$$u_1 = \begin{cases} \sigma^* x_1 x_2 / \eta E & x_2^2 \leq \eta^2 \\ \sigma^* [x_1 x_2 + (x_2 - \eta)^2 \cot 2\theta] / \eta E & x_2 > \eta \end{cases} \quad (29)$$

$$u_2 = \begin{cases} -\sigma^* [\nu x_2 + (x_1^2 - L^2)] / 2\eta E & x_2^2 \leq \eta^2 \\ -\sigma^* [\nu(x_2 - (x_2 - \eta)^2) + (x_2 - \eta)^2 + x_1^2 - L^2] / 2\eta E & x_2 > \eta \end{cases} \quad (30)$$

In similar fashion, the remaining aspects of the solution may be obtained for this special case.

### III. Elastic-Plastic Solution With Linear Work-Hardening

In the previous section, solutions were obtained for the stresses and displacements of a single crystal elastic-perfectly plastic beam in pure bending. The analysis is now extended to include the effects of work-hardening.

The plastic strains are given by the flow law

$$\dot{e}_{ij}'' = \frac{\frac{\partial f}{\partial \sigma_{ij}} \left( \frac{\partial f}{\partial \sigma_{mn}} \dot{\sigma}_{mn} \right)}{\frac{\partial f}{\partial \sigma_{pq}} h_{pq}} \quad (31)$$

instead of eq (21). We assume a linear isotropic hardening of an initial Mises yield surface, so the yield function is given by eq (9) and

$$h_{pq} = \alpha \frac{\partial f}{\partial \sigma_{pq}}. \quad (32)$$

The plastic strain is then

$$e_{11}'' = \sin^2 2\theta (\sigma_{11} - \sigma^*)/2\alpha \quad (33)$$

$$e_{22}'' = -\sin^2 2\theta (\sigma_{11} - \sigma^*)/2\alpha \quad (34)$$

$$e_{12}'' = \sin 4\theta (\sigma_{11} - \sigma^*)/4\alpha \quad (35)$$

in the regions where plastic deformation has occurred. These strains are obtained from the corresponding rate quantities by interpreting  $(\cdot)$  as differentiation with respect to  $\eta$  and by integrating subject to the requirement that the plastic strains vanish at the elastic-plastic interface.

The bending stress distribution in the plastically deforming region is found by employing the linear strain gradient assumption (19). The stress-strain relations are found to be

$$\sigma_{11} = \sigma^* (\eta + \beta x_2) / \eta (1 + \beta) \quad (36)$$

where

$$S_{11}/\beta = \sin^2 2\theta / 2\alpha. \quad (37)$$

Having determined the stress distribution in both elastic and plastic zones, the interface may now be located by requiring equilibrium with the externally applied bending moment,

$$M = \sigma^* t [3c^2\eta + 2\beta c^3 - \eta^3] / 3\eta (1 + \beta). \quad (38)$$

The cubic equation may be solved to obtain  $\eta(M)$ , but it is inconvenient to do so. However, the moment-curvature relation can be found by substituting from eqs (11) and (18) into eq (38) to obtain

$$M = -EIK[3(K^*/K) - (K^*/K)^3 + 2\beta]/2(1+\beta) \quad (39)$$

relating the applied moment to the resulting curvature and the curvature at the initiation of plastic flow,  $K^*$ .

The elastic core displacement solutions and centerline moment-curvature relation for the perfectly-plastic case (16, 17, 18) remain valid provided (15) is replaced by (38). To obtain the displacement in the plastic zone, we add the plastic strains previously determined to the elastic components computed from Hooke's laws.

$$e_{11} = S_{11}\sigma^*x_2/\eta \quad (40)$$

$$e_{22} = \sigma^*[S_{11} + S_{21} + (\beta S_{21} - S_{11})x_2/\eta]/(1+\beta) \quad (41)$$

$$e_{12} = \sigma^* \left[ -S_{11} \cot 2\theta + \frac{S_{61}}{2} + \left( \frac{S_{61}\beta}{2} + S_{11} \cot 2\theta \right) \frac{x_2}{\eta} \right] / (1+\beta) \quad (42)$$

and integrate the total strains subject to the appropriate continuity conditions at the interface. Thus,

$$u_1 = \sigma^* \left[ S_{11} \left( x_1 x_2 + \frac{(x_2 - \eta)^2}{1+\beta} \cot 2\theta \right) + \frac{S_{61}}{2} \left( x_2 - \frac{(x_2 - \eta)^2}{1+\beta} \right) \right] / \eta \quad (43)$$

and

$$u_2 = \sigma^* \left[ \frac{S_{21}}{2} \left( x_2 - \frac{(x_2 - \eta)^2}{1+\beta} \right) - \frac{S_{11}}{2} \left( x_1^2 - L^2 + \frac{(x_2 - \eta)^2}{1+\beta} \right) \right] / \eta. \quad (44)$$

The above results reduce to the perfectly-plastic solutions when  $\beta \rightarrow 0$ , i.e., as the tangent modulus vanishes.

#### IV. Dislocation Theory Solution

In the following section the theory of continuous distributions of dislocations developed by Kröner [3] and Bilby et al. [4] is used to obtain the results of the previous calculations in terms of dislocation content and distribution. The assumptions of the problem considered are essentially the same as for the continuum plasticity treatment. In addition, it is assumed that the plastic zone contains a continuous distribution of edge dislocations lying parallel to  $x_3$ , the axis of bending, and having

Burgers vectors of strength  $\bar{b}$  which have components  $(b_1, b_2, 0)$ . Thus in the plastic region the state of dislocation tensor has components

$$A_{mn} = \begin{pmatrix} 0 & 0 & b_1 N_3 \\ 0 & 0 & b_2 N_3 \\ 0 & 0 & 0 \end{pmatrix}, \quad (45)$$

where  $b_i$  are the components of  $\bar{b}$  along  $x_i$ , and  $N_3$  is the net number of dislocations intersecting unit area normal to  $x_3$ , i.e., the net density of excess dislocations of like sign. In the elastic portion of the beam the state of dislocation is zero. Finally, it is assumed that the state of stress is independent of  $x_1$ .

With the preceding assumptions the relevant equations reduce to [4, 5]

$$\sigma_{11,2} = -E(K_{31}^L + b_1 N_3) \quad (46)$$

$$0 = -E(K_{32}^L + b_2 N_3). \quad (47)$$

The component of the lattice curvature tensor,  $K_{31}^L$ , is the curvature of the neutral axis of the beam as shown by the following argument. Consider a strip of material in the plastic region having an original length,  $l$ , parallel to  $x_1$  and a thickness  $dx_2$  along  $x_2$  as shown in figure 2. The difference in the total strain between the top and bottom surfaces is

$$de_{11} = -Kdx_2 \quad (48)$$

where  $K$  is the curvature of the neutral axis. This difference is composed of a dislocation component, or plastic strain

$$de''_{11} = \frac{b_1 N_3 l dx_2}{l} \quad (49)$$

and a lattice strain component  $de'_{11}$ , which is elastic. Thus

$$de'_{11} = -(K_{31} + b_1 N_3) dx_2, \quad (50)$$

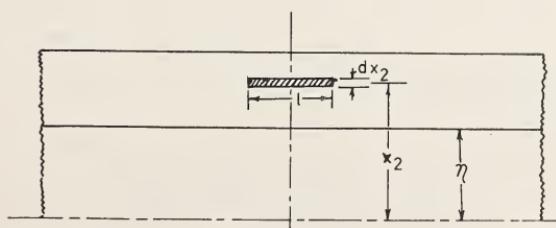


FIGURE 2. Model for decomposition of strain into plastic (dislocation) and elastic (lattice) components.

and by Hooke's Law

$$\sigma_{11,2} = -E(K + b_1 N_3), \quad (51)$$

showing that the lattice curvature appearing in eq (46) and the curvature of the neutral axis are identical.

In the plastic region the assumed stress distribution fixes the relation between the dislocation density and the curvature of the neutral axis.

In particular

$$-K = b_1 N_3 \quad (52)$$

in the plastic region.

The internal stress at a distance  $y$  from the neutral axis can be obtained by integrating eq (51) from  $x_2 = 0$  to  $x_2 = y$ ,

$$\sigma_{11} = -E \int_0^y (K + b_1 N_3) dx_2, \quad (53)$$

where the first term in the integrand gives the stress which would exist if the material obeyed Hooke's Law at  $x_2 = y$ , and the second term is the "stress relief" due to the dislocation stress field. The internal resisting moment,  $M$ , for a beam of rectangular cross section having thickness,  $t$ , along the  $x_3$  direction, can be obtained in the usual manner:

$$M = -2 \int_A \sigma_{11} y dA = 2E \int_0^c \int_0^y y(K_{31} + b_1 N_3) dx_2 dy, \quad (54)$$

where again the first term is the "Hookean" moment,  $M_E$ , and the second is the moment due to the stress fields of the dislocation array,  $M_p$ .

It is interesting to consider the significance of the integrals involving the dislocation distribution. Since  $N_3 = 0$  when  $y < \eta$ ,

$$\int_0^y N_3 dx_2 = \mathcal{N}(y) \quad (55)$$

is the net number of dislocations intersecting an area having dimensions of unity along  $x_1$  and  $(\eta - y)$  along  $x_2$ . The second integration gives the first moment of  $\mathcal{N}(y)$  about the axis of bending.

Integrating by parts

$$\int_\eta^c y \mathcal{N}(y) dy = [c^2 \mathcal{N}(c) - \int_\eta^c y^2 N_3 dy]/2, \quad (56)$$

where the first term involves the total number of dislocations (per unit length along  $x_1$ ) in the plastic zone, and the integral is the second moment of the dislocation density,  $N_3$ , about the axis of bending. Both of these

quantities can be determined analytically for particular dislocation distributions or experimentally on deformed specimens.

For the present problem, the dislocation density in the plastic region is constant (cf. eq (46)), hence

$$\mathcal{N}(y) = N_3(y - \eta) = -K(y - \eta)/b_1, \quad (57)$$

and the moment due to the stress field of the dislocation array is

$$M_p = -EKt[2c^3 - 3c^2\eta + \eta^3]/3. \quad (58)$$

The Hookean moment is simply

$$M_E = EKI, \quad (59)$$

and the net moment,  $M$ , is given by

$$M = M_E + M_p = EKt\eta[3c^2 - \eta^2]/3, \quad (60)$$

in agreement with the result of the continuum plasticity calculation.

Linear work-hardening can be introduced directly from eq (46). The physical consequences of such an assumption will now be examined. Let

$$\sigma_{11,2} = -r = -E(K + N_3b_1) \quad (61)$$

in the plastic zone. From eq (36) it is evident that

$$-r = \sigma^* \beta / \eta (1 + \beta). \quad (62)$$

The dislocation density is, then

$$N_3 = [(r/E) + K]/b_1, \quad (63)$$

which is evidently constant for a given curvature. The excess dislocation density,  $r/Eb_1$ , is thus proportional to the work-hardening rate. Hence, in a plastic region the rate of work-hardening can be determined by experimental measurements of  $K$  and  $N_3$  at various points in the region. The moment and curvature for the elastic-plastic beam can be found as before. In terms of  $r$

$$\frac{M}{t} = \{\sigma^*[3c^2 - \eta^2] + r[2c^3 - c^2\eta + \eta^3]\}/3. \quad (64)$$

The moment-curvature relation follows from the substitutions

$$c/\eta = K/K^* \text{ and } M^* = \sigma^* c^2 t$$

$$M = \frac{M^*}{3} \left[ 3 - \left( \frac{K^*}{K} \right)^2 \right] + \frac{M^* r}{3E} \left[ \frac{1}{K^*} - \frac{1}{K} + \frac{(K^*)^2}{K^3} \right] \quad (65)$$

where  $M^*$  and  $K^*$  are the moment and curvature at the instant of yielding of the outer fiber.

The moment-curvature relation can be expressed in terms of the dislocation density in the plastic region by substituting eqs (11) and (18) into eq (66):

$$\frac{M}{M^*} = \frac{1}{3} \left[ 3 - \left( \frac{K^*}{K} \right)^2 + \frac{(K + N_3 b_1)(K^3 - K^* K^2 + K^{*2})}{K^* K^3} \right]. \quad (66)$$

Note that for no work-hardening  $K = -N_3 b_1$  and the above reduces to the elastic-perfectly plastic result.

The above treatment now permits an interpretation of the empirical parameter  $\beta$  of the continuum plasticity result in terms of the dislocation content. From eqs (61) and (62),

$$\beta = \left( 1 + \frac{K}{N_3 b_1} \right); \quad (67)$$

thus  $\beta$  is a measure of the net dislocation density present in excess of that required to produce bending with a zero gradient of residual bending stress in the plastic region.

The advantage of the dislocation approach is to allow a physical interpretation of the assumptions of continuum plasticity. In the present case the assumption of a constant bending stress in the plastic region implies the following picture of deformation by bending. When a critical value of lattice strain,  $e_{11}^*$ , is obtained at the outer fiber of the beam, additional deformation may only be accomplished by the addition of dislocations. Clearly this is equivalent to assuming a critical shear strain on the active slip system. Furthermore, the dislocations must be arranged in such a manner that the lattice strain remains equal to the critical value throughout the plastic region. At first glance it seems unlikely that a uniform distribution of dislocation would satisfy such a requirement. It is therefore of interest to examine this point and to determine the effect of plastic deformation occurring by slip on planes inclined at various angles to the neutral axis. In the following sections, it is shown that the distribution of dislocations given by eq (52) does, in fact, give the correct stress distribution in the plastic region. Also, the effect of allowing the distribution to become discrete by introducing slip bands is examined.

The stress field of an edge dislocation in an infinite half-space has been given by Head for arbitrary orientation of the Burgers vectors to the free surface [6]. In the present case the results must be modified to correspond to the central plane of a beam in plane stress. This results in replacing the factor  $E/2(1 - \nu^2)$  in Head's results by  $E/2$ .

If the dislocations in the plastic region are uniformly distributed with a density given by eq (52), then the net Burgers vector of all dislocations crossing an element of area  $dz_1 dz_2$  is

$$B_1 = -Kdz_1 dz_2. \quad (68)$$

The stress field of such a "bundle" of edge dislocations is obtained by replacing the Burgers vector of an individual dislocation with Burgers vector parallel to the free surface with  $B_1$ . The stress field of the two-dimensional array is then obtained by integrating the field of these bundles over the entire plastic region. It is easily shown that  $\sigma''_{12}$  and  $\sigma''_{22}$  vanish for a beam having infinite length along  $x_1$ . The evaluation of  $\sigma''_{11}$  is somewhat more subtle, however. The stress components of dislocations lying near a free surface can be written in the usual manner as the stress components in an infinite body plus image terms. The image terms arise in part from image dislocations of opposite sense placed at equal distances on the opposite side of the free surface. Consider the contributions to the stress component  $\sigma''_{11}$  at the point  $(x_1, x_2)$  in the plastic region shown. The point lies in the tensile stress field of dislocations between  $x_2$  and  $c$ , but in the compressive stress field of their images. Although these do not cancel for a single dislocation, they do for an infinite array along the  $x_1$  axis or for a finite array in an infinite half-space, illustrated schematically in figure 3a. The point lies in the compressive stress field of dislocations between  $x_2$  and  $\eta$  and in the compressive field of their images as well. These superimpose to give the net stress component calculated below.

The value of the stress component depends on whether the general point is nearer or farther from the free surface than the dislocations. In the former case the stress fields of the image dislocations cancel those in the plastic region, while in the latter they add to give

$$\sigma''_{11} = \frac{EK}{4\pi} \int_{\eta}^{x_2} 4\pi dz_2; z_2 < x_2. \quad (69)$$

Since both  $x_2$  and  $z_2$  lie between  $c$  and  $\eta$ , the region in which  $z_2 < x_2$  is  $\eta < z_2 < x_2$ . Finally, the stress component is

$$\sigma''_{11} = EK(x_2 - \eta). \quad (70)$$

The stress in the plastic zone is then given by the sum of the stress which would exist at any point if Hookean behavior were obeyed (the "applied elastic stress" referred to by Mura [8]) and the stress due to the dislocation array. Thus,

$$\sigma_{11} = -EKx_2 + EK(x_2 - \eta) = -EK\eta = \sigma^*. \quad (71)$$

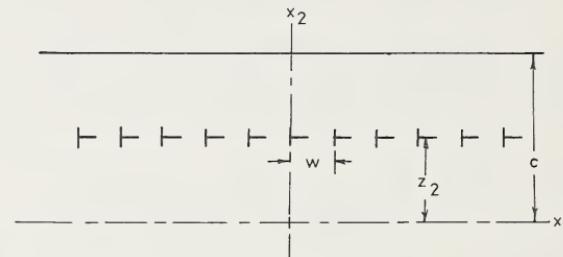
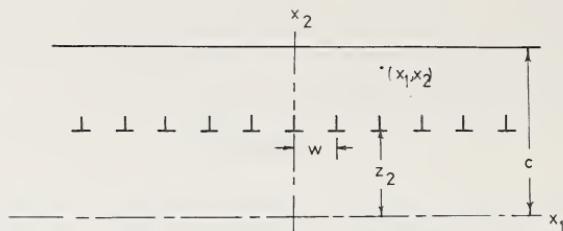


FIGURE 3(a). Infinite array of uniformly spaced edge dislocations with Burgers vectors parallel to a free surface.

FIGURE 3(b). Infinite array of uniformly spaced edge dislocations with Burgers vectors perpendicular to a free surface.

Since  $\eta$  is the elastic-plastic interface, the product  $K\eta$  is the critical lattice strain for yielding,  $e_{11}^*$ , which is constant. The yield stress is simply  $-EK\eta$ , that is, the value of the elastic stress at the elastic-plastic interface.

## V. Effect of Slip Geometry

In the following sections, the effect of slip geometry is considered. First note that in the present case the component of the net Burgers vectors parallel to the  $x_2$  axis can be expressed in terms of the curvature  $K$ :

$$B_2 = -K \cot \theta dx_1 dx_2. \quad (72)$$

Integration of the stress components as before shows that no net stress is developed due to  $B_2$ , as noted previously by Read [5].

The constancy of the stress component  $\sigma_{11}''$  can be interpreted as a constant resolved shear stress on the slip plane in the slip direction. This shear stress is

$$k = -(EK\eta)mn = \sigma^* \sin 2\theta/2. \quad (73)$$

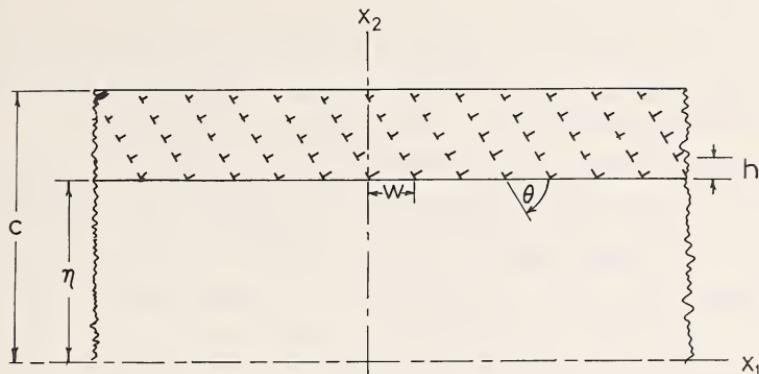


FIGURE 4. Edge dislocations in uniformly spaced slip bands.

The stress tending to produce climb can also be obtained by the usual transformation of stress components:

$$\sigma'_{11} = \sigma^* m^2 = \sigma^* \cos^2 \theta. \quad (74)$$

Thus introducing the concept of a continuous distribution of slip planes does not change the results. This observation was first made by Gardner [7].

The effect on introducing a discrete array of slip bands can be determined from an analysis of the stress field of the array shown in figure 4. The average dislocation density is assumed to be the same as that of the continuous array, thus

$$wh = w^2 \sin 2\theta/2 = 1/N_3 = -b_1/K. \quad (75)$$

The two-dimensional array shown can be analyzed as a distribution of infinite arrays which lie parallel to the free surface and which are composed of dislocations having a uniform spacing  $w$  along  $x_1$ . If we assume that the zeroth array is centered at  $(0, \eta)$ , the  $n$ th array is centered at  $(ns, \eta + nh)$  where  $s = h \tan \theta$ . The number of such arrays is

$$N = (c - \eta)/h. \quad (76)$$

Note that  $w$  and  $h$  are related to the curvature by eq (75).

The stress field of such a two-dimensional array is obtained in two steps. First, the stress field of the infinite array parallel to the free surface and centered at  $(0, \eta)$  is obtained by direct summation. Then the distribution of arrays is approximated by a continuous distribution along  $x_2$ , so that the Burgers vectors of dislocations in the array become

$$b_1(x_2) = \frac{b_1 dx_2}{h}; b_2(x_2) = \frac{b_1 \tan \theta dx_2}{h}; \quad (77)$$

the stress components are then integrated over the plastic region. The result for the continuous distribution can be obtained by taking the limit as  $w \rightarrow 0$ , while keeping  $K$  and  $b_1$  constant. The stress fields for the infinite arrays shown in figures 3a and 3b are given in [9].

The stress field of the two-dimensional array shown in figure 4 is obtained by replacing the Burgers vectors of individual dislocations in the array by eq (77) and integrating over the range  $\eta \leq z_2 \leq c$ . The results are given in [9]. Although the discrete distribution produces nonzero stress components other than  $\sigma_{11}^{(1)}$ , in all cases the limits as  $w \rightarrow 0$  of the components reduce to the continuous results, as they must.

The residual stress distribution in a plastically bent beam with zero net moment about  $x_3$  can be obtained by superimposing a Hookean state of stress arising from the application of a moment equal and opposite to that given by eq (66). Such a state of stress is

$$\sigma_{11} = -Mx_2/I, \quad (78)$$

all other components being zero. The net stress is then

$$\sigma_{11}^0 = \begin{cases} \sigma^* - r(x_2 - \eta) - Mx_2/I & \eta \leq x_2 \leq c \\ -EKx_2[2 - (3K^*/K) + (K^*/K)^3]/2 & 0 \leq x_2 < \eta. \end{cases} \quad (79)$$

The change in curvature when the external moment is removed (producing zero net moment) is simply

$$\Delta K = -M/EI, \quad (80)$$

hence the curvature of a bent elastic-plastic beam without external loads can be calculated in terms of the position of the elastic-plastic interface.

## VI. Summary

The elastic-plastic pure bending of a simply supported prismatic beam subjected to external moments on either end has been investigated from the viewpoints of continuum plasticity and dislocation theory, assuming plane stress and a constant bending stress in the plastic region. In the former case solutions are presented for a particular case of elastic anisotropy corresponding to the bending of an hexagonal close-packed metal by single slip. The yield criterion applied was that of a critical resolved shear stress on a slip system such that the slip direction is normal to the axis of bending. Strains and displacements in the elastic and plastic regions and the moment-curvature relation are obtained for both nonwork-hardening and linear work-hardening models of material behavior.

The dislocation approach employs the same assumptions (except for elastic anisotropy) to obtain the moment curvature relation and the state of dislocation in the plastic region. Also, a relation is obtained between the externally applied moment and various properties of the dislocation distribution. The relation is independent of any assumption concerning the yielding or flow behavior. Phenomenological coefficients appearing in the continuum plasticity treatment of linear work-hardening are shown to be related to the excess net dislocation density above that required to produce bending with a zero stress gradient in the plastic region. It is also shown that the model of no work-hardening corresponds to assuming a maximum lattice shear strain on the slip system.

The stress field of the two-dimensional dislocation array calculated from the assumed lattice stress distribution is shown to provide the required stress relief from the Hookean stress, i.e., that associated with Hookean behavior up to the total shape strain. It is also noted that a discrete distribution of dislocations in slip bands gives rise to nonzero components of the stress tensor in the plastic region other than the bending stress,  $\sigma_{11}$ . However, in the limit as the distribution becomes continuous, these go to zero.

The distribution of residual stresses in bent elastic-plastic beam with no applied moment and the change and curvature when an external moment is removed are calculated.

## VII. Acknowledgement

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# GENERALIZED STRESS AND NON-RIEMANNIAN GEOMETRY

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The general non-Riemannian approach to the geometry of a solid with lattice defects is briefly discussed. Non-Riemannian geometry is applied to the treatment of statics. The "stress" curvature tensor has the meaning of a generalized stress tensor with 27 components, while the associated Einstein tensor represents the classical stress tensor. The "stress" connexion expresses the generalized moment stress having 27 components. Its torsion tensor is the classical couple stress tensor.

The identities of the curvature tensors are identified with the static equilibrium conditions. Using a stress function density instead of a metric tensor, it is shown that the equilibrium conditions can always be identically fulfilled. A consistent theory involving lattice defects must necessarily involve also generalized moment stresses and generalized stresses.

**Key words:** Affine connection; continuum mechanics; non-Riemannian geometry; stress.

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## Introduction

Kondo [1] was probably the first to recognize that the geometry of an imperfect crystalline body can be appropriately represented in terms of a general non-Riemannian space. The notion was independently discovered by Bilby, Bullough, and Smith [2] and has since been very much developed, especially by the groups of Bilby [3] and Kröner [4], and from a somewhat different viewpoint by the school of Kondo [5, 6]. Recently, Bilby et al. [7] extended the analysis to include nonmetric connexions, and thus obtained an adequate continuum description of the geometrical properties of both dislocations and point defects. A fairly representative and up-to-date bibliography may be found in references [3, 6, 7].

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The importance of including couple stresses in a consistent continuum theory of lattice defects was pointed out by Kröner [4, 8]. Meanwhile, the theory of couple stresses, originated by E. and F. Cosserat [9], has been developed by a number of workers, from whom we shall mention only Erickson and Truesdell [10], Mindlin and Tiersten [11], and Toupin [12]. It must, however, be emphasized that the theory of couple stresses has been developed from an extremely phenomenological point of view, mainly in order to match the needs of the theory of thin shells. Of greatest importance in the present context is a paper by Eringen and Suhubi [13], who succeeded in eliminating the indeterminacies hitherto encountered in couple stress theories. They presented their results in a form which, though not explicitly stated by the authors, is suitable for direct interpretation in terms of continuously distributed lattice defects. Very recently Cohen and DeSilva [14], dealing with thin shells, introduced a stress tensor of valence 3 having 27 components, and thus presented the static counterpart of Bilby's geometrical theory [7].

Kröner [15, 16] and Eshelby [17] have put forward the application of three-dimensional tensorial stress functions to the determination of internal stresses in imperfect crystalline bodies. This has been done by generalizing the classical Beltrami-Michell equations to include incompatible strains. The stress functions can then be expressed in terms of the geometrical incompatibilities.

In the present paper we shall "geometrize the statics," i.e., we shall treat stress-functions, couple stresses and stresses as geometric quantities. This will enable us to apply the established formalism of nonriemannian differential geometry and thereby show that it is always possible to fulfill identically the static equilibrium conditions by deriving the stresses from stress-functions. Moreover, since the curvature tensor of the discussed space is identified with the stress tensor, the theory yields in a straightforward way the generalized 27-component stress of Cohen and DeSilva [14].

The terminology, the mathematical representation, and in particular the tensor notation will, except for minor deviations, closely adhere to those adopted by Schouten [18, 19]. The physical interpretation will follow the lines of the analyses by Kröner [4] and Bilby et al. [7].

## I. Geometry

For reference purposes and in order to clarify the notations, we shall briefly recall the essentials of the geometrical theory.

We imagine the solid under consideration to be initially a perfect stress-free crystal containing no extramatter. This *ideal* state will be labeled

[A]. The *plastic* (or dislocation) distortion P brings the solid into the *dislocated* state (first intermediate or first natural state according to Kröner [4]), labeled [A]. The introduction of extramatter, represented by the distortion Q, brings about a state which will be called *natural* (second intermediate or second natural in Kröner's terminology) and labeled [a]. Kröner calls the distortion Q quasiplastic and Bilby extramatter distortion. I suggest to coin the term "*qlastic*" distortion. This would fit the patterns "elastic" and "plastic" and might be interpreted as an abbreviation for quasiplastic reminding us of Q, and also reminiscent of the Greek word  $\kappa\lambda\alpha\sigma\tau\sigma\zeta$ =broken. Finally the *elastic* distortion E fits the plastically and qlastically distorted solid into ordinary Euclidian space and induces in it the *final* state, labeled [a]. The qlastic and elastic distortions Q, E, together form the *lattice* distortion L. The superposition of the plastic, qlastic and elastic distortions is the *total* distortion T.

All quantities referring to the above described fundamental states [A], [A], [a] and [a] will be denoted by *CAPITAL ITALICS*, *CAPITAL SCRIPT*, *smallscript* and *small italics*, respectively. The states themselves may for simplicity be specified by these terms if so desired. For symbols not specifically related to a particular state we chose a neutral type, namely Greek or ROMAN. Thus an arbitrary state will be denoted by [a] or [A].

The linear elements specifying the mutual position of two nearby particles (material points) of the solid in the states [A], [A], [a], [a] will be denoted by  $dX^\kappa$ ,  $d\mathcal{X}^\kappa$ ,  $d\mathcal{r}^\kappa$ ,  $dx^\kappa$ , respectively. Now we can write down the formal definitions of the fundamental distortions and their inverses (it is assumed that these always exist):

$$\begin{aligned}
 d\mathcal{X}^\kappa &= P_{\cdot\lambda}^\kappa dX^\lambda, & dX^\lambda &= D_{\cdot\kappa}^\lambda d\mathcal{X}^\kappa, & P_{\cdot\mu}^\kappa D_{\cdot\lambda}^\mu &= I_\lambda^\kappa, \\
 d\mathcal{r}^\kappa &= Q_{\cdot\lambda}^\kappa d\mathcal{X}^\lambda, & d\mathcal{X}^\lambda &= O_{\cdot\kappa}^\lambda d\mathcal{r}^\kappa, & Q_{\cdot\mu}^\kappa O_{\cdot\lambda}^\mu &= I_\lambda^\kappa, \\
 dx^\kappa &= E_{\cdot\lambda}^\kappa d\mathcal{r}^\lambda, & d\mathcal{r}^\lambda &= \mathcal{E}_{\cdot\kappa}^\lambda dx^\kappa, & E_{\cdot\mu}^\kappa \mathcal{E}_{\cdot\lambda}^\mu &= I_\lambda^\kappa, \\
 dX^\kappa &= L_{\cdot\lambda}^\kappa dx^\lambda, & dx^\lambda &= T_{\cdot\kappa}^\lambda dX^\kappa, & L_{\cdot\mu}^\kappa T_{\cdot\lambda}^\mu &= I_\lambda^\kappa.
 \end{aligned} \tag{1.1}$$

The inverse of a distortion D is here denoted by  $\mathbb{D}$  (upside down). The identity will be denoted by I having as its inverse  $\mathbb{I}$  again. This notation has proved to be very convenient. In accordance with their physical meaning, the distortions will always be treated as point transformations, and it is therefore the kernels that must be distinguished by different types. Our equations refer to some fixed but quite arbitrary coordinate system, ( $\kappa$ ). This fact is stressed by choosing neutral, viz,

Greek types for the indices. Of course, one will usually choose a coordinate system in which one of the fundamental states will be described most simply (say the final state in the Eulerian description and the ideal state in the Lagrangian description). This coordinate system will accordingly be labeled  $(K)$ ,  $(\mathcal{K})$ ,  $(\mathcal{A})$  or  $(k)$  and one will have, for instance

$$d\mathcal{E}^k = P^k_l dX^l \quad (1.2)$$

for the Eulerian definition of the plastic distortion etc.

Static quantities will, nevertheless, usually be denoted by Greek letters, in order to adhere to common usage. This will, however, cause no confusion, since the statics will throughout be given in the final state representation.

To every point transformation there belongs a certain coordinate transformation, such that the coordinate system is dragged along by the point transformation. Formally this is expressed by the equations:

$$\begin{aligned} d\xi^K &= \delta_{\kappa}^K dX^{\kappa}, \\ d\xi^{\mathcal{K}} &= \delta_{\kappa}^{\mathcal{K}} d\mathcal{X}^{\kappa}, \\ d\xi^{\mathcal{A}} &= \delta_{\kappa}^{\mathcal{A}} d\mathcal{A}^{\kappa}, \\ d\xi^k &= \delta_{\kappa}^k dx^{\kappa}, \end{aligned} \quad (1.3)$$

where now the kernel has become neutral (Greek). Using this trick, the fundamental distortions will now be written:

$$\begin{aligned} I_{\mathcal{L}}^{\mathcal{K}} &= \delta_{\kappa}^{\mathcal{K}} P_{\lambda}^{\kappa} \delta_{\mathcal{L}}^{\lambda}, & I_{\mathcal{K}}^L &= \delta_{\lambda}^L d_{\kappa}^{\lambda} \delta_{\mathcal{K}}^{\kappa}, \\ I_{\mathcal{L}}^{\mathcal{A}} &= \delta_{\kappa}^{\mathcal{A}} Q_{\lambda}^{\kappa} \delta_{\mathcal{L}}^{\lambda}, & I_{\mathcal{A}}^{\mathcal{L}} &= \delta_{\lambda}^{\mathcal{L}} O_{\kappa}^{\lambda} \delta_{\mathcal{A}}^{\kappa}, \\ I_{\mathcal{L}}^k &= \delta_{\kappa}^k E_{\lambda}^{\kappa} \delta_{\mathcal{L}}^{\lambda}, & I_k^{\mathcal{L}} &= \delta_{\lambda}^{\mathcal{L}} \mathcal{E}_{\kappa}^{\lambda} \delta_k^{\kappa}, \\ I_l^{\mathcal{K}} &= \delta_{\kappa}^{\mathcal{K}} L_{\lambda}^{\kappa} \delta_l^{\lambda}, & I_l^L &= \delta_{\lambda}^L T_{\kappa}^{\lambda} \delta_k^{\kappa}. \end{aligned} \quad (1.4)$$

This is the method adopted by Kröner. Bilby's notation is redundant, since he usually writes the equivalents of  $dX^k$ ,  $d\mathcal{X}^{\mathcal{K}}$ ,  $d\mathcal{A}^{\mathcal{A}}$ ,  $dx^k$  etc.

When dealing with more general problems involving an arbitrary number of point and/or coordinate transformations, it will be worthwhile to have a more fancy notation. One then replaces the kernel letters of the transformations by two-index symbols, such as

$$[\mathcal{A} \cdot] \cdot \lambda \equiv P^{\kappa} \cdot \lambda \quad (1.5)$$

etc., clearly indicating that the plastic distortion  $P$  transforms the state  $[A]$  into  $[\mathcal{A}]$ . Here the sign  $\equiv$  stands for “equal by definition.” Usually one will, of course, have to label the states by an index. Obviously, this notation extends the advantages of the kernel-index method to point transformations. Since we are, however, dealing only with a few fundamental distortions, we shall not use this method, in order to keep the notation as simple as possible to match our present needs.

We shall denote the distance between two fixed neighboring elements in the fundamental states by  $dL$  etc., and for each state we shall define a corresponding metric tensor  $A_{\kappa\lambda}$  etc. by the relations

$$\begin{aligned} dL^2 &= A_{\kappa\lambda} dX^{\kappa} dX^{\lambda}, \\ d\mathcal{L}^2 &= \mathcal{A}_{\kappa\lambda} d\mathcal{X}^{\kappa} d\mathcal{X}^{\lambda}, \\ d\ell^2 &= a_{\kappa\lambda} d\alpha^{\kappa} d\alpha^{\lambda}, \\ dl^2 &= a_{\kappa\lambda} dx^{\kappa} dx^{\lambda}. \end{aligned} \quad (1.6)$$

These metric tensors are essentially arbitrary and may for convenience be chosen as Kronecker deltas in some fixed coordinate system. Thus:

$$A_{\kappa\lambda} = \mathcal{A}_{\kappa\lambda} = a_{\kappa\lambda} = a_{\kappa\lambda}^* = \delta_{\kappa\lambda}. \quad (1.7)$$

Really meaningful metric tensors are however obtained when the length in a given state (e.g.,  $dL$ ) is related to the linear elements in another state (e.g.,  $dx^{\kappa}$ ). Thus we shall have for instance:

$$\begin{aligned} dL^2 &= G_{\kappa\lambda} dx^{\kappa} dx^{\lambda} = H_{\kappa\lambda} dX^{\kappa} dX^{\lambda}, \\ d\mathcal{L}^2 &= \mathcal{G}_{\kappa\lambda} d\mathcal{X}^{\kappa} d\mathcal{X}^{\lambda} = \mathcal{H}_{\kappa\lambda} dX^{\kappa} dX^{\lambda}, \\ d\ell^2 &= g_{\kappa\lambda} d\alpha^{\kappa} d\alpha^{\lambda} = h_{\kappa\lambda} dX^{\kappa} dX^{\lambda}, \\ dl^2 &= g_{\kappa\lambda} dx^{\kappa} dx^{\lambda} = h_{\kappa\lambda} dX^{\kappa} dX^{\lambda}. \end{aligned} \quad (1.8)$$

Here, of course, one of the metric tensors is still arbitrary, and one has

$$g_{\kappa\lambda} = a_{\kappa\lambda}, \quad H_{\kappa\lambda} = A_{\kappa\lambda}. \quad (1.9)$$

The metric tensors can be expressed in terms of the fundamental distortions. Since, for instance,

$$dL^2 = A_{\kappa\lambda} dX^\kappa dX^\lambda = A_{\kappa\lambda} L^\kappa_\nu dx^\mu L^\lambda_\nu dx^\nu = G_{\mu\nu} dx^\mu dx^\nu,$$

we obtain

$$G_{\mu\nu} = L^\kappa_\mu A_{\kappa\lambda} L^\lambda_\nu,$$

$$\mathcal{G}_{\mu\nu} = T^\kappa_\mu \mathcal{A}_{\kappa\lambda} T^\lambda_\nu,$$

(1.10)

$$\mathcal{F}_{\mu\nu} = E^\kappa_\mu \alpha_{\kappa\lambda} E^\lambda_\nu,$$

$$g_{\mu\nu} = I^\kappa_\mu a_{\kappa\lambda} I^\lambda_\nu = a_{\mu\nu}.$$

Now we can define the strain tensors as usual. The Eulerian strain tensors are defined by the relations

$$d\mathcal{L}^2 - dL^2 = (\mathcal{G}_{\kappa\lambda} - G_{\kappa\lambda}) dx^\kappa dx^\lambda \equiv 2\pi_{\kappa\lambda} dx^\kappa dx^\lambda,$$

$$d\ell^2 - d\mathcal{L}^2 = (\mathcal{F}_{\kappa\lambda} - \mathcal{G}_{\kappa\lambda}) dx^\kappa dx^\lambda \equiv 2q_{\kappa\lambda} dx^\kappa dx^\lambda,$$

$$dl^2 - d\ell^2 = (g_{\kappa\lambda} - \mathcal{F}_{\kappa\lambda}) dx^\kappa dx^\lambda \equiv 2\epsilon_{\kappa\lambda} dx^\kappa dx^\lambda, \quad (1.11)$$

$$dl^2 - dL^2 = (g_{\kappa\lambda} - G_{\kappa\lambda}) dx^\kappa dx^\lambda \equiv 2\tau_{\kappa\lambda} dx^\kappa dx^\lambda,$$

$$dl^2 - d\mathcal{L}^2 = (g_{\kappa\lambda} - \mathcal{G}_{\kappa\lambda}) dx^\kappa dx^\lambda \equiv 2\lambda_{\kappa\lambda} dx^\kappa dx^\lambda.$$

Hence, the Eulerian plastic, plastic, elastic, total and lattice strain tensors are, respectively:

$$\pi_{\kappa\lambda} = \frac{1}{2} (\mathcal{G}_{\kappa\lambda} - G_{\kappa\lambda}),$$

$$q_{\kappa\lambda} = \frac{1}{2} (\mathcal{F}_{\kappa\lambda} - \mathcal{G}_{\kappa\lambda}),$$

$$\epsilon_{\kappa\lambda} = \frac{1}{2} (g_{\kappa\lambda} - \mathcal{F}_{\kappa\lambda}), \quad (1.12)$$

$$\tau_{\kappa\lambda} = \frac{1}{2} (g_{\kappa\lambda} - G_{\kappa\lambda}),$$

$$\lambda_{\kappa\lambda} = \frac{1}{2} (g_{\kappa\lambda} - \mathcal{G}_{\kappa\lambda}).$$

In an analogous way one defines the lagrangian strain tensors

$$\begin{aligned} \Pi_{\kappa\lambda} &\equiv \frac{1}{2} (\mathcal{H}_{\kappa\lambda} - H_{\kappa\lambda}), \\ Q^{\kappa\lambda} &\equiv \frac{1}{2} (\mathcal{H}_{\kappa\lambda} - \mathcal{H}_{\kappa\lambda}), \\ E_{\kappa\lambda} &\equiv \frac{1}{2} (h_{\kappa\lambda} - \mathcal{H}_{\kappa\lambda}), \\ T_{\kappa\lambda} &\equiv \frac{1}{2} (h_{\kappa\lambda} - H_{\kappa\lambda}), \\ \Lambda_{\kappa\lambda} &\equiv \frac{1}{2} (h_{\kappa\lambda} - \mathcal{H}_{\kappa\lambda}). \end{aligned} \quad (1.13)$$

The connexions associated with the fundamental states are defined as

$$\begin{aligned} B_{\kappa\lambda}^{\mu} &\equiv I_{\cdot\nu}^{\mu} \partial_{\kappa} I_{\cdot\lambda}^{\nu} \equiv 0, \\ \mathcal{B}_{\kappa\lambda}^{\mu} &\equiv d_{\cdot\nu}^{\mu} \partial_{\kappa} P_{\cdot\lambda}^{\nu}, \\ \mathcal{A}_{\kappa\lambda}^{\mu} &\equiv d_{\cdot\rho}^{\mu} \bar{O}_{\cdot\nu}^{\rho} \partial_{\kappa} Q_{\cdot\sigma}^{\nu} P_{\cdot\lambda}^{\sigma}, \\ b_{\kappa\lambda}^{\mu} &\equiv L_{\cdot\nu}^{\mu} \partial_{\kappa} T_{\cdot\lambda}^{\nu}. \end{aligned} \quad (1.14)$$

The connexion  $b_{\kappa\lambda}^{\mu}$  is the most important one. With the restriction to holonomic coordinate systems, every connexion can be written as the sum of a Riemannian connexion and a tensor:

$$\begin{aligned} \mathcal{B}_{\kappa\lambda}^{\mu} &= \mathcal{G}^{\mu\sigma} (\mathcal{G}_{\{\kappa\sigma\lambda\}} - \mathcal{S}_{\{\kappa\sigma\lambda\}}), \\ \mathcal{A}_{\kappa\lambda}^{\mu} &= \mathcal{G}^{\mu\sigma} (\mathcal{G}_{\{\kappa\sigma\lambda\}} - \mathcal{A}_{\{\kappa\sigma\lambda\}} + \mathcal{G}_{\{\kappa\sigma\lambda\}}), \\ b_{\kappa\lambda}^{\mu} &= g^{\mu\sigma} (g_{\{\kappa\sigma\lambda\}} - s_{\{\kappa\sigma\lambda\}} + q_{\{\kappa\sigma\lambda\}}). \end{aligned} \quad (1.15)$$

Here we have defined

$$2g_{\kappa\lambda\mu} \equiv \partial_{\kappa} g_{\lambda\mu}, \quad (1.16)$$

$$s_{\kappa\lambda\mu} \equiv b^{\mu}_{[\kappa\lambda]}, \quad (1.17)$$

$$s_{\kappa\lambda\mu} \equiv g_{\mu\sigma} s_{\kappa\lambda}{}^{\sigma}, \quad (1.18)$$

$$2q_{\kappa\lambda\mu} \equiv -\overset{b}{\nabla}_\kappa g_{\lambda\mu} = -\partial_\kappa g_{\lambda\mu} + b_{\kappa\lambda}^\sigma g_{\sigma\mu} + b_{\kappa\mu}^\sigma g_{\sigma\lambda}, \quad (1.19)$$

$$\phi_{\{\kappa\lambda\mu\}} \equiv \phi_{\kappa\lambda\mu} - \phi_{\lambda\mu\kappa} + \phi_{\mu\kappa\lambda}, \quad (1.20)$$

and analogous definitions for quantities associated with other states.

The *torsion* tensor  $s_{\kappa\lambda\mu}$  describes the distribution of dislocations and the *ammetry* tensor  $q_{\kappa\lambda\mu}$  describes the distribution of extramatter. It should be emphasized that the *physical* entities, i.e., the lattice defects, are always represented by *tensors*.

Since the solid that has undergone a total distortion again fits into the Euclidean space, the connexion  $b_{\kappa\lambda}^\mu$  must be integrable. The integrability condition is the vanishing of the associated curvature tensor

$$c_{\kappa\lambda\mu}^\nu \equiv 2\partial_{[\kappa} b_{\lambda]\mu}^\nu + 2b_{[\kappa|\sigma|}^\nu b_{\lambda]\mu}^\sigma. \quad (1.21)$$

Hence the *fundamental geometric equation*, or else the *generalized compatibility condition* is

$$c_{\kappa\lambda\mu}^\nu = 0, \quad (1.22)$$

where now the curvature tensor  $c_{\kappa\lambda\mu}^\nu$  has to be expressed in terms of the distributions of lattice defects.

A general curvature tensor can always be expressed as the sum of a Riemannian curvature tensor  $r_{\kappa\lambda\mu}^\nu$  and terms depending on the non-Riemannian, tensorial part of the connexion:

$$c_{\kappa\lambda\mu}^\nu = r_{\kappa\lambda\mu}^\nu + 2\overset{g}{\nabla}_{[\kappa} t_{\lambda]}^\nu + 2t_{[\kappa|\sigma|}^\nu t_{\lambda]\mu}^\sigma, \quad (1.23)$$

where

$$r_{\kappa\lambda\mu}^\nu \equiv 2\partial_{[\kappa} g_{\lambda]\mu}^\nu + 2g_{[\kappa|\sigma|}^\nu g_{\lambda]\mu}^\sigma, \quad (1.24)$$

$$g_{\kappa\lambda}^\mu \equiv g^{\mu\sigma} g_{\{\kappa\sigma\lambda\}}, \quad (1.25)$$

$$t_{\kappa\lambda}^\mu \equiv g^{\mu\sigma} (-s_{\{\kappa\sigma\lambda\}} + q_{\{\kappa\sigma\lambda\}}), \quad (1.26)$$

and  $\overset{g}{\nabla}$  is the operator of the covariant derivative with respect to the Riemannian connection  $g_{\kappa\lambda}^\mu$ .

Instead of (1.22) we can now write the equation

$$r_{\kappa\lambda\mu}^\nu = -2\overset{g}{\nabla}_{[\kappa} t_{\lambda]\mu}^\nu + 2t_{[\kappa|\sigma|}^\nu t_{\lambda]\mu}^\sigma. \quad (1.27)$$

Here the right-hand side defined by the defect-distribution tensor  $t_{\kappa\lambda}^\mu$  can be interpreted as the incompatibility associated with the lattice defects.

Since the identities valid for the Riemann tensor  $r_{\kappa\lambda\mu}{}^\nu$  restrict the number of its essential components to 6, it can be equivalently represented by the associated symmetric Einstein tensor

$$k_{\kappa\lambda} \equiv r_{\sigma\kappa\lambda}{}^\sigma - \frac{1}{2} g_{\kappa\lambda} g^{\mu\nu} r_{\sigma\mu\nu}{}^\sigma. \quad (1.28)$$

Performing the operations prescribed by (1.28) on the right-hand side of (1.27) we obtain the usual symmetric incompatibility tensor  $i_{\kappa\lambda} = i_{\lambda\kappa}$ , so that we have six conditions

$$k_{\kappa\lambda} = i_{\kappa\lambda}. \quad (1.29)$$

Equations (1.27) however yields 18 additional relations with a zero left-hand side.

## II. Classical Statics

We can now proceed towards our goal, namely the geometrization of statics. We shall, however, not treat the most general case at once, but we shall start with a demonstration of our procedure in the instance of classical elasticity theory (CET). Thus we shall have the advantage of considerable simplicity, while retaining most of the essential features of our program. We shall throughout stick to the eulerian representation, since the equilibrium of forces is maintained in the final state  $[a]$ .

In the framework of CET the state of stress of a deformed solid body is described by the *stress tensor density*  $\hat{\sigma}_{\kappa\lambda}$ ; this is a symmetric tensor density of weight +1. The weight of a density will be denoted by the number of carets above the kernel letter for positive weights, or below the kernel letter for negative weights. Thus  $\hat{g}$  denotes a scalar density of weight +2,  $\hat{\mathcal{Q}}_{\kappa\lambda\mu\nu}$  a 4-valent covariant tensor density of weight -1 (or tensor capacity of weight 1). This notation perfectly fits our purpose, since we shall not need weights higher than 2.

The static equilibrium conditions in CET are

$$\nabla_\kappa \hat{\sigma}^{\kappa\lambda} + \hat{f}^\lambda = 0, \quad (2.1)$$

$$\hat{\sigma}^{[\kappa\lambda]} = 0, \quad (2.2)$$

where  $\hat{f}^\lambda$  is the vector density of volume forces of weight +1.

The equilibrium conditions (2.1), (2.2), respectively, bear a striking similarity to the Bianchi identity and the fourth identity for the Riemann

tensor, when written out for the Einstein tensor. Essentially the three remaining identities for the Riemann tensor are also contained here, since the construction of an Einstein tensor equivalent to the Riemann tensor is only possible when these identities hold.

The analogy between the static equilibrium conditions and the curvature identities is not at all accidental and we shall make it the essential point of our program.

First we shall reconstruct from  $\hat{\sigma}^{\kappa\lambda}$  the full Riemann tensor or rather its density. We shall apply the Levi-Civita tensor densities defined by

$$\hat{e}^{\kappa\lambda\mu} = \hat{e}^{[\kappa\lambda\mu]}, \quad \hat{e}^{123} \equiv +1, \quad (2.3)$$

$$\hat{e}_{\kappa\lambda\mu} = \hat{e}_{[\kappa\lambda\mu]}, \quad \hat{e}_{123} \equiv +1. \quad (2.4)$$

Now we construct the 4-valent covariant stress tensor density

$$\sigma_{\kappa\lambda\mu\nu} \equiv \hat{e}_{\kappa\lambda\rho} \hat{e}_{\mu\nu\sigma} \hat{\sigma}^{\rho\sigma} \quad (2.5)$$

and the corresponding representation of the volume force density

$$f_{\kappa\lambda\mu\nu} \equiv \hat{e}_{\kappa\lambda} \hat{e}_{\mu\nu\sigma} \hat{f}^{\sigma}. \quad (2.6)$$

Rewriting eq (2.1) in this representation we obtain

$$\nabla_{[\kappa} \sigma_{\lambda]\mu\nu} = - f_{\kappa\lambda\mu\nu}, \quad (2.7)$$

which has, except for the signs of density, already the form of a general Bianchi identity:

$$\nabla_{[\kappa} C_{\lambda]\mu\nu} = 2S_{[\kappa} \sigma_{\lambda]\sigma\mu\nu}, \quad (2.8)$$

since by definition

$$f_{\kappa\lambda\mu\nu} = f_{[\kappa\lambda]\mu\nu}. \quad (2.9)$$

The Bianchi-identity (2.8) can be written in a more convenient form, using the operator  $\nabla^2$  defined for tensors alternating in the first 2 indices:

$$\nabla^2_{[\kappa} C_{\lambda]\mu\nu} \equiv \nabla_{[\kappa} C_{\lambda]\mu\nu} - 2S_{[\kappa} \sigma_{\lambda]\sigma\mu\nu}, \quad (2.10)$$

(for a general definition of  $\overset{n}{\nabla}$  cf. ref. 19, p. 149 ff). Then we have instead of (2.8)

$$\overset{2}{\nabla}_{[\iota} C_{\kappa\lambda]\mu\nu} = 0. \quad (2.11)$$

It is easy to see from the comparison of (2.8) and (2.9) that a given volume force density  $\hat{f}^\lambda$  induces in addition to the Riemannian connection  $g_{\kappa\lambda}^\mu$  a semisymmetrical tensorial term

$$p_{\kappa\lambda}^\mu \equiv p_{[\kappa} I_{\lambda]}^\mu, \quad (2.12)$$

with

$$p_\kappa \equiv \frac{3}{2} \varrho_{\kappa\lambda} \hat{f}^\lambda, \quad (2.13)$$

where  $\varrho_{\kappa\lambda}$  is the inverse of the stress tensor density  $\hat{\sigma}^{\kappa\lambda}$ , and thus is defined by

$$\varrho_{\kappa\mu} \hat{\sigma}^{\mu\lambda} = I_\kappa^\lambda. \quad (2.14)$$

A nonvanishing volume force density implies a nonsingular stress tensor density and therefore the existence of the inverse  $\varrho_{\kappa\lambda}$  in all cases of interest.

From a practical point of view the representation of the volume force density  $\hat{f}^\lambda$  by the vector  $p_\kappa$  is as good as useless, since in order to determine  $p_\kappa$  one has first to compute  $\hat{\sigma}^{\kappa\lambda}$  and  $\varrho_{\kappa\lambda}$ , which are ultimately determined by  $\hat{f}^\lambda$ . However, it shows that assuming a general connexion, one already covers the case of nonvanishing volume forces, and therefore the treatment can in principle be simplified. Since, moreover, we are primarily interested in internal stresses due to lattice defects, it will be fully justified to simplify our exposure by assuming

$$\hat{f}^\lambda = 0. \quad (2.15)$$

Now the equilibrium condition (2.1) becomes

$$\nabla_\kappa \hat{\sigma}^{\kappa\lambda} = 0. \quad (2.16)$$

Ever since Beltrami [20] it has been well known that this equation can be identically fulfilled by deriving the stress tensor  $\sigma^{\kappa\lambda}$  from a symmetric stressfunction density of weight -2:

$$\sigma^{\kappa\lambda} = \frac{1}{4} \hat{e}^{\kappa\mu\rho} \hat{e}^{\lambda\nu\sigma} \nabla_\mu \nabla_\nu \gamma_{\rho\sigma}, \quad (2.17)$$

where

$$\sigma^{\kappa\lambda} \equiv \frac{\hat{\sigma}^{\kappa\lambda}}{\sqrt{\hat{g}}} \quad (2.18)$$

$$\hat{g} \equiv \frac{1}{6} \hat{e}^{\alpha\beta\gamma} \hat{e}^{\kappa\lambda\mu} g_{\alpha\kappa} g_{\beta\lambda} g_{\gamma\mu}$$

$$= \text{Det } (g_{\kappa\lambda}). \quad (2.19)$$

Since one will usually choose  $g_{\kappa\lambda} = \delta_{\kappa\lambda}^*$ , the definitions (2.18), (2.19) do not, in fact, complicate matters.

It can now immediately be recognized that the relation between  $\gamma_{\kappa\lambda}$  and  $\hat{\sigma}^{\kappa\lambda}$  is essentially the same as between the density  $g_{\kappa\lambda}/\hat{g}$  derived from a Riemannian metric tensor  $g_{\kappa\lambda}$  and the associated Einstein tensor  $g^{\kappa\lambda}$ .

Let us now proceed to construct the theory, first for CET. The basic quantity is the symmetric stressfunction tensor density  $\gamma_{\kappa\lambda}$  of weight -2, which is assumed to be a function of the coordinates differentiable as many times as necessary. The tensor (density)  $\gamma_{\kappa\lambda}$  and its inverse  $\hat{\gamma}^{\kappa\lambda}$  will be used instead of fundamental tensors to raise and lower indices. This can be interpreted as defining in the manifold of  $x^\kappa$  a new "stress" metric  $\gamma_{\kappa\lambda}$  not directly connected with the strain metric  $g_{\kappa\lambda}$ . While  $\gamma_{\kappa\lambda}$  is a bicapacity with respect to  $g_{\kappa\lambda}$  it will be a tensor with respect to itself.

From  $\gamma_{\kappa\lambda}$  we construct first a Riemannian connexion (density of weight -2):

$$\beta_{\kappa\lambda\mu} \equiv \frac{1}{2} \partial_{\kappa} \gamma_{\lambda\mu}, \quad (2.20)$$

By raising the index  $\lambda$  in (2.20) we obtain the connexion

$$\beta_{\kappa\mu}^\nu \equiv \hat{\lambda}^{\nu\sigma} \beta_{\kappa\sigma\mu} = \frac{1}{2} \hat{\lambda}^{\nu\sigma} \partial_{\kappa} \gamma_{\sigma\mu}. \quad (2.21)$$

We form the Riemannian curvature tensor  $\rho_{\kappa\lambda\mu}^{\nu}$  associated with the connexion  $\beta_{\kappa\lambda}^{\mu}$ , according to the definition

$$\rho_{\kappa\lambda\mu}^{\nu} \equiv 2\partial_{[\kappa}\beta_{\lambda]\mu}^{\nu} + 2\beta_{[\kappa|\sigma|\beta_{\lambda]\mu}^{\sigma}} \quad (2.22)$$

and now construct the tensor (density)

$$\rho_{\kappa\lambda\mu\nu} \equiv \gamma_{\nu\sigma}\rho_{\kappa\lambda\mu}^{\sigma} \quad (2.23)$$

Instead of (2.22) one can, with the same result, also define:

$$\rho_{\kappa\lambda\mu\nu} \equiv 2\partial_{[\kappa}\beta_{\lambda]\mu\nu} + 2\hat{\lambda}^{\rho\sigma}\beta_{[\kappa|\rho\nu|\beta_{\lambda]\mu\sigma}}. \quad (2.24)$$

Now obviously,  $\rho_{\kappa\lambda\mu}^{\nu}$  is a Riemann tensor, and therefore the density  $\rho_{\kappa\lambda\mu\nu}$  fulfills the identities

$$\begin{aligned} \text{(I)} \quad & \rho_{(\kappa\lambda)\mu\nu} = 0, \\ \text{(II)} \quad & \rho_{[\kappa\lambda\mu\nu]} = 0, \\ \text{(III)} \quad & \rho_{\kappa\lambda(\mu\nu)} = 0, \\ \text{(IV)} \quad & \rho_{\kappa\lambda\mu\nu} = \rho_{\nu\mu\kappa\lambda}, \end{aligned} \quad (2.25)$$

and the identity of Bianchi in the form

$$\nabla_{[\kappa}\rho_{\lambda]\mu\nu} = 0. \quad (2.26)$$

From the identities (I), (II), (III) (2.25) it follows that  $\rho_{\kappa\lambda\mu\nu}$  can equivalently be replaced by the associated Einstein tensor. In the 3-dimensional case this can be constructed in a most simple way by means of the Levi-Civita density, as follows:

$$\sigma^{\alpha\beta} \equiv \frac{1}{4}\hat{e}^{\alpha\kappa\lambda}\hat{e}^{\beta\mu\nu}\rho_{\kappa\lambda\mu\nu}, \quad (2.27)$$

and

$$\hat{\sigma}^{\kappa\lambda} \equiv \sqrt{\hat{g}} \sigma^{\kappa\lambda}.$$

In terms of  $\hat{\sigma}^{\kappa\lambda}$  the Bianchi identity and the identity (IV) become

$$\nabla_\kappa \hat{\sigma}^{\kappa\lambda} = 0, \quad (2.29)$$

$$\hat{\sigma}^{[\kappa\lambda]} = 0. \quad (2.30)$$

The tensor density  $\hat{\sigma}^{\kappa\lambda}$  must obviously be identified with the stress tensor density. One sees that the stress tensor plays the part of the Einstein tensor (or if written with the 4-index notation, the Riemann tensor) in a space where the stressfunction density  $\gamma_{\kappa\lambda}$  corresponds to  $g_{\kappa\lambda}/\hat{g}$ .

We have now essentially achieved our goal, in that we have shown that a stress tensor (density) can always be constructed as the curvature tensor (density) associated with a symmetric stressfunction tensor (density) as metric tensor. This construction automatically ensures the fulfillment of the equilibrium conditions (2.29), (2.30), identical with (2.16) and (2.2). At this point one has to use the constituting equations, which define  $\hat{\sigma}^{\kappa\lambda}$  in terms of the elastic strain tensor  $\epsilon_{\kappa\lambda}$  (and vice versa). According to (1.12) we have in the case of CET

$$\epsilon_{\kappa\lambda} = \frac{1}{2} (g_{\kappa\lambda} - G_{\kappa\lambda}), \quad (2.31)$$

where  $g_{\kappa\lambda}$  (or alternatively  $G_{\kappa\lambda}$ ) is an arbitrary symmetric tensor and may in some coordinate system be chosen as

$$g_{\kappa\lambda}^* = \delta_{\kappa\lambda}. \quad (2.32)$$

Therefore the constituting equations define  $G_{\kappa\lambda}$  in terms of  $\hat{\sigma}^{\kappa\lambda}$ . We shall assume, for the sake of simplicity, the constituting equations to be in the form of Hooke's law

$$\begin{aligned} \hat{\sigma}^{\kappa\lambda} &= \hat{C}^{\kappa\lambda\mu\nu} \epsilon_{\mu\nu}, \\ \epsilon_{\mu\nu} &= \mathcal{Q}_{\mu\nu\kappa\lambda} \hat{\sigma}^{\kappa\lambda}. \end{aligned} \quad (2.33)$$

We obtain

$$\begin{aligned} G_{\mu\nu} &= g_{\mu\nu} - 2\epsilon_{\mu\nu} \\ &= g_{\mu\nu} - 2\mathcal{Q}_{\mu\nu\kappa\lambda} \hat{\sigma}^{\kappa\lambda}. \end{aligned} \quad (2.34)$$

Now we form the Riemann tensor  $R_{\kappa\lambda\mu}{}^\nu$  associated with  $G_{\mu\nu}$  according to the usual rules. Again we may replace the Riemann tensor  $R_{\kappa\lambda\mu}{}^\nu$  by its associated Einstein tensor  $K_{\kappa\lambda} = K_{\lambda\kappa}$ . Since both the initial state  $[A]$  and the final state  $[a]$  fit into the Euclidean space, we have the 6 compatibility conditions

$$K_{\kappa\lambda} = 0. \quad (2.35)$$

When  $K_{\kappa\lambda}$  is expressed through (2.34) in terms of  $\hat{\sigma}^{\kappa\lambda}$  these equations are the Beltrami equations. If, moreover, we express here  $\hat{\sigma}^{\kappa\lambda}$  through (2.28), (2.24) and (2.20) in terms of  $\hat{\gamma}_{\kappa\lambda}$ , we obtain 6 partial differential equations of the 4th order for the 6 functions  $\hat{\gamma}_{\kappa\lambda}$ . However, since a coordinate transformation involves 3 arbitrary parameters, we can choose in a particular coordinate system 3 of the components of  $\hat{\gamma}_{\kappa\lambda}$  at will, and fulfill 3 equations identically. For a Cartesian coordinate system the choice is either Maxwell's ( $\hat{\gamma}_{\kappa\lambda} = 0, \kappa \neq \lambda$ ) or Morera's ( $\hat{\gamma}_{\kappa\kappa} = 0$ ). This topic has been extensively discussed by many authors (cf. ref. 16, p. 55 ff.).

### III. Generalized Stress

We are now ready to generalize our results to the case that is of real interest, namely when the connexion  $\beta_{\kappa\lambda}^\mu$  is neither symmetric nor metric, i.e., there are nontrivial distributions of dislocations and point defects throughout the solid, which, as will be seen, are equivalent to couple stresses and double force stresses.

Let us assume a stress connexion  $\beta_{\kappa\lambda}^\mu$  defined throughout the solid. The connexion defines a covariant derivative. Let us introduce a symmetric stressfunction tensor (density)  $\hat{\gamma}_{\kappa\lambda}$  and its inverse  $\hat{\lambda}^{\kappa\lambda}$ .

Let us now define the ammetry  $\psi_{\kappa\lambda\mu}$  of  $\hat{\gamma}_{\kappa\lambda}$  with respect to  $\beta_{\kappa\lambda}^\mu$ :

$$\psi_{\kappa\lambda\mu} \equiv -\frac{1}{2} \hat{\nabla}_\kappa^\beta \hat{\gamma}_{\lambda\mu}. \quad (3.1)$$

As before we now obtain

$$\beta_{\kappa\lambda}^\mu = \hat{\lambda}^{\mu\sigma} \left( \frac{1}{2} \partial_{[\kappa} \hat{\gamma}_{\sigma\lambda]} - \zeta_{[\kappa\sigma\lambda]} + \psi_{[\kappa\sigma\lambda]} \right), \quad \zeta_{\kappa\lambda\mu} \equiv \hat{\gamma}_{\mu\sigma} \beta_{[\kappa\lambda]}^\sigma. \quad (3.3)$$

The connexion  $\beta_{\kappa\lambda}^\mu$  is now expressed in terms of the stressfunctions  $\hat{\gamma}_{\kappa\lambda}$ , their derivatives  $\psi_{\kappa\lambda\mu}$  and the associated torsion tensor  $\zeta_{\kappa\lambda}^\mu$ .

Now let us form the curvature tensor  $\chi_{\kappa\lambda\mu}{}^\nu$  belonging to  $\beta_{\kappa\lambda}^\mu$  and  $\hat{\gamma}_{\kappa\lambda}$ :

$$\chi_{\kappa\lambda\mu}{}^\nu \equiv 2\partial_{[\kappa} \beta_{\lambda]}^\nu + 2\beta_{[\kappa|\sigma} \beta_{\lambda]\mu}^\sigma, \quad (3.4)$$

or

$$\underset{\circ}{\chi}_{\kappa\lambda\mu\nu} \equiv 2\partial_{[\kappa}\underset{\circ}{\beta}_{\lambda]\mu\nu} + 2\hat{\lambda}^{\rho\sigma}\underset{\circ}{\beta}_{[\kappa|\rho\nu}|\underset{\circ}{\beta}_{\lambda]\mu\sigma}, \quad (3.5)$$

where

$$\underset{\circ}{\beta}_{\kappa\lambda\mu} \equiv \underset{\circ}{\gamma}_{\mu\sigma}\underset{\circ}{\beta}_{\kappa\lambda}^{\sigma}. \quad (3.6)$$

The tensor (density)  $\underset{\circ}{\chi}_{\kappa\lambda\mu\nu}$ , by virtue of its definition, fulfills the identities

$$(I) \quad \underset{\circ}{\chi}_{(\kappa\lambda)\mu\nu} = 0,$$

$$(II) \quad \underset{\circ}{\chi}_{[\kappa\lambda\mu]\nu} = 2\overset{2}{\nabla}_{[\kappa}\underset{\circ}{\zeta}_{\lambda\mu]\nu}, \quad (3.7)$$

$$(III) \quad \underset{\circ}{\chi}_{\kappa\lambda\mu\nu} = 2\overset{2}{\nabla}_{[\kappa}\underset{\circ}{\psi}_{\lambda]\mu\nu} + 2\underset{\circ}{\zeta}_{\kappa\lambda}^{\rho}\underset{\circ}{\psi}_{\rho\mu\nu}$$

and the Bianchi identity

$$\overset{2}{\nabla}_{[\iota}\underset{\circ}{\chi}_{\kappa\lambda]\mu\nu} = 0. \quad (3.8)$$

The identity (I) of (3.7) shows that  $\underset{\circ}{\chi}_{\kappa\lambda\mu\nu}$  has 27 (rather than 81) independent components and the identities (II) and (III) of (3.7) and (3.8) represent 30 equations for the 33 functions of  $\underset{\circ}{\beta}_{\kappa\lambda}^{\mu}$  (27 functions) and  $\underset{\circ}{\gamma}_{\kappa\lambda}$  (6 functions). Since 3 components of  $\underset{\circ}{\gamma}_{\kappa\lambda}$  can still be chosen, we have the appropriate number of equations. These identities represent the generalized equilibrium conditions (eqs (4.1), (4.11) in ref. 14).

The interpretation of  $\underset{\circ}{\chi}_{\kappa\lambda\mu\nu}$  is as follows. The Einstein tensor

$$\tau^{\alpha\beta} \equiv \frac{1}{4}\hat{e}^{\alpha\kappa\lambda}\hat{e}^{\beta\mu\nu}\underset{\circ}{\chi}_{\kappa\lambda\mu\nu} \quad (3.9)$$

represents the stress tensor which, however, is not symmetric, since an identity of the form (IV) (2.25) does not hold.

One can of course express  $\underset{\circ}{\chi}_{\kappa\lambda\mu\nu}$  as the sum of a Riemann tensor density  $\underset{\circ}{\rho}_{\kappa\lambda\mu\nu}$  and a non-Riemannian part  $\underset{\circ}{\phi}_{\kappa\lambda\mu\nu}$ :

$$\underset{\circ}{\chi}_{\kappa\lambda\mu\nu} = \underset{\circ}{\rho}_{\kappa\lambda\mu\nu} + \underset{\circ}{\phi}_{\kappa\lambda\mu\nu}. \quad (3.10)$$

Then the Einstein tensor

$$\sigma_{\kappa\lambda}^{\alpha\beta} \equiv \frac{1}{4} \hat{e}^{\alpha\kappa\lambda} \hat{e}^{\beta\mu\nu} \rho_{\mu\nu}^{\kappa\lambda} \quad (3.11)$$

corresponding to  $\rho_{\kappa\lambda\mu\nu}$  will correspond to the classical symmetric stress tensor and all nonclassical terms will be associated with  $\phi_{\kappa\lambda\mu\nu}$ .

The tensor density

$$\chi_{\kappa\lambda(\mu\nu)} = \phi_{\kappa\lambda(\mu\nu)} \quad (3.12)$$

may be conveniently called *double stress* [14], since it corresponds to the distribution of double forces due to point defects, as can be immediately seen from (III) (3.7).

In the phenomenological treatment of Eringen and Suhubi [13] the quantities corresponding to  $\beta_{\kappa\lambda\mu}$ ,  $\tau^{\kappa\lambda}$  and  $\sigma^{\kappa\lambda}$  are called first stress moments, macrostress and microstress average, respectively.

The interpretation of  $\zeta_{\kappa\lambda\mu}$  and  $\psi_{\kappa\lambda\mu}$  is quite obvious. Forming the tensor

$$\mu^{\alpha\beta\gamma} \equiv \frac{1}{2} \hat{e}^{\alpha\kappa\lambda} \hat{e}^{\beta\gamma\mu} \zeta_{\kappa\lambda\mu}, \quad (3.13)$$

we obtain the familiar couple stress tensor  $\mu^{\alpha\beta\gamma}$ , where  $\alpha$  labels the plane and  $\beta\gamma$  the couple. Therefore,  $\zeta_{\kappa\lambda\mu}$  expresses the same physical quantity, but here  $\kappa\lambda$  labels the plane and  $\mu$  the couple.

The tensor  $\psi_{\kappa\lambda\mu}^{\alpha\beta}$  must be found in a different way, namely

$$\psi^{\alpha\beta} \equiv \frac{\hat{\lambda}^{\alpha\lambda} \hat{\chi}^{\beta\mu} \psi_{\kappa\lambda\mu}}{\hat{g}} \quad (3.14)$$

Now  $\psi_{\kappa\lambda\mu}^{\alpha\beta}$  represents the torqueless moment stress labeled by  $\alpha\beta$  on the plane  $\kappa$ . Hence  $\psi_{\kappa\lambda\mu}^{\alpha\beta}$  corresponds to distributions of extramatter, i.e., foreign atoms, vacancies, etc. The quantity  $\psi_{\kappa\lambda\mu}^{\alpha\beta}$  or  $\psi_{\kappa\lambda\mu}$  is very convenient from a practical point of view, since the effect of point defects is usually given in terms of the double force distribution, which can be directly measured (cf. refs. 4; 16, p. 148 ff; 21; 22).

The next step to be taken is to express the static quantities  $\chi_{\kappa\lambda\mu\nu}$ ,  $\beta_{\kappa\lambda}$ , etc. in terms of geometric quantities, or vice versa. This can be done if an energy function is given for the solid in terms of these quantities (and possibly the entropy). This has been done by Eringen and Suhubi [13] who, however, give a very vague phenomenological interpretation.

If the energy density  $\hat{w}$  as a function of the elastic stress tensor, the torsion tensor (representing the dislocation density) and the ammetry tensor (representing the extramatter distribution) is

$$\hat{w} = \hat{w}(\epsilon_{\kappa\lambda}, s_{\kappa\lambda}^\mu, q_{\kappa\lambda\mu}), \quad (3.15)$$

then

$$\hat{\sigma}^{\kappa\lambda} = \frac{\partial \hat{w}}{\partial \epsilon_{\kappa\lambda}}, \quad (3.16)$$

$$\hat{\zeta}_{\cdot\mu}^{\kappa\lambda} = \frac{\partial \hat{w}}{\partial s_{\kappa\lambda}^\mu}, \quad (3.17)$$

$$\hat{\phi}_{\kappa\lambda\mu} = \frac{\partial \hat{w}}{\partial q_{\kappa\lambda\mu}}, \quad (3.18)$$

where, of course, the densities, are obtained from the corresponding tensor by multiplication with  $\sqrt{\hat{g}}$ .

These equations show that a distribution of dislocations is intimately connected with the presence of couple stresses, and a distribution of extramatter is in a similar way connected with the presence of torqueless moment stresses. Hence any consistent continuum theory of dislocations must necessarily take into account the couple stresses, and a theory accounting for extramatter is necessarily ammetric both in the geometric and in the static connexions. The energy contributions of the moment stresses are usually small, and Kröner [4] developed a successful theory in which he dealt with 15 geometric functions  $\epsilon_{\kappa\lambda}, s_{\kappa\lambda}^\mu$ , but took into account only 6 static functions  $\hat{\sigma}^{\kappa\lambda}$ . He was, however, fully aware of the inconsistency of his approach. It should, nevertheless, be emphasized that the present general approach has a great physical value, since it allows a continuum mechanical treatment of inelastic quantities associated with lattice defects. Nowadays it is possible to determine the energy function  $\hat{w}$  (3.14), since the intrinsic inelastic energy terms of grain boundaries and point defects can be measured with a fair degree of accuracy.

Let us return to the determination of stresses. Equations (3.16), (3.17), (3.18) can be solved for  $\epsilon_{\kappa\lambda}, s_{\kappa\lambda}^\mu$ , and  $q_{\kappa\lambda\mu}$  in terms of  $\hat{\sigma}^{\kappa\lambda}, \hat{\zeta}_{\cdot\mu}^{\kappa\lambda}, \hat{\psi}^{\kappa\lambda\mu}$ , and

$\hat{\sigma}^{\kappa\lambda}$  can, through (3.11), be expressed in terms of  $\gamma_{\kappa\lambda}$ , with the associated Riemann tensor density

$$\rho_{\kappa\lambda\mu\nu} = \partial_{[\iota} \partial_{\kappa]} \gamma_{\mu\nu} + \frac{1}{2} \hat{\lambda}^{\rho\sigma} \partial_{[\kappa} \gamma_{\rho\nu]} \partial_{\lambda]} \gamma_{\mu\sigma]}. \quad (3.19)$$

inserting now into (1.22) and the Bianchi identity, we obtain

$$c_{\kappa\lambda\mu\nu} = 0, \quad (3.20)$$

$$\overset{2}{\nabla}_{[\iota} c_{\kappa\lambda]\mu\nu} = 0, \quad (3.21)$$

where  $c_{\kappa\lambda\mu\nu}$  is expressed in terms of 33 static quantities  $\gamma_{\kappa\lambda}$ ,  $\zeta_{\kappa\lambda\mu}$ ,  $\psi_{\kappa\lambda\mu}$ . Equations (3.11) represent 27 equations, (3.27) 6 equations, in all 33 equations for 33 functions. Since a coordinate transformation involves 3 arbitrary parameters, 3 of the functions  $\gamma_{\kappa\lambda}$  can be chosen at will to fulfill 3 equations identically. Equations (3.20) are partial differential equations of 2nd order for  $\zeta_{\kappa\lambda\mu}$  and  $\psi_{\kappa\lambda\mu}$ , and of 4th order for  $\gamma_{\kappa\lambda}$ ; eqs (3.21) are higher by one order.

Our procedure may be written in a concise symbolical form. Let us put down the constituting equations in the symbolical form

$$(\sigma, \beta) = C(\epsilon, b), \quad (3.22)$$

$$(\epsilon, b) = \mathcal{O}(\sigma, \beta), \quad (3.23)$$

and denote the formation of the curvature tensor associated with the metric tensor (density)  $g$  and the connection  $b$  by the *Riemann-Christoffel operator*  $R$ .

$$R = R(g, b). \quad (3.24)$$

Then the equations for the determination of generalized stresses become

$$R[\mathcal{O}R(\gamma, \beta), \mathcal{O}\beta] = 0. \quad (3.25)$$

Kröner [15, 16] found these equations for the linear Euclidean case and wrote the equivalent of

$$Ink[\mathcal{O}Ink\gamma, s] = 0 \quad (3.26)$$

(eq (II.17) in ref. 16, p. 54). It can be seen that the Riemann-Christoffel operator  $R$  is the full generalization of Kröner's incompatibility operator  $Ink$ .

#### IV. Conclusion

The statics of general continuum mechanics of solids with distributions of lattice defects can be developed in full analogy with the geometry. Theorems known from the differential geometry of non-Riemannian space ensure that the method of generalized stress functions can always be applied, together with a stress connexion representing the generalized moment stresses. In other words, the static equilibrium conditions can always be identically fulfilled by stress functions and moment stresses. The stress tensor has in this theory 27 components, the new 18 components being due to lattice defect distributions. A full and consistent continuum theory of lattice defects must involve both a full geometric and a full stress connexion, each having 27 components, i.e., it must be based on a non-Riemannian, nonsymmetric and nonmetric space.

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## Discussion on Papers by C. Teodosiu, and C. S. Hartley and M. A. Eisenberg, Including Two Written Contributions by S. I. Ben-Abraham.

SIMMONS: I would like to address a comment to Dr. Teodosiu and make some general comments on the non-linear problem for dislocations. First I would like to say that Signorini's scheme that Dr. Teodosiu has put forth is a very nice extension of the technique that was done and given by Willis where the iteration scheme was given on the distortion.<sup>1</sup> Dr. Bullough and I have appearing in the Orowan Commemorative Volume another discussion of the deformation of the non-linear continuum,<sup>2</sup> and in this paper we take into explicit account the shape changes of the body. We give there an iterative scheme which is equivalent to the Signorini scheme and includes a derivation of the shape change also in the final state problem if one is given a little bit of extra information concerning the plastic deformation that gives rise to the final state. We call that particular scheme a final state problem if you're given the dislocations in the final state, and you are given a little bit of information as to how you got those, then you can calculate both the distortions and strains of the final state as well as the dislocation density. We also formulate the so-called initial state problem for non-linear problems. That is to say, if you put in a given type of plastic deformation field and then ask what will be the resulting dislocation field and the resulting strain field, then we present a scheme for also obtaining that type of result which I think does not appear in the literature. Finally, we discuss a topic which I notice Dr. Teodosiu took care to properly treat, namely the use of the appropriate strain tensor. For isotropic bodies one can use either the Cauchy strain tensor or the Green's strain tensor, that is the final or initial state strains; this is not true for anisotropic bodies in the non-linear case, where the Green's or initial state strain measure must be employed.

I would also like to comment on what is a more difficult problem for the non-linear distortion or strain field associated to singular dislocations, something which is not often brought out, and I would like to say it this way if I may: Because of the feed-back or the non-superimposability of strain fields in the non-linear theory, a singular dislocation, described basically by a distribution—or delta function—in the linear theory,

<sup>1</sup> Willis, J. R., *Int. J. Engrg. Sci.* **5**, 171 (1967).

<sup>2</sup> Bullough, R., and Simmons, J. A., in *Physics of Strength and Plasticity*, A. Argon, Ed. (MIT Press, Cambridge, Mass., 1969) p. 47.

produces a globally different distortion field than one in which you smear out the core. You don't have anything like the Burger's cut-off situation that you do in linear theory. That is to say, if one looks at the results of, for instance, Seeger and Mann, or Pfleiderer, Seeger and Kröner,<sup>3</sup> where the non-linear problem has been solved for a dislocation with a hollow core at whose surface the tractions were set at zero, one finds that the first order corrections diverge everywhere in the whole body as the core size goes to zero. This is unlike the ordinary Burger's cut-off situation where, of course, the answer goes to infinity at the core, but elsewhere doesn't change at all.

In the case of the non-linear theory as you vary the core size the answer blows up *everywhere* which means, of course, that the core size is an exceedingly sensitive parameter in such a theory. We feel that the only way to treat this problem is to go to the formulation which includes essentially a continuum analogue of the Peierls problem. In the non-linear theory you have to actually introduce a dislocation along a slip plane, and you have to put down explicitly an expression for the misfit energy along that slip plane. You, then, can solve the problem by minimizing the total energy of the body: You assume a certain continuous distribution of plastic deformation which will produce the dislocation. You, then, everywhere (except in the misfit energy region) solve the non-linear problem to attain the total non-linear elastic energy—this is not supposed to be practical; this is in principle—you add to that the amount of misfit energy which is associated to the particular slip distribution you put in, and this gives you an amount of total energy in the body. You then have to—by hook or by crook—start varying the slip distribution that you have put in the body, and therein find the correct strain distribution everywhere in the body as that which is produced by the particular slip distribution which minimizes the total energy.

If one had only some really reasonable physical meaning for a continuous distribution in a real body or if you assume such a distribution, then, of course, the problem disappears. But, as I said, unlike the linear theory where at any distance away the solution doesn't really depend much on how you perturb the solution, it does in a non-linear theory in that you get entirely different answers depending on exactly what particular distribution of continuously distributed dislocations you put near the core.

So, this is a very much more difficult problem than in the linear case, and I would be interested to hear from Dr. Teodosiu any comments concerning how one can treat such a singular dislocation, because I think

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<sup>3</sup> Seeger, A., and Mann, E., Z. Naturf. **14a**, 154 (1959); Pfleiderer, H., Seeger, A., and Kröner, E., Z. Naturf. **15a**, 758 (1960).

the problem of treating singular dislocations in non-linear theory is much more difficult than it appears at first blush.

TEODOSIU: I agree completely with this comment. However, we have considered only a continuous distribution of dislocations, and the problem of how to treat a singular dislocation in this scheme is a more complicated one which has to be solved. With respect to this stress about the singularity, I feel that Professor Kröner may have something to say about this.

KRÖNER: I just agree with you; one has to work it out.

GRUNER: I would like to address a question to Dr. Teodosiu. The assumption underlying your theory is that the superimposed waves do not alter the dislocation arrangement. One should, however, think that a strong wave would change the configuration and the number of the dislocations as well.

TEODOSIU: Our assumption was only that the superimposed displacement field does not produce any plastic flow. This was a simplifying assumption. Of course, the local dislocation density is influenced because the Burgers vectors, themselves, deform together with the material, and the surfaces to which the dislocation density is referred also deform together with the material. But our assumption was only that we have no plastic flow accompanying the superimposed displacement field. Of course, maybe you are speaking about a more complicated problem we have not approached so far.

MURA: I have a small comment on the last paper by Professors Hartley and Eisenberg. You said you used Professor Head's solution because you have a free surface. However, it was unnecessary to use this solution; you can have the same results by using the simple solution of the infinitely extended medium. If you sum up the infinite body solutions for the edge dislocations in the upper and lower plastic domains of the beam, all stress components except  $\sigma_{11}$  vanish. But, since you only need the formal tractions  $\sigma_{22}$  and  $\sigma_{21}$  to vanish on the surface of the beam, you obtain in the simple way the proper stress field for the dislocations in the beam.

FOX: I really just want to make a comment concerning the remarks of Dr. Teodosiu on the presence of the plastic strain in the constitutive equations for the theory of the elastic-plastic continuum in finite deformation. I would certainly agree that there are obviously many factors which influence the yield criterion and which should therefore appear in the constitutive equations—including the hardening law. I would also agree that the dislocation density and higher order gradients, if you wish, should go

in as well. I think that in non-linear continuum theories these days we have got the apparatus for making them as complicated as you like. It seemed to me that the total plastic strain was the most fundamental variable we have, and that is why I simply put that in and nothing else; but certainly put in the others if you wish. Admittedly the total plastic strain would depend upon the history of the deformation, but I see no reason why this should exclude its presence from the constitutive equations.

TEODOSIU: I think the problem, here, is not to complicate the theory, but only to obtain something which can describe the real behavior of materials. If we want to describe the plastic state only by using the dislocation densities, it would, of course, not be possible, because on a macroscopic scale we have a vanishing dislocation density. So we have to introduce some measures of more complicated dislocation arrangements. Unfortunately, we have, so far, few indications from experiments as to which are the significant dislocation arrangements for plastic flow: first in a single crystal and further in a polycrystalline material. In the meantime, as theoreticians, we only have to think about the invariant measures we could introduce in these conditions.

Now about plastic flow, if we have a perfect lattice which glides in a parallel set of planes [like a deck of cards], then the internal structure remains the same, so I see no reason for which the response of the material at any two points will be different, except, of course, if we approach the boundary of a finite body; but far from the boundary the structure being the same after plastic flow, the response, I think, must also be the same. It, therefore, seems to me that, as Professor Kröner pointed out in 1963, plastic strain has no reasonable place in the work hardening law, but we have to introduce some measures of the interior structure of the body, such as the density of dislocation loops, density of pile ups, etc.

BULLOUGH: I just wanted to comment how pleasant it was to see, at last, someone trying to really test the value of the theory of continuous distributions of dislocations. I wonder if Professor Hartley could elaborate a little on precisely how he intends to complete the work. What he said was interesting, but it wasn't clear how he was testing the distribution calculation.

HARTLEY: One of the things that we had hoped to do by getting some indication of what the phenomenological parameters appearing in continuum elasticity treatments meant in terms of dislocation theory was to introduce perhaps more realistic approximations to flow laws for real materials based on what we know about dislocation behavior from other studies. The other thing was to examine in more detail what some of the

assumptions of continuum plasticity mean in terms of dislocation behavior and see if we can use what we know about the behavior of individuals and groups of dislocations to make a more realistic continuum theory.

WEINER: [Written contribution] I would like to insert here a reference to the dissertation of Dr. J. M. Santiago.<sup>4</sup> This dissertation contains a very clear discussion of continuous distributions of dislocations together with some valuable original contributions.

BEN-ABRAHAM: [The following two discussions are written contributions. The first discussion is devoted to "The Importance of Scale."] In recent years and months, many among us have come to question the validity of continuum theories of lattice defects for real solids. The 1967 IUTAM Symposium (held in Freudenstadt and Stuttgart, Germany) was symptomatic. While mathematicians and continuum mechanists "by birth" presented highly sophisticated theories, some of those "born physicists" staged a concentrated attack from quite a few directions on the very relevance of those theories.

To make my point clear, let me quote an almost childish example. In order to define a dislocation density in a meaningful way one has to choose the mathematical line element large compared to the mean spacing of dislocations. Since the average dislocation spacing in metals will usually be anywhere from  $10^{-6}\text{m}$  to  $10^{-9}\text{m}$ , the "mathematically infinitesimal" line element should be at least of the order of  $10^{-4}\text{m}$ , which is fairly big by any standard. The torque stresses associated with dislocation densities must be considered on the same scale, while on any smaller scale one must resolve them into force stresses. This has been recognized as early as 1958 by Kröner.

Things are, of course, different with spin type torques, as has been pointed out again by Kröner (1967). However, it would be rather artificial to associate these spin torques with some kind of "micro-dislocations." At any rate, I feel that such a procedure would only obscure matters rather than contribute to our physical insight.

The situation, though, is somewhat better with regard to point defects and the associated symmetries and torqueless moment stresses, since they appear already at the atomic level. Nevertheless, a macroscopic continuum theory is hardly able to distinguish between the effects of impurities and inclusions.

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<sup>4</sup> Santiago, J. M., Mechanics and Thermodynamics of Continuously Dislocated Crystals, Columbia University Ph. D., 1962 (University Microfilms, Inc., Ann Arbor, Michigan, No. 63-1522).

Credit must be given to Kondo who, once more, was the first to recognize the importance of distinguishing “levels” in the geometry of mathematically continuous bodies. He also emphasized that the same physical phenomenon may be adequately described by quite different geometric entities at different levels. However, he did not specify actual scales.

Krumhansl (1967) clarified matters quite a bit from the physicist’s point of view. He suggested to distinguish between the atomic or micro scale, the macro scale, and, what he called a “milli” scale in between. For such a rough distinction, however, one should rather prefer a more “mod” and less specific term like “mini” or “midi.”

However, I can’t see a good reason why one should not be more specific and, taking the meter as a basic unit, talk of a meter or macro scale ( $10^0\text{m}$ ), a milli scale ( $10^{-3}\text{m}$ ) meaning exactly what it says. The latter would normally correspond to small crystals or moderately large crystal grains. Continuum theories of lattice defects would then be adequate at the micro scale ( $10^{-6}\text{m}$ ), while atomic phenomena would take place at the nano ( $10^{-9}\text{m}$ ) or possibly pico ( $10^{-12}\text{m}$ ) scale.

Admittedly, this looks very much like just playing with words. Yet, it should be borne in mind that our primary concern is to build bridges between the various levels both in the sense of constructing the connecting theories and in the more human sense of establishing meaningful interaction between scholars who concentrate their efforts at the different levels. By the way, the terms “macro” and “micro” are so often being utterly misused that literally “One man’s micro is another one’s macro.” Therefore, I believe it won’t do any harm to have a clear cut common language.

Essentially, one would like to predict the behavior of bodies at the macro level from laws assumed to be valid at the nano level, or deduce nano phenomena from macro experiments. Things usually turn out to be all right when it is possible to bridge the gap directly from nano to macro, i.e., when the averages of nano phenomena directly yield the right macroscopic results.

One should look more carefully at this apparently trivial truism. One point we should be aware of is our obsession with 19th century physics and our reluctance to enter the 20th century. Let me point out in parentheses that continuum mechanical theories, no matter how sophisticated and elaborate, belong to the past century, which of course, doesn’t mean that they cannot be very useful tools if properly used. Yet, it should be clear from the start that any consistently continuum formulation must necessarily neglect relevant information about discrete phenomena. Moreover, there is a lower bound of scale to the validity of continuum theories which presents another highly effective communica-

tion barrier since it may vary in wide limits according to the particular case in question.

Now, when is it actually possible to bridge the gap from nano to macro by a single span? It is possible in the case of additive quantities having a single sign (such as mass) or in the case of quantities of both signs when we are interested only in their net bulk value and their manifestations on the surface of the macroscopic body (such as electric charge).

Matters are quite different with lattice defects, in particular dislocations. These occur typically at the micro level where they have distinct discrete properties. They are of either sign, or even worse, they are vector-like. We are interested in the entirety of their effects upon bulk behavior. And, last but not least, they significantly interact among themselves and with other entities. Consequently, a defect density defined at the milli level, even if by some odd chance different from zero, will by no means convey relevant information at the macro level.

Of course, an attempt to work out a nano or micro theory to describe milli and macro phenomena would be both impossible and futile. So, one has to compromise. We have to work at the particular level we are interested in, however, expressing in an appropriate way relevant information from a lower level. For instance, at the milli level we must still keep separate the densities of different kinds of defects and we must introduce various "effective fields" to describe interactions. Sometimes we have to resort to rather artificial devices like stress moments of higher orders, and often introduce most arbitrary force laws and constitutive equations. This is exactly the strength and the weakness of the new continuum theories. It is the physicist's primary task to find physical justifications of those phenomenological quantities and to establish which one is relevant, and when any particular term can be safely discarded.

Now, we do have a fine precedent in the relationship between thermodynamics and statistical mechanics. I would especially like to draw attention to the theory of superparamagnetism where the three levels of atoms, magnetic particles and bulk are clearly distinguished and statistical averagings are used twice.

This brings me to my final point. The processing of information from a lower level to be fed to a higher one invariably involves some averaging. In this process one has to be extremely careful not to average out relevant information to zeros, and, to be sure to take into account any statistical correlation.

[The second written contribution is devoted to "Plastic Flow—An Unsolved Problem."]

The primary goal of dislocation theory has always been and still is to pre-

dict the process of plastic straining in a given solid body under given conditions of stress. During a few decades we have come to understand the fundamental process of plastic deformation, namely glide. We have been successful in discovering and, at least in part, explaining the role played by dislocations in grain boundaries, diffusion, crystal growth, epitaxy, properties of semiconductors and dielectrics, etc. Dislocation theory has been interacting quite fruitfully with various fields of pure and applied mathematics, mainly tensor calculus, differential geometry and the theory of generalized functions. And last, but not least, some ideas born within dislocation theory might prove useful for solving some fundamental problems of physics in the general theory of relativity and particle physics.

Yet, we have to admit that in spite of lengthy and concentrated efforts of a great many workers in the field (whose list is too long to be cited without possibly hurting someone), and although these efforts were often successful in details, we are as far as ever from our primary goal. Plastic flow is still an unsolved problem. At the very best, we now understand how complex the problem in reality is.

The advent of the theory of continuous distributions of dislocations (credit is given to all pioneers without quoting names) inspired great hopes which, alas, proved to be exaggerated. Some important fundamental results have been obtained, and as a byproduct, it has been recognized that the relationship between the continuum mechanics of a solid body and hydrodynamics is a fundamental one rather than a superficial analogy. Since then, this point of view has obtained independent support from studies of a quite different kind.

Yet, the continuum theory of lattice defects (in general, and dislocations in particular) has a very serious limitation which, in my opinion, makes it almost useless for meaningful application to all but a few very special problems of practical interest. The continuum theory of lattice defects is, in fact, an extension of classical elasticity in which the geometric (or kinematic) equations have non-vanishing right hand sides. These right hand sides, representing the distributions of defects, are the very crux of the theory. However, the theory is by its very nature macroscopic and thus meaningful only on a scale large compared with interatomic distances or, even worse, on a scale large compared with the average spacing of lattice defects. Since in plastic deformation all possible mobile dislocations of both signs participate, the inevitable result is that the relevant average dislocation density on a sufficiently large scale for the theory to be applicable, becomes very nearly zero.

The way out of this dilemma is to adopt the point of view of plasma physics, i.e., to maintain, at least to a certain degree, the individuality of different particles—in the present case dislocations.

This leads us to consider the behavior of dislocations on at least three distinct levels: (1) individual; (2) statistical; (3) continuum.

The level of individual dislocations can be roughly subdivided according to the method of approach into: (a) atomistic; and (b) elastic.

The elastic (or quasielastic, Peierls-type) theory of individual dislocations is now well established and well understood. The atomistic treatment has become feasible through the development of computer science and is at present in steady progress.

At the other extreme we have the continuum theory. In its "plasma" version one must keep separated the densities of different Burgers vectors and dislocation types and work with a quasineutral, rather than neutral, continuum. Of course, the conventional continuum theory of lattice defects becomes a necessary prerequisite just as the Maxwell theory is for plasma physics. By this approach one is, of course, adding tremendous difficulties.

The author has tried to work along these lines only to discover that a plasma of dislocations in a tractable approximation does not describe a solid but rather a liquid. This leads us directly to the dislocation theory of melting most clearly formulated by Kuhlmann-Wilsdorf.<sup>5</sup> Rapid plastic flow of a solid then appears as a highly non-equilibrium process in which the crystal on some planes shows liquid behavior in one dimension. It is clear that experimentally such a state can be most easily realized during creep which also bears the most pronounced resemblance to the flow of liquids. Low rate plastic flow appears as the same phenomenon, however, sporadic. From the "plasma" point of view it is similar to a glow discharge.

I feel that one should take the dislocation theory of melting for granted and therefrom deduce conclusions about plastic behavior rather than the other way around.

The remaining item in our classification, namely the statistical theory of dislocations, has been put forward mainly by Akulov.<sup>6</sup> Yet, credit should be given to a significant and increasing number of physicists who are now aware that the behavior of a large number of dislocations as encountered in plastic flow is by no means the simple sum of the behaviors of individual dislocations. The present author feels that Akulov's conclusions are basically right but they have no sound physical foundation.

In discussions with Professor Gilman<sup>7</sup> we concluded that the right answer to problems of plasticity might very probably be furnished by the

<sup>5</sup> Kuhlmann-Wilsdorf, D., *Phys. Rev.* **140**, A1599 (1965).

<sup>6</sup> Akulov, N. S., *Phil. Mag.* **9**, 767 (1964).

<sup>7</sup> Gilman, J. J., in *Dislocation Dynamics*, Rosefield, A. R., Hahn, G. T., Bement, A. L., Jr., and Jaffee, R. I., Eds. (McGraw-Hill Book Co., N.Y., 1968) p. 3.

theory of traffic flow. However, first it is necessary to find a proper physical justification.

A very strong argument in favor of collective effects and the dislocation theory of melting comes along the lines pursued by Professor Maradudin, Professor Weiner's group and others. A dislocation can be described in terms of a localized mode of crystal vibrations. As the density of dislocations increases the localized modes start to overlap. This physically means that we have significant non-local and non-linear interactions between dislocations. With a further increase of dislocation density the localized modes fill out the entire crystal and thus cease to be localized. Instead, a new phonon spectrum, that of the liquid, is established.

It should be noted that since the self-energy of a dislocation is roughly proportional to the square root of the dislocation density, one has to expect dislocation multiplication to be a self-enhancing process, provided enough energy is supplied by an external source, e.g., an applied stress. As the temperature rises, the shear modulus slightly decreases and the process is further enhanced. Moreover, large deflections of atoms from their equilibrium positions become more frequent. A large deflection of two neighboring atoms in opposite directions essentially represents an elementary dislocation loop. Thus we have a purely thermal mechanism of dislocation multiplication. At the melting point, the process becomes spontaneous and self-sustaining. Below the melting point it will be active only locally as long as a sufficiently high stress is being applied. After removing the stress, the excess dislocations will mutually annihilate at a very fast rate. Recently Adler et al.<sup>8</sup> found spontaneous local slipping in a model for solid bcc He<sup>4</sup> just below the melting point. Their experiment seems to be a direct proof of the discussed mechanism of plasticity and melting.

With Gilman, we tried to find justifications for the application of traffic flow theory to plasticity.

We considered two edge dislocations on a common slip plane or on closely spaced parallel slip planes. An elementary but tedious analysis yields the answer that during acceleration of the dislocations by an applied stress very violent transient oscillatory phenomena occur. These lead to significant radiation losses. The motion of the two dislocations is quite similar to that of a car being tailed by another car and is directly interpretable in terms of traffic flow.

We also studied the behavior of a finite array of dislocations under applied stress. The analysis can be carried out for a finite dislocation wall.

<sup>8</sup> Adler, B. J., Gardner, W. R., Hoffer, J. K., Phillips, N. E., Young, D. A., Phys. Rev. Letters **21**, 732 (1968).

but the answer will be *a fortiori* valid for a two-dimensional array. It turns out that an applied stress will pull the dislocations out of the wall one by one rather than moving the whole wall. Once the wall is in motion it will undergo oscillations. Again, the result is increased damping per effective amount of slip. The motion of dislocations again follows a traffic pattern.

Further, we speculated that in a crystal heavily dislocated by repeated plastic flow one might find more or less regular "crystalline" arrays of dislocations. These in turn would necessarily become dislocated. Thus, one should observe "hyperdislocations" (dislocations in dislocation arrays). The action of an applied stress should be concentrated on the hyperdislocations thus producing a collective effect while having the appearance of a single glide but governed by the effective mass of the array and the collective losses. This is one possible way to account for the discrepancy between measured and calculated damping constants.



# VII FIELD THEORIES II

*Chairman:*

J. A. SIMMONS



# THE ELASTIC FIELD OF MOVING DISLOCATIONS AND DISCLINATIONS

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The previous work and the present stage of study on the elastic field of moving dislocations and disclinations are reviewed. Emphasis will be placed upon the general method and approach using Green's tensor functions and Fourier integrals. The previous solutions for individual problems are reviewed as examples of this unified approach.

Key words: Anisotropic elasticity; dislocation dynamics; dislocations; Green's tensors.

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## I. Introduction

The purpose of this paper is to review the various works of dynamic field theory of dislocation by introducing a most general approach, namely, continuously distributed dislocations.

The field equation of elasticity for an infinitely extended medium will be solved in a general form for an arbitrarily prescribed plastic distortion or given dislocation density tensors and dislocation flux (velocity) tensors. By using the result, the elastic strain energy and kinetic energy of the medium will be expressed in terms of the dislocation density and the velocity tensors.

The concept of force acting on dislocations is also discussed in connection with the concept of the energy dissipation of a system. The analysis is extended to the motion of disclinations.

The most fundamental contribution to the dynamic field theory of dislocations was made by Frank, Eshelby, Nabarro, and Leibfried. They considered the simplest case of a straight discrete dislocation or Peierls dislocation. In this paper such specification is avoided and a more general configuration of dislocations is considered.

The stress singularity at the center of the dislocation and the multi-valued nature of the displacement can be avoided by treating discrete dislocations as special cases of continuously distributed dislocations. The method of continuously distributed dislocations is also useful when the relationship between continuum plasticity and dislocation theory is considered.

The plastic deformation of crystals is described by the creation of slip planes and their extension, which corresponds to the creation of dislocations (or disclinations) and the motion of dislocations (or disclinations), respectively. The motion of an edge-type disclination is quite similar to that of a dislocation where the Burgers rotational vector and the center of rotation are conserved during the motion. Since any other cases of disclination motion require a special caution, attention will first be centered only on the case of dislocations. The result will be extended to the case of disclinations in the following section.

Denoting the direction of a line segment of a dislocation by  $\nu$ , the Burgers vector by  $\mathbf{b}$ , and the velocity of the segment by  $\mathbf{V}$ , the time rate of plastic distortion caused by the motion of the segment can be described by

$$\dot{\beta}_{ji}^* = -\epsilon_{jih} V_l \nu_h b_i, \quad (1)$$

where  $\epsilon_{ijk}$  is the unit permutation tensor. When an arbitrary point  $P$  in an actual deforming body at time  $t$  is considered, there are several dislocation lines at  $P$  which have various Burgers vectors  $\mathbf{b}, \mathbf{b}' \dots$ , directions  $\nu, \nu' \dots$ , and velocities  $\mathbf{V}, \mathbf{V}' \dots$ . The total Burgers vector of the dislocations threading an infinitesimal surface element  $\Delta S$  at  $P$  can be expressed as

$$B_i = \alpha_{hi} \Delta S_h, \quad (2)$$

where

$$\alpha_{hi} = \nu_h b_i + \nu'_h b'_i + \dots \quad (3)$$

The rate of plastic distortion (1) can be expressed as

$$\dot{\beta}_{ji}^* = -\epsilon_{jih} V_{lhi} \quad (4)$$

by defining

$$V_{lhi} = V_l \nu_h b_i + V'_l \nu'_h b'_i + \dots \quad (5)$$

By assuming that dislocations are continuously distributed in the material, tensors  $\alpha_{ij}$  and  $V_{ijk}$  are defined as continuous functions of the coordinates and time and called the dislocation density tensor (after Nye [1]) and the dislocation flux (velocity) tensor [2], respectively.

Let the dislocation density tensor change by an amount  $\dot{\alpha}_{ij}$  per unit time. The growth rate of the total Burgers vector of the dislocations threading an arbitrary open surface  $S$  is  $\int_S \dot{\alpha}_{hi} dS_h$  and can be considered as the

result of the dislocations moving through the boundary of the surface  $S$ . Since only the dislocation velocity component which is normal both the

boundary line of  $S$  and to the direction of the line of dislocation can contribute to the growth, then

$$\int_S \dot{\alpha}_{hi} dS_h = \oint \epsilon_{lmk} V_{lm} dl_k \quad (6)$$

where  $d\mathbf{l}$  is the line element of the boundary of  $S$ . Applying Stokes' theorem to the right side of eq (6) leads to the result

$$\dot{\alpha}_{hi} = \epsilon_{hik} \epsilon_{lmk} V_{lm},_l \quad (7)$$

or, by using (4)

$$\dot{\alpha}_{hi} = -\epsilon_{hik} \beta_{ki,l}^* \quad (8)$$

or, by integrating with time

$$\alpha_{hi} = -\epsilon_{hik} \beta_{ki,l}^* \quad (9)$$

where “ $l$ ” stands for the differentiation with respect to coordinate  $x_l$ . Equation (9) was obtained by Kröner [3] and equivalent relations, under more general conditions, were studied by Kondo [4] and Bilby [5] from the geometrical point of view. Equation (7) was obtained by Kosevich [6] and Mura [2] independently. An equation similar to (7) and the analogy with Maxwell's equation was studied by Holländer [7] and the geometrical theory valid for large deformations was developed by Amari [8] and Günther [9].

In this paper, only small deformations will be considered. It is assumed that displacements of material,  $U_i$ , are continuous and continuously differentiable functions of the coordinates and time. A finite amount of a slip, which leads to a discontinuous displacement, is replaced by an infinite number of slip surfaces with infinitesimal gliding such that it gives the same macroscopic average effect to the deformation caused by the discontinuous displacement. This infinitesimal slip model (or continuously distributed dislocation model), however, does not exclude the investigation of a finite discrete slip, because the slip can be expressed by the Dirac delta function,  $\delta$ , and the Heaviside step function,  $H$ , which are treated as continuous functions.

The distortion of materials  $U_{i,j}$  is not only caused by the infinitesimal gliding (plastic) but also by the superimposed elastic distortion  $\beta_{ji}$ , namely

$$U_{i,j} = \beta_{ji}^* + \beta_{ji}. \quad (10)$$

The term *elastic* has a meaning only for the symmetric part of  $\beta_{ji}$ , which is related to stress  $\sigma_{ij}$  by Hooke's law

$$\sigma_{ij} = C_{ijkl}\beta_{kl}. \quad (11)$$

Since  $U_{i,j}$  and  $\beta_{ji}^*$  can be well defined,  $\beta_{ji}$  may be defined as the difference between  $U_{i,j}$  and  $\beta_{ji}^*$ .

## II. Disclinations

It has been well known in theory of elasticity that there are two types of Volterra's dislocations: the translational type and the rotational type. Although the translational type of dislocation has been known simply as the dislocation in crystals, little attention has been paid to the latter type of dislocations, which will be called the disclination. Recently, in his book, Nabarro [10] introduced some applications of disclinations [11, 12, 13] to liquid crystalline structures. The application will be extended to solids, particularly to the problem of torsion in crystal bars.

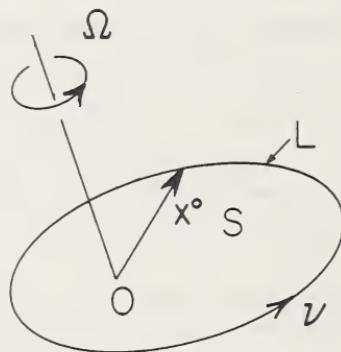


FIGURE 1. A disclination with a rotational Burgers vector  $\Omega$  and a center of rotation  $O$ .

A line of a disclination is defined as a boundary  $L$  of an open surface  $S$  inside of a material (fig. 1) where the displacement  $U_i$  has a multiple-value,

$$[U_i] = \epsilon_{ijk}\Omega_j x_k^0 \quad (12)$$

equal to the difference of  $U_i$  defined above  $S$  and below  $S$ . It is created by twisting the two surfaces on  $S$  by  $\Omega$  about a center of rotation  $O$ . Here,  $x^0$  is the radial vector of a point in question measured from  $O$ , and  $\epsilon_{ijk}$  is the unit permutation tensor. In order to define a disclination uniquely, the center of rotation, rotational vector  $\Omega$ , and the direction of disclination line  $\nu$  must be given. Going around a linking circuit (the Burgers

circuit) in the direction of rotation of a right-handed screw advancing along the direction of the disclination, the ending point of the Burgers circuit is displaced by (12) relative to the beginning point of the circuit.

A force on the disclination can be defined in a manner similar to the Peach-Koehler force on a dislocation. Under a stress field  $\sigma_{ij}$ , when a line element  $\nu dl$  of the disclination is displaced by  $\mathbf{V}$  without changing  $\Omega$  and the center of rotation, the work done by  $\sigma_{ij}$  can be written as

$$\Delta W = \oint_L -\sigma_{ij}\epsilon_{imn}\Omega_m x_n^0 \epsilon_{jpq} V_p \nu_q dl = \oint_L -\epsilon_{jpq} \nu_q M_{jm} \Omega_m V_p dl, \quad (13)$$

where

$$M_{jm} = \sigma_{ji}\epsilon_{imn}x_n^0 \quad (14)$$

is a moment about the center of rotation. The force  $\mathbf{f}$  is defined by

$$\Delta W = \oint_L f_p V_p dl$$

and, therefore,

$$f_p = -\epsilon_{pj}\nu_q M_{jm} \Omega_m, \quad (15)$$

or

$$\mathbf{f} = -\nu \times (\mathbf{M} \cdot \boldsymbol{\Omega}). \quad (15)'$$

The simplest example of (15) is the motion of a circular disclination whose center is the center of rotation. When  $\boldsymbol{\Omega}$  is normal to the circular plane, the disclination receives a uniform central force  $M\Omega$ , under a twisting moment  $M$ , about the center of rotation.

When the center of rotation moves from 0 to  $0'$ , a distance  $\Delta x^0$ , without motion of the disclination line, the work done by  $\sigma_{ij}$  is

$$\Delta W = \int_S \sigma_{ij}\epsilon_{imn}\Omega_m \Delta x_n^0 dS_j. \quad (16)$$

Then, the force on the center of rotation is

$$f_n^0 = \int_S \sigma_{ij}\epsilon_{imn}\Omega_m dS_j \quad (17)$$

by defining  $\Delta W = f_n^0 \Delta x_n^0$ .

Another type of motion of the disclination is possible when a change in  $\boldsymbol{\Omega}$  is considered. A more complicated motion may be the combination of the above three cases. The discussions in the following sections will

be limited to the cases where centers of rotation and the Burgers rotational vectors,  $\Omega$ , are conserved during motion. Then, the discussion on dislocations can be extended to the case of disclinations.

The plastic distortion caused by a disclination is

$$\beta_{ji}^* = -n_j \epsilon_{ikl} \Omega_k x_l^0 \quad (18)$$

where  $n_i$  is the normal vector of the twisted surface  $\mathbf{S}$ . Its time rate of change due to a motion of disclination line with a velocity  $\mathbf{V}$  is

$$\dot{\beta}_{ji}^* = -\epsilon_{jih} V_l \nu_h \epsilon_{imn} \Omega_m x_n^0. \quad (19)$$

The equation similar to (7) is derived as

$$\dot{\theta}_{hi} = \epsilon_{hik} \epsilon_{mnk} (V_m \theta_{ni}), \quad (20)$$

where  $\theta_{hi} = \nu_h \Omega_i$ . The  $\theta_{hi}$  is called the disclination density tensor when a continuous distribution of disclinations can be considered.

Differentiation of (19) with respect to the coordinate of the center of rotation leads to

$$-\partial \dot{\beta}_{ji}^* / \partial x_n^0 = \epsilon_{jih} V_l \theta_{hm} \epsilon_{imn} \quad (21)$$

or

$$(1/2) \epsilon_{imn} \dot{\beta}_{ji,n}^* = -\epsilon_{lhi} V_l \theta_{hm} \quad (21)'$$

where  $\partial / \partial x_n^0$  is replaced by  $\partial / \partial x_n$  because of  $x_n^0 = x_n - x_n(0)$ . From (20) and (21)', we have

$$\dot{\theta}_{hi} = -(1/2) \epsilon_{hik} \epsilon_{inj} \dot{\beta}_{kj,ln}^* \quad (22)$$

or

$$\theta_{hi} = -(1/2) \epsilon_{hik} \epsilon_{inj} \beta_{kj,ln}^* \quad (22)'$$

which<sup>1</sup> corresponds to (9). The plastic distortion caused by a disclination can also be obtained by a proper choice of a continuous distribution of dislocations. This equivalent  $\alpha_{ij}$  is obtained from (9) and (22)'. Substituting (9) into (22)' leads to

$$\theta_{hi} = (1/2) \epsilon_{inj} \alpha_{hj,n} \quad (23)$$

whose symmetric part becomes the incompatibility tensor.

<sup>1</sup> By defining  $(1/2) \epsilon_{inj} \beta_{kj,n}^* \equiv \kappa_{ki}^p$ , (22)' becomes the same expression by deWit in this Proceeding [14].

### III. Elastic Fields

General expressions of solutions will be reviewed for the elastic field caused by the motion of dislocations or disclinations. For simplicity, the material is assumed to be infinitely extended and free from external stresses.

Suppose that a plastic distortion is known as a function of the co-ordinates and time as a result of dislocation or disclination motion. It will be given in the form of Fourier integrals,

$$\beta_{ji}^*(x, t) = \iint_{-\infty}^{\infty} \bar{\beta}_{ji}^*(k, \omega) \exp \{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} d\omega \quad (24)$$

$$\bar{\beta}_{ji}^*(k, \omega) = (2\pi)^{-\nu-1} \iint_{-\infty}^{\infty} \beta_{ji}^*(x', t') \exp \{-i(\omega t' + \mathbf{k} \cdot \mathbf{x}')\} dx' dt'$$

where  $\mathbf{k} \cdot \mathbf{x} = k_1 x_1 + k_2 x_2 + k_3 x_3$ ,  $d\mathbf{k} = dk_1 dk_2 dk_3$ ,  $d\mathbf{x}' = dx'_1 dx'_2 dx'_3$ , and  $\nu = 3$  for a three-dimensional case, or  $\mathbf{k} \cdot \mathbf{x} = k_1 x_1 + k_2 x_2$ ,  $d\mathbf{k} = dk_1 dk_2$ ,  $d\mathbf{x}' = dx'_1 dx'_2$ , and  $\nu = 2$  for a two-dimensional case.

The equation of motion

$$\sigma_{pq, q} = \rho \ddot{U}_p \quad (25)$$

is to be solved with (9) and (10), where  $\rho$  is a constant density of the material.

The solution is easily found as [15, 16]

$$U_m(x, t) = -i \iint_{-\infty}^{\infty} k_l C_{klj} L_{mk}(k, \omega) \bar{\beta}_{ji}^*(k, \omega) \exp \{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} d\omega, \quad (26)$$

where

$$L_{mk}(k, \omega) = \epsilon_{kst} \epsilon_{mnr} K_{sn} K_{tr} / (2 \epsilon_{pqr} K_{p1} K_{q2} K_{r3}) \quad (27)$$

and

$$K_{sn} = C_{sjnl} k_j k_l - \rho \omega^2 \delta_{sn}. \quad (28)$$

For isotropic materials, (27) becomes

$$L_{mk}(k, \omega) = \frac{\delta_{km} \{(\lambda + 2\mu) k^2 - \rho \omega^2\} - k_k k_m (\lambda + \mu)}{(\mu k^2 - \rho \omega^2) \{(\lambda + 2\mu) k^2 - \rho \omega^2\}} \quad (29)$$

with  $k^2 = k_1^2 + k_2^2 + k_3^2$ , where  $\lambda$  and  $\mu$  are the Lamé constants and  $\delta_{ij}$  is the Kronecker delta.

The solution (26) can be rewritten as

$$U_m(x, t) = - \iint_{-\infty}^{\infty} C_{klji} G_{mk, l}(x - x', t - t') \beta_{ji}^*(x', t') d\mathbf{x}' dt' \quad (30)$$

by defining

$$G_{mk}(x - x', t - t') = (2\pi)^{-\nu-1} \iint_{-\infty}^{\infty} L_{mk}(k, \omega) \exp \{i\omega(t - t') + i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')\} d\mathbf{k} d\omega \quad (31)$$

and  $G_{mk, l}$  means  $\partial G_{mk} / \partial x_l = -\partial G_{mk} / \partial x'_l$ . The function  $G_{mk}$  is called the Green's tensor function.

The elastic distortion is derived from the above result by differentiating with respect to  $x_n$  and subtracting  $\beta_{nm}^*$ ,

$$\beta_{nm}(x, t) = \iint_{-\infty}^{\infty} [k_n k_l C_{klji} L_{mk}(k, \omega) - \delta_{jn} \delta_{im}] \bar{\beta}_{ji}^*(k, \omega) \exp \{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} d\omega, \quad (32)$$

or

$$\beta_{nm}(x, t) = - \iint_{-\infty}^{\infty} C_{klji} G_{mk, ln}(x - x', t - t') \beta_{ji}^*(x', t') d\mathbf{x}' dt' - \beta_{nm}^*(x, t). \quad (33)$$

The basic idea leading to (30) has been used by Nabarro [17] for the case when an infinitesimal dislocation loop is created suddenly in an isotropic medium (see also Kosevich and Natsik [18], Gutzwiller [19], Willis [20] and [2]). For a static case, the static Green's tensor is used, which is obtained from (31) by taking  $\omega = 0$ , dropping the integral with respect to  $\omega$ , and changing the factor  $(2\pi)^{-\nu-1}$  to  $(2\pi)^{-\nu}$  (see Eshelby [21], Indenbom [22], Kroupa [23]).

The result in this section can be applied to any case independent of how  $\beta_{ji}^*$  is interpreted as, for instance, a thermal expansion, phase-transformation distortion, inclusion misfit strain, or any other inelastic distortions. However, here particular interest lies in the case where  $\beta_{ji}^*$  is caused by the motion of dislocations or disclinations. Then, the solutions (26), (30), (32), (33) may be expressed in terms of velocity and density tensors of these line imperfections instead of  $\beta_{ji}^*$ . The result will be useful in the following sections.

When  $\beta_{ji}^*$  and  $\beta_{ji}^*$  are eliminated from these expressions by using (4) and (9), Mura [2] has obtained the following result by a semi-intuitive approach (later the result was confirmed by Bross [24] and Willis [25]).

$$U_m(x, t) = \iint_{-\infty}^{\infty} C_{klkj} H_{mk, l}(x - x', t - t') \epsilon_{jnh} V_{nhi}(x', t') d\mathbf{x}' dt' \quad (34)$$

$$\begin{aligned} \beta_{nm}(x, t) = & \iint_{-\infty}^{\infty} [\epsilon_{njh} C_{klkj} G_{mk, l}(x - x', t - t') \alpha_{hi}(x', t') \\ & + \rho \dot{G}_{im}(x - x', t - t') \epsilon_{nli} V_{lhi}(x', t')] d\mathbf{x}' dt'. \end{aligned} \quad (35)$$

where

$$H_{mk}(x - x', t - t') = \int_{-\infty}^t G_{mk}(x - x', t - t') dt, \quad (36)$$

or the Fourier expressions

$$\begin{aligned} U_m(x, t) = & \iint_{-\infty}^{\infty} (1/\omega) k_l C_{klkj} L_{mk}(k, \omega) \epsilon_{jnh} \bar{V}_{nhi}(k, \omega) \\ & \exp \{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} d\omega \end{aligned} \quad (37)$$

$$\begin{aligned} \beta_{nm}(x, t) = & i \iint_{-\infty}^{\infty} [\epsilon_{njh} C_{klkj} L_{mk}(k, \omega) k_l \bar{\alpha}_{hi}(k, \omega) \\ & + \rho \omega L_{im}(k, \omega) \epsilon_{nli} \bar{V}_{lhi}(k, \omega)] \exp \{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} d\omega \end{aligned} \quad (38)$$

where

$$\begin{aligned} V_{nhi}(x, t) &= \int_{-\infty}^{\infty} \bar{V}_{nhi}(k, \omega) \exp \{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} d\omega \\ \alpha_{hi}(x, t) &= \int_{-\infty}^{\infty} \bar{\alpha}_{hi}(k, \omega) \exp \{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} d\omega \end{aligned} \quad (39)$$

and

$$\begin{aligned} \bar{V}_{nhi}(k, \omega) &= (2\pi)^{-\nu-1} \iint_{-\infty}^{\infty} V_{nhi}(x', t') \exp \{-i(\omega t' + \mathbf{k} \cdot \mathbf{x}')\} d\mathbf{x}' dt' \\ \bar{\alpha}_{hi}(k, \omega) &= (2\pi)^{-\nu-1} \iint_{-\infty}^{\infty} \alpha_{hi}(x', t') \exp \{-i(\omega t' + \mathbf{k} \cdot \mathbf{x}')\} d\mathbf{x}' dt' \end{aligned} \quad (40)$$

It is important to notice that the difference between a non-state and state quantity can be seen in solutions (37) and (38). The elastic distortion (38) is a state quantity, but the displacement (37) is not. The difference becomes clear when a static case is derived from the above result as a limiting process. While the elastic distortion in the static state can be obtained directly from (38) by taking  $\bar{V}_{ijk}=0$  and  $\omega=0$ , the displacement in that state must be specified in (37) by choosing a proper path for  $V_{ijk}$  which has brought the dislocations to their static configuration under

consideration. In other words, the displacement cannot be determined unless the motion of dislocations is specified. The difference also becomes clear when an oscillating case is considered. In this case, (37) gives only a time-dependent part of displacement: on the contrary (38) yields both the time-dependent and time-independent parts of the elastic distortion. To get the time-independent part of the displacement from (37), the dislocations are brought to the oscillating position under consideration through a progression of infinitesimal steps.

For the case of disclinations, the solution similar to (34) is obtained from (19),

$$U_m(x, t) = \iint_{-\infty}^{\infty} C_{klkj} H_{mk, l}(x - x', t - t') \epsilon_{jnh} \epsilon_{ist} V_n \theta_{hs}(x', t') x_t^0(x', t') d\mathbf{x}' dt'. \quad (41)$$

For a single disclination loop, (30) and (18) give

$$U_m(x, t) = \iint_S^{\infty} C_{klkj} G_{mk, l}(x - x', t - t') \epsilon_{ihs} \Omega_h x_n^0(x', t') dS_j(x', t') dt' \quad (42)$$

where  $dS_j$  is a surface element of the twisted plane  $S$ .

#### IV. Uniform Motion

In the following sections, some specifications will be imposed on the results given in the last section.

When all dislocations are moving uniformly with a constant velocity  $\mathbf{V}$ , definitions (3) and (5) lead to

$$V_{hi}(x, t) = V_i \alpha_{hi}(x, t), \quad (43)$$

and

$$\alpha_{hi}(x, t) = \alpha_{hi}(\mathbf{x} - \mathbf{V}t), \quad (44)$$

because a dislocation configuration at point  $x$  at time  $t=0$  is the same as that a point  $\mathbf{x} - \mathbf{V}t$  at time  $t=t$ . Let the distribution of dislocations at  $t=0$  given by  $\alpha_{hi}(x)$  be noted, then

$$\alpha_{hi}(x) = \int_{-\infty}^{\infty} \bar{\alpha}_{hi}(k) \exp(i\mathbf{k} \cdot \mathbf{x}) d\mathbf{k},$$

$$\bar{\alpha}_{hi}(k) = (2\pi)^{-\nu} \int_{-\infty}^{\infty} \bar{\alpha}_{hi}(x') \exp(-i\mathbf{k} \cdot \mathbf{x}') d\mathbf{x}', \quad (45)$$

The distribution at  $t = t$  is

$$\alpha_{hi}(x, t) = \int_{-\infty}^{\infty} \bar{\alpha}_{hi}(k) \exp \{i\mathbf{k}(\mathbf{x} - \mathbf{V}t)\} d\mathbf{k} \quad (46)$$

and the flux is

$$V_{hi}(x, t) = V_l \int_{-\infty}^{\infty} \bar{\alpha}_{hi}(k) \exp \{i\mathbf{k}(\mathbf{x} - \mathbf{V}t)\} d\mathbf{k} \quad (47)$$

Comparing them with (39), it can be seen that

$$\bar{V}_{hi} = V_l \bar{\alpha}_{hi}(k), \quad (48)$$

and the integral sign with respect to  $\omega$  drops out. Then, (37) and (38) become

$$U_m(x, t) = - \int_{-\infty}^{\infty} (1/\mathbf{k} \cdot \mathbf{V}) k_l C_{klkj} L_{mk}(k, -\mathbf{k} \cdot \mathbf{V}) \epsilon_{jnh} V_n \bar{\alpha}_{hi}(k) \exp \{i\mathbf{k}(\mathbf{x} - \mathbf{V}t)\} d\mathbf{k} \quad (50)$$

and

$$\beta_{nm}(x, t) = i \int_{-\infty}^{\infty} [\epsilon_{njh} C_{klkj} L_{mk}(k, -\mathbf{k} \cdot \mathbf{V}) k_l - \rho \mathbf{k} \cdot \mathbf{V} L_{im}(k, -\mathbf{k} \cdot \mathbf{V}) \epsilon_{nlh} V_l] \bar{\alpha}_{hi}(k) \exp \{i\mathbf{k}(\mathbf{x} - \mathbf{V}t)\} d\mathbf{k} \quad (51)$$

where  $\bar{\alpha}_{hi}(k)$  is known from the distribution at  $t = 0$  and  $L_{mk}(k, -\mathbf{k} \cdot \mathbf{V})$  is given by (27) and  $\omega = -\mathbf{k} \cdot \mathbf{V}$ .

The solution for a static case is easily obtained as a limiting case  $\mathbf{V} \rightarrow 0$ . It should be noticed in (50) that the limiting value of  $V_n/(\mathbf{k} \cdot \mathbf{V})$  does depend only on the direction of  $\mathbf{V}$ .

The first analytical solution was obtained by Frank [26] for a straight screw dislocation. In this case, all components of  $\alpha_{ij}$  are zero except

$$\begin{aligned} \alpha_{33}(x) &= b_3 \delta(x_1) \delta(x_2) \\ \bar{\alpha}_{33}(k) &= b_3 (2\pi)^{-2} \end{aligned} \quad (52)$$

with non-zero  $V_1$  and  $d\mathbf{k} = dk_1 dk_2$ ,  $k_3 = 0$ . Eshelby [27] extended the Frank solution to an edge dislocation. In the preceding analysis, (50) and (51) with non-zero components of  $\bar{\alpha}_{31} = b_1 (2\pi)^{-2}$  and  $V_1$  yield the solution. When non-zero components  $\bar{\alpha}_{31} = b_1 (2\pi)^{-2}$  and  $V_2$  are chosen, the solution is for the case of climb motion which agrees with Weertman's

solution [28]. Eshelby [27] extended the static solution of Peierls dislocation to the dynamic case of uniform motion (see also Leibfried and Dietz [29]).

For anisotropic materials, the denominator of  $L_{mk}(k, -\mathbf{k} \cdot \mathbf{V})$  is the sixth order homogeneous polynomial of  $k_i$  which has no analytical zero points except for a few cases of special elastic constants with higher symmetry. Bullough and Bilby [30] extended the two-dimensional static analysis of Eshelby, Read, and Shockley [31] to the dynamic case. The method employed by Bullough and Bilby has been applied to a fast-moving dislocation by Weertman [32, 33] and also applied to the investigation of the Weertman effect [34] by Teutonico [35, 36, 37].

Sáenz [38] and Stroh [39] discussed the limitation of dislocation velocities. The denominator of  $L_{mk}$  becomes zero for these limited values of velocity. The dislocations moving with higher velocities than these critical velocities are called supersonic dislocations. Eshelby [40] first showed the analytical solution for a supersonic screw dislocation, whereas Weertman [41] extended it to cover an edge dislocation.

Now, the energy of moving dislocations will be discussed under the absence of applied stresses. Consider two distributions of dislocations  $\alpha_{ij}(x, t)$  and  $\alpha'_{ij}(x, t)$  which are uniformly moving with velocity  $\mathbf{V}$  and  $\mathbf{V}'$  respectively. The interaction elastic strain energy between them is defined as

$$E_I = \int_{-\infty}^{\infty} C_{pqmn} \beta_{qp}(x, t) \beta'_{nm}(x, t) d\mathbf{x}, \quad (53)$$

where  $\beta'_{ij}$  is the elastic distortion caused by  $\alpha'_{ij}$ . For any function  $f(k)$ ,

$$\iint_{-\infty}^{\infty} f(k') \exp \{i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{x}\} d\mathbf{x} d\mathbf{k}' = (2\pi)^v f(-k), \quad (54)$$

therefore, (53) can be written as follows after the substitution of (51) and the similar formula for  $\beta'_{nm}$ ,

$$E_I = (2\pi)^v \int_{-\infty}^{\infty} C_{pqmn} [\epsilon_{qjh} C_{ktij} L_{pk}(k, -\mathbf{k} \cdot \mathbf{V}) k_l - \rho \mathbf{k} \cdot \mathbf{V} L_{ip}(k, -\mathbf{k} \cdot \mathbf{V}) \epsilon_{qth} V_l] \\ [\epsilon_{nj'h'} C_{k'l'i'j'} L_{mk'}(k, -\mathbf{k} \cdot \mathbf{V}') k_l - \rho \mathbf{k} \cdot \mathbf{V}' L_{i'm}(k, -\mathbf{k} \cdot \mathbf{V}') \epsilon_{nl'h'} V'_l] \\ \bar{\alpha}_{hi}(k) \bar{\alpha}'_{h'i'}(-k) \exp \{-i\mathbf{k} \cdot (\mathbf{V} - \mathbf{V}') t\} d\mathbf{k}. \quad (55)$$

Further modification can be made by using

$$\begin{aligned}\bar{\mathbf{k}} &= \mathbf{k}/k, & \bar{\mathbf{k}} \cdot \bar{\mathbf{k}} &= 1, \\ \bar{\mathbf{r}} &= \mathbf{r}/r, & \bar{\mathbf{r}} \cdot \bar{\mathbf{r}} &= 1.\end{aligned}\quad (56)$$

Then (55) can be written as

$$\begin{aligned}E_I &= -i(2\pi)^{-\nu} C_{pqmn} \int \int_{-\infty}^{\infty} \alpha_{hi}(x) \alpha'_{h'i'}(x') / r d\mathbf{x} d\mathbf{x}' \oint [\epsilon_{qjh} C_{klj} L_{pk}(\bar{\mathbf{k}}, -\bar{\mathbf{k}} \cdot \mathbf{V}) \bar{k}_l \\ &\quad - \rho \bar{\mathbf{k}} \cdot \mathbf{V} L_{ip}(\bar{k}, -\bar{\mathbf{k}} \cdot \mathbf{V}) \epsilon_{qlh} V_l] [\epsilon_{nj'h'} C_{k'l'i'j'} L_{mk'}(\bar{\mathbf{k}}, -\bar{\mathbf{k}} \cdot \mathbf{V}') \bar{k}_{l'} \\ &\quad - \rho \bar{\mathbf{k}} \cdot \mathbf{V}' L_{i'm}(\bar{k}, -\bar{\mathbf{k}} \cdot \mathbf{V}') \epsilon_{nl'h'} V_{l'}] dA / (\bar{\mathbf{k}} \cdot \bar{\mathbf{r}}),\end{aligned}\quad (57)$$

where

$$\mathbf{r} = (\mathbf{x} - \mathbf{x}') + (\mathbf{V} - \mathbf{V}')t. \quad (58)$$

The integral  $\oint dA$  is a surface integral defined on a unit sphere at the origin of  $\mathbf{k}$ -space. During the derivation of (57), the fact that  $k_l k_{l'} L_{mk}(k, -\bar{\mathbf{k}} \cdot \mathbf{V})$  is a ratio of two homogeneous polynomials with the same order was used. The  $\mathbf{r}$  is a distance between two dislocation segments at time  $t = t$ . The above result leads to the line integral expression [42] when two dislocation loops are considered to be in a static state ( $\mathbf{V} = \mathbf{V}' = 0$ ).

The elastic strain energy for one distribution  $\alpha_{ij}(x, t)$  is easily obtained as a special case of (57) by assuming  $\alpha_{ij} = \alpha'_{ij}$ ,  $\mathbf{V} = \mathbf{V}'$  and by multiplying by the factor 1/2.

Similarly, the interaction kinetic energy is defined as

$$K_I = \rho \int_{-\infty}^{\infty} \dot{U}_m(x, t) \dot{U}'_m(x, t) d\mathbf{x} \quad (59)$$

where  $\dot{U}'_m$  is the velocity of material caused by  $\alpha'_{ij}$ . Equation (59) can be written as

$$\begin{aligned}K_I &= (2\pi)^{\nu} \rho V_n V'_n \int_{-\infty}^{\infty} k_l k_{l'} C_{klj} C_{k'l'i'j'} L_{mk}(k, -\bar{\mathbf{k}} \cdot \mathbf{V}) L_{mk'}(k, -\bar{\mathbf{k}} \cdot \mathbf{V}') \\ &\quad \epsilon_{jnh} \epsilon_{j'n'h'} \bar{\alpha}_{hi}(k) \bar{\alpha}'_{h'i'}(-k) \exp \{-i\bar{\mathbf{k}} \cdot (\mathbf{V} - \mathbf{V}')t\} d\mathbf{k}\end{aligned}\quad (60)$$

or

$$\begin{aligned}K_I &= -i(2\pi)^{-\nu} \rho V_n V'_n \int_{-\infty}^{\infty} \alpha_{hi}(x) \alpha'_{h'i'}(x') / r d\mathbf{x} d\mathbf{x}' \oint \bar{k}_l \bar{k}_{l'} C_{klj} C_{k'l'i'j'} L_{mk}(\bar{\mathbf{k}}, -\bar{\mathbf{k}} \cdot \mathbf{V}) \\ &\quad L_{mk'}(\bar{k}, -\bar{\mathbf{k}} \cdot \mathbf{V}') \epsilon_{jnh} \epsilon_{j'n'h'} dA / (\bar{\mathbf{k}} \cdot \bar{\mathbf{r}})\end{aligned}\quad (61)$$

The kinetic energy for  $\alpha_{hi}(x, t)$  is similarly obtained from the above result by assuming  $\alpha_{ij} = \alpha'_{ij}$ ,  $\mathbf{V} = \mathbf{V}'$  and by multiplying the factor  $1/2$ . When the velocity  $\mathbf{V}$  is negligibly small compared with the sound velocities, the approximation

$$L_{mk}(k, -\mathbf{k} \cdot \mathbf{V}) \approx L_{mk}(k, 0) \quad (62)$$

can be used for (60) and (61). Then, the integrals in the  $\mathbf{k}$  space become independent of  $\mathbf{V}$  for  $\mathbf{V} = \mathbf{V}'$ . The kinetic energy, therefore, is expressed by a quadratic form of  $V_m$ . The effective mass of  $\alpha_{hi}$  is easily defined as the coefficient of  $(1/2)\rho V_n V_{n'}$  in that expression.

## V. Oscillation

When all dislocations are oscillating with a constant frequency  $\omega$  and a small amplitude, the velocity tensor can be approximated by

$$V_{thi}(x, t) = V_l \exp(i\omega t) \alpha_{hi}(x) \quad (63)$$

where  $\mathbf{V}$  is a constant velocity amplitude. The distribution of dislocations is independent of time under the above assumption and, therefore, it is denoted by  $\alpha_{hi}(x)$ . When  $\alpha_{hi}(x)$  is given as (46), eq (63) is expressed as

$$V_{thi}(x, t) = V_l \int_{-\infty}^{\infty} \bar{\alpha}_{hi}(k) \exp\{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} \quad (64)$$

and therefore

$$\bar{V}_{thi} = V_l \bar{\alpha}_{hi}(k) \quad (65)$$

Then, solutions (37) and (38) can be written as

$$U_m(x, t) = \int_{-\infty}^{\infty} (1/\omega) k_l C_{klj} L_{mk}(k, \omega) \epsilon_{jnh} V_n \bar{\alpha}_{hi}(k) \exp\{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} \quad (66)$$

$$\begin{aligned} \beta_{nm}(x, t) = i \int_{-\infty}^{\infty} [\epsilon_{njh} C_{klj} L_{mk}(k, \omega) k_l \\ + \rho \omega L_{im}(k, \omega) \epsilon_{nlt} V_l] \bar{\alpha}_{hi}(k) \exp\{i(\omega t + \mathbf{k} \cdot \mathbf{x})\} d\mathbf{k} \end{aligned} \quad (67)$$

As mentioned before, (66) yields only the time-dependent part of the displacement. On the other hand, (67) includes both the time-dependent and time-independent parts of the elastic distortion.

An example of a straight screw dislocation has been solved by Eshelby [43]. Kiusalaas and Mura [44] obtained an analytical solution for an edge dislocation. These solutions can be easily obtained from (66) by putting  $\bar{\alpha}_{33} = b_3(2\pi)^{-2}$  or  $\bar{\alpha}_{31} = b_1(2\pi)^{-2}$ , and  $k_3 = 0$ ,  $V_2 = V_3 = 0$ ,  $d\mathbf{k} = dk_1 dk_2$ . It is rather surprising that, compared with the case of uniform motion, very few examples of oscillations have been exactly solved.

The elastic strain energy,  $E$ , and the kinetic energy,  $K$ , can be obtained by a similar method as was used in the case of uniform motion. It will be necessary, however, in the products  $(1/2)C_{pqmn}\beta_{qp}\beta_{nm}$  and  $(1/2)\rho\dot{U}_m\dot{U}_m$  to take the real part of each factor of the products.

The result is expressed as

$$E = \frac{(2\pi)^\nu}{2} \int_{-\infty}^{\infty} C_{pqmn} [\epsilon_{qjh} C_{klkj} L_{pk}(k, \omega) k_l + \rho \omega L_{ip}(k, \omega) \epsilon_{qjh} V_i] \\ [\epsilon_{nj'h'} C_{k'l'i'j} L_{mk'}(k, \omega) k_{l'} - \rho \omega L_{i'm}(k, \omega) \epsilon_{nl'h'} V_{l'}] \bar{\alpha}_{hi}(k) \bar{\alpha}_{h'i}(-k) \cos^2 \omega t d\mathbf{k} \quad (68)$$

and

$$K = \frac{-(2\pi)^\nu}{2} \rho V_n V_{n'} \int_{-\infty}^{\infty} k_l k_{l'} C_{klkj} C_{k'l'i'j} L_{mk}(k, \omega) L_{mk'}(k, \omega) \\ \epsilon_{jnh} \epsilon_{j'n'h'} \bar{\alpha}_{hi}(k) \bar{\alpha}_{h'i}(-k) \sin^2 \omega t d\mathbf{k}. \quad (69)$$

For the simple example of a straight screw dislocation which is oscillating with a small amplitude  $A$ ,  $\bar{\alpha}_{33}(k) = \bar{\alpha}_{33}(-k) = b_3(2\pi)^{-2}$ ,  $V_1 = A i \omega$ . Then (68) and (69) give

$$E = \frac{\mu b_3^2}{8\pi} \{2 \log R/\epsilon_0 - A^2 (\omega/c)^2\} \cos^2 \omega t \\ K = \frac{\mu b_3^2}{8\pi} A^2 (\omega/c)^2 \log R/\epsilon_0 \sin^2 \omega t \quad (70)$$

where  $\mu$  is the shear modulus,  $c$  the shear wave velocity, and  $R$  and  $\epsilon_0$  are the cut-off radius of the material size and the dislocation core radius, respectively.

For oscillating disclinations, a similar result is obtained from (41). The time-dependent part of displacement is

$$U_m(x, t) = \iint_{-\infty}^{\infty} C_{klkj} H_{mk}, l(x - x', t - t') \epsilon_{jnh} \epsilon_{ist} V_n \exp(i\omega t') \theta_{hs}(x') x_t^0(x') d\mathbf{x}' dt'. \quad (71)$$

## VI. Forces

When a material is subjected to an applied stress, the total stress field is simply a sum of the applied stress  $\tau_{ij}$  and the internal stress  $\sigma_{ij}$  caused by dislocations or disclinations. The applied stress is defined as that stress which is *elastically* in equilibrium under the applied boundary forces. The total stress is called the elasto-plastic stress.

Consider an arbitrary domain  $G$ , lying entirely within a given domain  $D$  of the material. The rate of work done by the total stress on the boundary  $\partial G$  of  $G$  is

$$\delta W/\delta t = \int_{\partial G} (\sigma_{ij} + \tau_{ij}) \dot{U}_i n_j dS. \quad (72)$$

The  $U_i$  is the total displacement, satisfying the field equations

$$\begin{aligned} \sigma_{ij,j} + \tau_{ij,j} &= \rho \ddot{U}_i \\ \dot{U}_{i,j} &= \dot{\beta}_{ji}^* + \dot{\beta}_{ji} + \dot{\gamma}_{ji} \end{aligned} \quad (73)$$

where  $\beta_{ji}$  and  $\gamma_{ji}$  are the elastic distortions related to  $\sigma_{ij}$  and  $\tau_{ij}$  by Hooke's law, respectively.

Applying Gauss' theorem of integration to (72) and using (73),

$$\delta W/\delta t = \dot{E} + \dot{K} + \int_G (\sigma_{ij} + \tau_{ij}) \dot{\beta}_{ji}^* d\mathbf{x} \quad (74)$$

where  $E$  and  $K$  are the elastic strain energy and the kinetic energy in  $G$  respectively, that is,

$$\begin{aligned} E &= \frac{1}{2} \int_G (\sigma_{ij} + \tau_{ij}) (\beta_{ji} + \gamma_{ji}) d\mathbf{x}, \\ K &= \frac{1}{2} \int_G \rho \dot{U}_i \dot{U}_i d\mathbf{x}. \end{aligned} \quad (75)$$

From (4), eq (74) can be written as

$$\delta W/\delta t - \dot{E} - \dot{K} = \int_G (f_l V_l + f'_l V'_l + \dots) d\mathbf{x} \quad (76)$$

where

$$\begin{aligned} f_l &= -(\sigma_{ij} + \tau_{ij}) \epsilon_{jlm} \nu_m b_l \\ f'_l &= -(\sigma_{ij} + \tau_{ij}) \epsilon_{jlm} \nu'_m b'_l \end{aligned} \quad (77)$$

are the Peach-Koehler force or the force defined by (15). According to the balance of energy, the right side of (76) is equal to the energy dissipated

in  $G$ , namely

$$\int_G (f_l V_l + f'_l V'_l \dots) d\mathbf{x} = \int_G Q d\mathbf{x} \quad (78)$$

where  $Q$  is the energy dissipated per unit volume and can not be negative according to the second law of thermodynamics. As reviewed by Lothe [45],  $Q$  can be evaluated *independently* by several models of energy dissipation. The most fundamental one will be the Zener thermoelastic dissipation proposed by Eshelby [43], later modified by Weiner [46]. Mason [47, 48] proposed the other models of dissipation caused by phonon viscosity and electron viscosity.

For most cases,  $Q$  is a quadratic form of the velocity of the dislocation. Then, eq (78) yields

$$f_l = \partial Q / \partial V_l, f'_l = \partial Q / \partial V'_l, \dots \dots \dots, \quad (79)$$

which is considered as the equilibrium of dislocation forces. When no energy dissipations are considered, the equilibrium can be written as

$$f_l = 0, f'_l = 0, \dots \dots \dots \quad (80)$$

Consider an infinitely extended body where dislocations are oscillating as described in the last section under the absence of applied stresses. Eshelby [43] pointed out that the average of  $\delta W / \delta t$  per period is positive (those for  $\dot{E}$  and  $\dot{K}$  are zero). From (76), it can be seen that the average of  $f_l V_l$  per period for  $\tau_{ij} = 0$  is positive. This energy dissipated is called the radiation energy. In order to keep the dislocations in such a state of periodic oscillation, the same amount of energy as dissipated must be supplied by the application of  $\tau_{ij}$ , which is determined from

$$f_l = -(\sigma_{ij} + \tau_{ij}) \epsilon_{jlm} \nu_h b_i = 0. \quad (81)$$

The  $\tau_{ij}$  is applied in the form of sound waves. Then, the dislocation stress field is interpreted as the scattering of the sound waves. This calculation has been done by Nabarro [49] and Leibfried [50]. Leibfried argued that the scattering of sound waves due to the thermal vibration of the atoms should lead to a drag force on a moving dislocation. It should be noticed that the resultant dissipation of energy under  $\sigma_{ij}$  and  $\tau_{ij}$  is zero in this case. A further investigation on the phonon scattering has been done by Ninomiya [51] by using a string model of a dislocation.

## VII. Conclusion

In this paper the differential geometry involved with dislocations and disclinations and the generalized mechanics of oriented media have not been discussed, since the emphasis of the present paper has been placed upon only the elastic field associated with these line imperfections in the framework of linear elasticity.

There are several problems remaining to be solved. Contrary to the case of dislocations, no observation of a disclination line has been reported beside the work done by Anthony, Essmann, Seeger, and Träuble [52]. If the Burgers vector is observed as a tangential vector along the singularity curve, the curve is a disclination. The atomic configuration associated with a disclination loop and the stability of the loop should be investigated in order to substantiate the physical realization of the disclination. The atomic misfit involves the whole plane bounded by the loop. Since all the atoms on the plane are displaced to a higher potential energy level, the Burgers rotational vector  $\Omega$  possibly changes its value during subsequent motion in order to reduce the potential energy.

Application of the theory of moving dislocations to the dynamic plasticity of metals has not been fully researched. The macroscopic theory of plastic waves due to von Karman and Duwez [53] should be reconsidered in the light of the behavior of accelerated dislocations. More practical applications of dislocation motion will be found in sheetdrawing, extrusion, and machining where the arrangement and oscillation of dislocations become the important factors.

Green's functions for anisotropic elasticity are the most fundamental functions for the analytical study of imperfections in crystalline materials. Contrary to the static case [54-57], very little work has been done on the dynamic case. A more comprehensive investigation seems to be necessary. Finally, it is proposed to study physical applications of a new concept of the *impotent* distribution of dislocations (Mura [58]). The impotent distribution of dislocations is constructed from (9) by using asymmetric plastic distortion tensor  $\beta_{ij}^* = -\beta_{ji}^*$ . Such a distribution of dislocations does not produce any displacement and stress fields in material.

## VIII. Acknowledgement

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## Discussion on Paper by T. Mura.

ARSENAULT: What can you say about the energy of the disclination?

MURA: I have not calculated the energy, yet, but if we consider the screw type of disclination in a finite cylinder, I think it is not too bad. Also, the edge type of disclination is not bad in an infinitely extended medium. Part of these calculations have actually been done.

ARSENAULT: Could you foresee a disclination as a twin fracture nucleus?

MURA: Yes, it might have applications to twinning, but I don't know about fracture.

SIMMONS: I'd like to ask a question for clarification in my own mind. One would have thought that the way to make a disclination would be by introducing a discontinuity in the rotation across a surface which then leads you directly to the concept of a curvature type element—in the Riemannian geometry sense. I was curious to see why you thought it necessary to put in a center of rotation in your definition. Would it not be easier if one just had this concept of a discontinuity in rotation on the surface without having to identify a center point?

MURA: Your question involves geometry and, as I said in my talk, research in dislocations might be done in three ways: geometry, elasticity and physics. The geometry is a chaos and the physics is a jungle; only the elasticity theory is clear. So I don't want to get into the geometric part of your question. However, I need a center of rotation to express the displacement jump at the discontinuity surface in terms of rotation. In your description, the center of rotation is on the discontinuity surface and at each discontinuity point, so you have no displacement jump in your formulation.

DE WIT: I also thought to make a comment on this point. There is a constant rotation associated with the discrete disclination and there is maybe not a center, but an axis of rotation which need not be fixed in space. It could be moved to a different location by adding some dislocations to the disclination, because you can move the axis by a translation.<sup>1</sup> So, Dr. Simmons' description differs from Professor Mura's by a dislocation distribution.

<sup>1</sup> See paper by R. de Wit in these Proceedings: eq (3.4) for the discrete case, or eq (7.4) for a continuous distribution.

MURA: I should apologize for not saying more clearly that I'm considering dislocations and disclinations separately. I have expressed the plastic distortion in one way or the other, so if you have motion of both dislocations and disclinations at the same time it cannot be as simple as the expressions I gave.

VON TURKOVICH: Would your velocity calculation be applicable to the case of a half mil where you can tie to the classical solution for slip lines?

MURA: Yes, it is applicable, but this is a special case which I haven't calculated.

BULLOUGH: I just wondered if, in your example you took on the opposite sides of a half plane a discrete semi-infinite row of evenly spaced edge dipoles with Burgers vectors perpendicular to the half plane and put your edge dislocation with Burgers vector in the plane at the end of the row, what does the stress field look like then?

MURA: As I said, if the row of dipoles is continuous, then the stress field is zero. If, however, the distribution is discrete, the stress field might be periodic over the half plane where dipoles are and have zero space average. In the half space away from the dipoles it should be almost zero, but I don't know without calculating how it falls off perpendicular to the half plane.

ESHELBY: Isn't the impotent dislocation array you're discussing just a narrow strip of material between the dipoles which has been rotated relative to the stuff outside—like inside a little grain? Then it's not surprising it has no strain field.

MURA: Right.

# KINEMATICS OF CONTINUOUSLY DISTRIBUTED DISLOCATIONS

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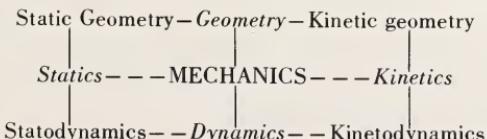
The general non-Riemannian approach to the geometry of a solid with lattice defects is extended to include the kinematics. The treatment is valid for both the motion of old defects and the creation of new ones. The change in a geometric quantity is described by a corresponding rate. The main quantities dealt with are distortion rates, stretching tensors and connexion rates, and new quantities called fluxions are introduced. In terms of these a fundamental kinematic law and continuity equations for the defect currents are set up and are found to be consistent with earlier results valid in special cases.

Key words: Affine connection; continuum mechanics; kinematics; non-Riemannian geometry.

## Introduction

The first attempt to develop a kinetic<sup>1</sup> theory of continuously distributed dislocations (CDD) was made in 1960 by Holländer [1, 2, 3], who used the close analogy to electrodynamics to put forward a linearized theory based on a set of equations following the pattern of Maxwell's equations. In 1962,

<sup>1</sup> We shall try to revive here a nomenclature advocated by Sir William Thompson (Lord Kelvin) and P. G. Tait and used by Grammel and Winkelmann. According to this nomenclature, *mechanics* is the science of motion and forces, and thus is divided into geometry and dynamics. *Geometry* deals with spatial relations, whereas *dynamics* deals with the action of forces. With regard to whether changes in time are considered or not, mechanics is divided into *statics* and *kinetics*. Consequently, we distinguish *static geometry* from *kinetic geometry* (commonly called "kinematics"), and *statodynamics* ("statics") from *kinetodynamics* ("dynamics"). This is visualized in the following diagram:



the same author [4] reformulated the kinematics to conform with the non-linear theory of CDD as developed by Bilby et al. [5, 6, 7, 8], and Kröner [9]. Holländer's work suffers from the typical inconsistencies and deficiencies of a first try. Nevertheless, it was the signal for the start of an intense activity in this field. Amari [10] and Simmons [11] introduced four-dimensional formalisms into the differential-geometric theory. Amari was able to develop a full kinematic theory in the linear approximation, while Simmons, working within a much wider framework, also arrived at the fundamental kinematic law. Kosevich [12, 13] rediscussed the linear theory and rediscovered Holländer's 1960 results. However, he extracted a consistent minimum set of equations, so that he could determine the elastic field of a given continuous distribution of dislocations undergoing prescribed motions. Bross [14] corrected Holländer's calculations and also convincingly showed that a four-dimensional approach could have only formal value. An original and very fruitful approach to the kinetics of CDD was proposed by Mura [15, 16, 17]. He formulated the problem in terms of integral equations and used the formalism of Green's functions to find interpretable solutions. Finally, Günther [18], in a comprehensive monograph presented what seems to be, to this date, the most exact, clear and elaborate formulation of the kinematics of CDD (KCDD). None of the aforementioned papers considered plastic distortion.

Bilby et al. [19] extended the static geometry of CDD to include non-metric connexions, and thus obtained an adequate continuum description of the geometrical properties of both dislocations and point defects in the static case.

In this account we shall deal with the kinematics of CDD at a stage of development corresponding to Günther [18]. However, necessary criticism shall not be withheld and original work concerned with the generalization to ammetric conditions will also be reported. A treatment of dynamics will not be included.

The mathematical presentation, and in particular the tensor notation will, except for minor deviations, adhere to those adopted by Schouten [20, 21]. The terminology and conventions concerning the distortions are explained in another paper presented at this conference [22].

## I. Four-Dimensional Formulation of Fundamental Equations

Let us consider an elastic crystalline medium  $M$  embedded in our real three-dimensional Euclidean space  $E3$ . The elements of  $M$ , called "points," shall be represented by (usually cartesian) coordinates in  $E3$ . The medium  $M$  has the following two basic properties:

(1) At each point of  $M$  is given a set of quantities  $\mu_1, \dots, \mu_r, \dots$  characterizing the elastic properties of  $M$ . In general, the  $\mu$ 's will be

functions of the points and the time, though usually they will be just the ordinary elastic constants of various orders.

(2) At each point of  $M$  is given a set of three independent preferred directions, i.e., the lattice orientation. In general,  $M$  will be in some strained and dislocated state.

In order to simplify the presentation, let us assume that the ideal lattice vectors form an orthonormal triple. The generalization to arbitrary lattices is almost trivial.

The crystalline medium  $M$  is transformed from the ideal state  $[A]$  to the final state  $[a]$  by the total distortion  $T^a_{\cdot b}$

We shall formally extend the E3 to a four-dimensional Minkowskian space  $\bar{E}4$  by including the time coordinate, conveniently defined by

$$x^0 \equiv ct, \quad (1.1)$$

where  $c$  is some constant having the dimensionality and the order of the speeds of sound in  $M$ . No special importance should be attached to either the definition (1.1) or the specific value of  $c$ . We shall elaborate on this point later.

The total distortion  $T^a_{\cdot b}$  will be artificially extended to a 4-distortion by the definition<sup>2</sup>

$$T^{\alpha}_{\cdot \beta} \equiv \begin{pmatrix} T^a_{\cdot b} & T^0_{\cdot b} = 0 \\ T^a_{\cdot 0} = v^a/c & T^0_{\cdot 0} = 1 \end{pmatrix}, \quad (1.2a)$$

with the inverse

$$L^{\alpha}_{\cdot \beta} = \begin{pmatrix} L^a_{\cdot b} & L^0_{\cdot b} = 0 \\ L^a_{\cdot 0} & L^0_{\cdot 0} = 1 \end{pmatrix}, \quad (1.2b)$$

where  $v^a = v^a(x^0, x^b)$  is the matter velocity. It can be easily shown that

$$L^a_{\cdot 0} = -L^a_{\cdot b}v^b/c \quad (1.2c)$$

The Eulerian metric will be given by the equation

$$g_{\alpha\beta} = L^{\kappa}_{\cdot \alpha} L^{\lambda}_{\cdot \beta} G_{\kappa\lambda}, \quad (1.3a)$$

<sup>2</sup> We shall agree that Roman indices take the values  $a, b, \dots = 1, 2, 3$ , while Greek indices shall take the values  $\alpha, \beta, \dots = 0, 1, 2, 3$ .

with the inverse

$$g^{\alpha\beta} = T^\alpha_\kappa T^\beta_\lambda \mathcal{D}^{\kappa\lambda}, \quad (1.3b)$$

where  $G_{\alpha\beta}$  is arbitrarily fixed by choosing a pseudo-Cartesian coordinate system such that

$$G_{\alpha\beta} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (1.4a)$$

with the inverse

$$\mathcal{D}^{\alpha\beta} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (1.4b)$$

A 4-connexion  $b_{\alpha\beta}^\gamma$  of distant parallelism can now be defined by

$$b_{\alpha\beta}^\gamma \equiv T^\gamma_\kappa \partial_\alpha L^\kappa_\beta. \quad (1.5a)$$

This connexion must satisfy the auxiliary conditions

$$\square_\alpha T^\gamma_\beta = 0, \quad (1.5b)$$

and

$$\square_\alpha g_{\beta\gamma} = 0, \quad (1.5c)$$

where  $\square_\alpha$  is the four-dimensional operator of the covariant derivative. From (1.2) it follows that

$$b_{\alpha\beta}^0 = 0, \quad (1.5d)$$

while in general  $b_{\alpha\beta}^c \neq 0$ .

Apart from  $b_{\alpha\beta}^\gamma$  we shall also define the 3-connexion

$${}^3b_{ab}^c \equiv T^c_{\cdot k} \partial_a L^k_{\cdot b}. \quad (1.6)$$

Now we define the 4- and 3-tensors of curvature, respectively, by

$$\frac{1}{2}c_{\alpha\beta\gamma}{}^\delta \equiv \partial_{[\alpha}b_{\beta]\gamma}{}^\delta + b_{[\alpha|\kappa|}b_{\beta]\kappa}{}^\delta, \quad (1.7)$$

$$\frac{1}{2}{}^3c_{abc}{}^d \equiv \partial_{[a}{}^3b_{b]c}{}^d + {}^3b_{[a|k|}{}^d {}^3b_{b]k}{}^c, \quad (1.8)$$

respectively.

The set of kinematic field equations is now obtained by extending the fundamental geometric law to four dimensions. At the same time one still has to postulate the validity of the static geometric law and the condition (1.5d). Summarizing, we have the equations

$$c_{\alpha\beta\gamma}{}^\delta = 0, \quad (1.9a)$$

$$b_{\alpha\beta}^0 = 0, \quad (1.9b)$$

$${}^3c_{abc}{}^d = 0. \quad (1.9c)$$

However, these equations are redundant and we have to select from among them a set of independent equations. We shall proceed to do so, but first let us give a geometric interpretation of (1.9).

Equation (1.9a) represents the necessary and sufficient conditions of distant parallelism in  $\bar{E}4$ . Yet, eq (1.9b) shows that the  $\bar{E}4$  is not genuinely four-dimensional, but at all times decomposes into the ordinary  $E3$  and the time axis. Then (1.9c) is the necessary and sufficient condition of distant parallelism in  $E3$ , now valid at all times.

## II. Independent Equations

The equations of general relativity corresponding to (1.9a) include four arbitrary parameters reflecting the equivalence of frames of reference. There is no such equivalence in KCDD. However, from the mathematical point of view, we do have four additional degrees of freedom. Let us clarify their significance.

From (1.2, 1.3, 1.4) it follows that

$$\mathcal{S}^{ab} = {}^3\mathcal{S}^{ab} - \frac{v^a v^b}{c^2}, \quad (2.1a)$$

$$\mathcal{S}^{0b} = -\frac{v^b}{c}, \quad (2.1b)$$

$$\mathcal{S}^{00} = -1, \quad (2.1c)$$

and hence

$$g_{ab} = {}^3g_{ab}, \quad (2.2a)$$

$$g_{0b} = -\frac{v^k}{c} g_{kb}, \quad (2.2b)$$

$$g_{00} = -1 + \frac{v^k v^l}{c^2} g_{kl}. \quad (2.2c)$$

Equation (2.2c), or any equivalent equation for that matter, fixes one of the four arbitrary parameters. The remaining three degrees of freedom have genuine physical significance. The corresponding parameters are determined by the equilibrium conditions

$$\partial_k \hat{\sigma}^{ka} - \hat{\rho} dv^a/dt = -\hat{f}^a, \quad (2.3)$$

where  $\hat{\sigma}^{ka}$  is the stress tensor density,  $\hat{\rho}$  the mass density, and  $\hat{f}^a$  the density of volume forces. With the constitutive equations

$$\hat{\sigma}^{ab} = \hat{\sigma}^{ab}(g_{kl}) \quad (2.4)$$

eq (2.3) represents three differential conditions determining the metric  $g_{ab}$  in a unique way.

We proceed to eliminate the redundant equations from the set (1.9). In order to do so we shall write down evidently independent equations and by successive scanning establish any additional conditions until the process is exhausted.

Equations (1.9) define the metric if the connexions  $b_{\alpha\beta}^\gamma$  and  ${}^3b_{ab}^c$  are decomposed into their Riemannian parts  $g_{\alpha\beta}^\gamma$  and  ${}^3g_{ab}^c$  and the torsion tensors  $s_{\alpha\beta}^\gamma$  and  ${}^3s_{ab}^c$ , respectively, i.e., if the dislocation density is given as a physical quantity. Thus

$$b_{\alpha\beta}^\gamma = g_{\alpha\beta}^\gamma + s_{\alpha\beta}^\gamma + s_{\beta\alpha}^\gamma + s_{\alpha\beta}^\gamma, \quad (2.5a)$$

$${}^3b_{ab}^c = {}^3g_{ab}^c + {}^3s_{ab}^c + {}^3s_{ab}^c + {}^3s_{ba}^c, \quad (2.5b)$$

where

$$g_{\alpha\beta}^\gamma \equiv \frac{1}{2} \partial^{\gamma\mu} \{ \partial_\alpha g_{\beta\mu} - \partial_\mu g_{\alpha\beta} + \partial_\beta g_{\mu\alpha} \}, \quad (2.6)$$

and

$$s_{\alpha\beta}^\gamma \equiv b_{[\alpha\beta]}^\gamma \quad (2.7)$$

with analogous definitions for  ${}^3g_{ab}^c$  and  ${}^3s_{ab}^c$ .

Now we have to find a physical interpretation for the 4-torsion  $s_{\alpha\beta}^\gamma$ .

From (1.2b, 1.5a, 1.6) it follows that

$$b_{ab}^c = {}^3b_{ab}^c, \quad (2.8)$$

and hence

$$s_{ab}^c = {}^3s_{ab}^c, \quad (2.9a)$$

which represents the dislocation density. Moreover, according to (1.5a)

$$s_{\alpha\beta}^0 = 0. \quad (2.9b)$$

Günther [18] also showed that

$$s_{.0c}^0 = -\frac{v^l}{c} s_{.1c}^0 \quad (2.9c)$$

$$s_{.bo}^0 = -\frac{v^m}{c} s_{.bm}^0, \quad (2.9d)$$

$$s_{.00}^0 = \frac{v^l v^m}{c} s_{.lm}^0. \quad (2.9e)$$

$$s_{.bc}^a = {}^3s_{.bc}^a + \frac{v^a}{c} s_{.bc}^0. \quad (2.9f)$$

Thus, any tensor component of  $s_{\alpha\beta}^{\gamma}$  having at least one 0 index either vanishes or can be reduced to  $s_{.bc}^0$ . Therefore, it is essential to find an interpretation to the latter, and, once this has been done, the entire 4-tensor of torsion becomes physically meaningful.

As, of course, anticipated,  $s_{.bc}^0$  turns out to represent the dislocation current. Components with more than one 0 index then stand for additional purely kinematical terms. Moreover, we see that an additional 0 index reduces the order of the component by a factor of  $v/c$ .

In addition to eqs (2.9) the only independent condition following from (1.9b) turns out to be

$$b_{(ab)}^0 = 0. \quad (2.10)$$

Clearly, (1.9c) is independent of (2.10). Thus we have the condition

$${}^3c_{abc}^d = 0. \quad (2.11)$$

Now we have to check the number of independent conditions imposed by (1.9a) in addition to (2.10, 2.11). This number is given by the number of independent components of  $c_{\alpha\beta\gamma}^{\delta}$ , determined by its symmetries.

By definition, the curvature tensor fulfills the *first identity*

$$c_{(\alpha\beta)\gamma}{}^\delta = 0 \quad (2.12)$$

and the *second identity*

$$c_{[\alpha\beta\gamma]}{}^\delta = 2 \nabla_{[\alpha} s_{\beta\gamma]}{}^\delta - 4 s_{[\alpha\beta}{}^\mu s_{\gamma]\mu}{}^\delta,$$

or

$$c_{[\alpha\beta\gamma]}{}^\delta = 2 \overset{2}{\nabla}_{[\alpha} s_{\beta\gamma]}{}^\delta. \quad (2.13)$$

Since the connexion  $b_{\alpha\beta}^\gamma$  is metric, the *third identity* is also valid in the form

$$c_{\alpha\beta(\gamma\delta)} = 0. \quad (2.14)$$

Thus, the fundamental kinematic law (1.9a) imposes only the condition

$$c_{[\alpha\beta\gamma]}{}^\delta = 0, \quad (2.15)$$

or, in terms of the torsion, i.e., the dislocation density and current

$$\overset{2}{\nabla}_{[\alpha} s_{\beta\gamma]}{}^\delta = 0. \quad (2.16)$$

However, the fundamental law of static geometry (2.11) already covers a part of (2.15), so that the additional content of (2.15) can be reduced to

$$c_{(0bc)}{}^d = 0. \quad (2.17)$$

From (2.14, 2.15) it follows that the curvature tensor also fulfills the *fourth identity*

$$c_{[[\alpha\beta|\gamma\delta]]} = 0. \quad (2.18)$$

The symmetry conditions limit the number of independent components of  $c_{\alpha\beta\gamma}^\delta$  to 21. Now (2.10) represents 6 equations, (2.11) 9 equations, and (2.17) 3 equations, in all 18 evidently independent equations. The remaining 3 parameters are fixed by (2.3).

Thus the full set of kinematic equations can be written as

$${}^3c_{abc}{}^d = 0, \quad (2.19a)$$

$$b_{(ab)}^0 = 0, \quad (2.19b)$$

$$c_{(0bc)}{}^d = 0. \quad (2.19c)$$

Günther presented a few more equivalent formulations such as

$${}^3c_{(ab)} = 0, \quad (2.20a)$$

$$c_{(ab)} = 0, \quad (2.20b)$$

$${}^3c_{[abc]d} = 0, \quad (2.20c)$$

$${}^3c_{[0bc]d} = 0, \quad (2.20d)$$

where

$${}^3c_{ab} \equiv {}^3c_{mab}{}^m, \quad (2.21a)$$

$$c_{ab} \equiv c_{\mu ab}{}^\mu \quad (2.21b)$$

are the three- and four-dimensional Ricci tensors, respectively, and

$${}^3c_{[0bc]d} \equiv c_{[0bc]}{}^n g_{dn} \quad (2.21c)$$

### III. Interpretation

Equation (2.19b) can be written in the explicit form

$$cb_{(ab)}^0 = \frac{1}{2} (\partial g_{ab}/\partial t + v^m \partial_m g_{ab}) + g_{m(a} \partial_{b)} v^m + 2cs_{(ab)}^0 = 0, \quad (3.1)$$

While eq (2.20d) becomes

$$\begin{aligned} 3c^3c_{[0ab]c} &= \partial^3 s_{abc}/\partial t - 2c \partial_{[a} s_{b]c}^0 + v^m \partial_m s_{abc} \\ &- 2^3s_{m[a|c} \partial_{b]} v^m + {}^3s_{abm} \partial_c v^m \\ &+ 2cs_{[a|m|} {}^3b_{b]c}^m + 2c {}^3s^m{}_{ab} s_{cm}^0 = 0. \end{aligned} \quad (3.2)$$

This equation is the key to the interpretation of  $s_{bc}^0$ . Taking into account (2.9a) and neglecting all nonlinear terms in (3.2) we obtain

$$\frac{\partial}{\partial t} s_{ab}{}^c = 2c \partial_{[a} s_{b]}^0. \quad (3.3)$$

Holländer [4] derived a continuity equation for dislocation currents which, in the linear approximation, reads

$$\frac{\partial}{\partial t} s_{ab}^c = \partial_{[a} j_{b]}^c. \quad (3.4)$$

where  $j_b^c$  is the dislocation current tensor defined as follows. Let  $\hat{k}^{abc}$  be the total Burgers vector in the  $c$  direction carried by dislocation lines in the  $b$  direction moving in the  $a$  direction and crossing in a unit of time a unit of length normal to the  $(bc)$  plane if  $b \neq c$ , and normal to the  $(ab)$  plane if  $b = c$ . Since the motion of dislocation in its line direction is unphysical  $\hat{k}^{abc}$  is completely determined. The plastic effects are given by the tensor density

$$\hat{j}^{abc} \equiv \hat{k}^{[ab]c} \quad (3.5)$$

which is then appropriately called the dislocation current density.

This can be equivalently replaced by the tensor

$$j_a^b = \epsilon_{kla} \hat{j}^{kbl} = \epsilon_{kla} \hat{k}^{kbl}, \quad (3.6)$$

called the dislocation current tensor. The latter is connected with the plastic distortion  $P_a^b$  by means of the equation

$$\partial P_a^b / \partial t = -j_a^b. \quad (3.7)$$

Generalizing the results of the linear theory we identify

$$2c s_{b}^0{}^c = j_b^c = -\partial P_a^c / \partial t. \quad (3.8)$$

Hence, eq (3.2) is the nonlinear continuum equation connecting the dislocation density with the dislocation current. Then eq (3.1) connects the strain and the matter velocity with the dislocation current.

#### IV. Comments

Günther [18] discussed the relationship of his results to earlier work by Amari [10], Holländer [1, 2, 3, 4], Bross [14], and Kosevich [12, 13].

In the linear approximation the fundamental equations reproduce Amari's results. However, Amari failed to recognize the importance of distinguishing between 3- and 4-quantities. Yet, this does not affect the validity of the results, since in the linear approximation the spacelike-part of any 4-quantity and the corresponding 3-quantity do indeed coincide.

On the other hand, however, probably due to the latter circumstance Amari did not select a set of independent equations, and so his formulation is redundant.

Bross [14] considered the case of vanishing impressed volume forces and a homogeneous isotropic hookeian medium. In this case, the equilibrium conditions (2.3), the constitutive equations (2.4) and the linearized equation

$$c_{ab} \equiv c_{\kappa ab}^{\kappa} = 0 \quad (4.1)$$

yield an equation for elastic waves in the presence of dislocations and dislocation currents:

$$\partial_k \partial^k \epsilon_{ab} + (1 + \lambda/\mu) \partial_a \partial_b \epsilon_k^k - (1/c_T^2) \partial^2 \epsilon_{ab} / \partial t^2 = t_{ab}, \quad (4.2)$$

where

$$\frac{1}{4} t_{ab} \equiv (1/c) \partial s_{(ab)}^0 / \partial t + \partial_k s^k_{(ab)} - \partial_{(a} s^k_{b)k}, \quad (4.3)$$

$c_T$  is the transversal wave velocity, and  $\lambda, \mu$  are the Lamé constants.

Equation (4.2) reduces to inhomogeneous wave equations if shape and volume deformations are taken separately. For  $\epsilon_k^k = 0$  we have

$$\partial_k \partial^k \epsilon_{ab} - (1/c_T^2) \partial^2 \epsilon_{ab} / \partial t^2 = t_{ab}, \quad (4.2a)$$

while by contraction of the indices  $a, b$  we obtain

$$\partial_k \partial^k \epsilon_l^l - (1/c_L^2) \partial^2 \epsilon_l^l / \partial t^2 = t_l^l, \quad (4.2b)$$

where  $c_L$  is the longitudinal wave velocity.

The equations derived by Bross are identical with (4.2) except that the right-hand sides were expressed in terms of the incompatibility.

Holländer [3, 4], Amari [10], Kosevich [12, 13] and Günther [18] all arrive in some form at the kinematical law in terms of elastic strains and dislocation currents

$$\nabla_{(a} v_{b)} + \frac{1}{2} \partial \epsilon_{ab} / \partial t = j_{(ab)} \quad (4.4)$$

and the continuity equations

$$\nabla_{[a} \nabla_{b]} v^c - \nabla_{[a} j_{b]}^c + \partial s_{ab}^c / \partial t = 0 \quad (4.5)$$

which here were given as (2.19c).

Günther used equations (4.2a, b) to justify his choice of

$$c = c_T. \quad (4.6)$$

Yet, he honestly admitted that such a choice was by no means necessary. His own analysis clearly shows that the “elastic spacetime” invariably degenerates into separate spacelike and timelike parts.

I wish to discuss this point in some detail. In my early work [1, 2, 3], I introduced a four-dimensional space-time continuum primarily as a heuristic means to find the right equations which subsequently should be physically justified. Yet, the particular choice (4.6) was made on the basis of the physical rather than formal similarity between fast dislocations and relativistic particles with full awareness of the significant differences. Indeed, the physical result that emerged was the clear recognition that a linearized theory could hold only for low velocities as well as small distortions, and then the particular choice of  $c$  becomes immaterial as long as  $c$  has the order of magnitude of the speed of sound.

It also became clear that upon deciphering the four-dimensional equations one is left with a great many redundant relations some of which are hard to interpret. In fact, I totally misinterpreted some quantities confusing distemperations with point defects [3].

It turns out that both Amari and Günther fell into this trap. Fortunately, they were more careful and did not jump to conclusions. Günther also endeavoured the painstaking job of separating the relevant equations.

Once the target equations have been established and it becomes necessary to justify and generalize them by referring to intuitive and, as far as possible, realistic physical and geometrical models, the four-dimensional formalism becomes more troublesome than helpful, and, it should be discarded. I believe so, and I did so [4].

However, there is one possibility of genuine application for the four-dimensional formalism. This comes about when one allows for distemperations.

Let us consider the following model which is admittedly highly artificial, but nevertheless quite illuminating. We take a soft ferromagnetic (or ferroelectric, for that matter) crystalline body. At equal intervals of time  $\tau$  we magnetize the body for a very short period  $\tau' \ll \tau$ . Accepting as spacetime events only happenings at lattice points during the magnetized periods  $\tau'$ , we convert the instantaneously body into a genuinely four-dimensional crystal. Now  $c$  will, of course, have to be the propagation velocity of the magnetization, rather than the speed of sound.

In our 4-crystal we can now introduce distemperations. An edge distemperation will be created if the crystal is divided into two parts 1 and 2.

The magnetizing pulses in  $l$  arrive at the basic frequency  $\nu = 1/\tau$ . In part 2 the frequency is shifted to  $\nu_+ = 1/(\tau+1)$  or  $\nu_- = 1/(\tau-1)$  until the pulses again coincide. A screw distemporation can be created making the pulses continuously lag in time around a given axis of propagation in such a way that along any axis of propagation the pulse spacing is  $\tau$  again. It should be pointed out that dislocations (including distemporations) in a four-dimensional medium are two-dimensional entities.

Taking into account the dispersivity of the medium and magneto-elastic interactions we would now have a genuine four-dimensional elastic crystalline medium. In this case the four-dimensional formalism would become really meaningful. The full set of equations would be just the set of independent four-dimensional equations, since none of them would overlap or become trivial.

Günther [18] also generalized his equations to include point defects. However, since his treatment of the subject is somewhat vague and, in the meantime, has been superseded by the introduction of nonmetric connexions by Bilby et al. [19], I prefer to report work done by myself on this subject in early 1966.

## V. Distortion Rates

Our starting point will be the fundamental distortions, as defined in GS. Thus we shall deal with the plastic, qlastic and elastic distortions, respectively denoted by  $P$ ,  $Q$ , and  $E$ . The distortions  $Q$  and  $E$  form together the lattice distortion  $L$ , while the superposition of all three fundamental distortions  $P$ ,  $Q$ , and  $E$  is the total distortion  $T$ .

The present complication is that the distortions are considered to be changing in time. We shall assume the distortions to be continuous and differentiable functions of time  $t$ . Consequently, we must introduce incremental distortions and distortion rates.

First of all, let us fix that any symbol referring to the time instant  $\tilde{t} + dt$  shall be distinguished by a tag to the left of the corresponding symbol that refers to the instant  $t$ . Thus we have for the states

$$[A] \equiv [A]_t, [{}'A] \equiv [A]_{t+dt}, \quad (5.1)$$

and for the line elements

$$dX^\kappa \equiv (dX^\kappa)_t, d'X^\kappa \equiv (dX^\kappa)_{t+dt}. \quad (5.2)$$

For convenience we shall also introduce what will be called *comple-*

mentary distortions by the definition:

$$\bar{D}^{\kappa}_{\lambda} \equiv T^{\kappa}_{\mu} D^{\mu}_{\lambda}, \quad (5.3)$$

wherefrom it follows that

$$\bar{D}^{\kappa}_{\mu} D^{\mu}_{\lambda} = T^{\kappa}_{\lambda}. \quad (5.4)$$

The distortion  $\bar{D}$  will be called the *complement* of  $D$ .

Since

$$T^{\kappa}_{\lambda} = E^{\kappa}_{\mu} Q^{\mu}_{\lambda} P^{\nu}_{\lambda}, \quad (5.5)$$

we have the relations

$$\bar{P}^{\kappa}_{\lambda} = E^{\kappa}_{\mu} Q^{\mu}_{\lambda} = L^{\kappa}_{\lambda},$$

$$\bar{Q}^{\kappa}_{\lambda} = P^{\kappa}_{\mu} E^{\mu}_{\lambda},$$

$$\bar{E}^{\kappa}_{\lambda} = Q^{\kappa}_{\mu} P^{\mu}_{\lambda},$$

$$\bar{T}^{\kappa}_{\lambda} = I^{\kappa}_{\lambda},$$

$$\bar{I}^{\kappa}_{\lambda} = T^{\kappa}_{\lambda} \quad (5.6)$$

The complementary distortions will prove to be useful in later work.

Now we can define the fundamental *distortion increments*  $dD$  by the relations

$$d'X^{\kappa} = (I^{\kappa}_{\lambda} + dI^{\kappa}_{\lambda}) dX^{\lambda},$$

$$d'\mathcal{X}^{\kappa} = (I^{\kappa}_{\lambda} + dP^{\kappa}_{\lambda}) d\mathcal{X}^{\lambda},$$

$$d'x^{\kappa} = (I^{\kappa}_{\lambda} + d\bar{E}^{\kappa}_{\lambda}) dx^{\lambda},$$

$$d'x^{\kappa} = (I^{\kappa}_{\lambda} + dT^{\kappa}_{\lambda}) dx^{\lambda}. \quad (5.7)$$

The ideal state  $[A]$  remains, of course unchanged, i.e.

$$[{}'A] = [A], \quad (5.8)$$

so that

$$d'X^\kappa = dX^\kappa, \quad (5.9)$$

and naturally,

$$dI^\kappa_\lambda = 0. \quad (5.10)$$

From (5.7) we obtain for the fundamental distortions at the time  $t + dt$ :

$$\begin{aligned} d'\mathcal{X}^\kappa &= 'P^\kappa_\lambda dX^\lambda, \\ d'\sigma^\kappa &= 'Q^\kappa_\lambda d\sigma^\lambda, \\ d'x^\kappa &= 'E^\kappa_\lambda dx^\lambda, \\ d'X^\kappa &= 'L^\kappa_\lambda dx^\lambda, \end{aligned} \quad (5.11)$$

where, obviously,

$$'D^\kappa_\lambda = D^\kappa_\lambda + dD^\kappa_\lambda. \quad (5.12)$$

Now we introduce the *distortion rates*, or for short, *distorates*  $\dot{D}$ . We define

$$\begin{aligned} dP^\kappa_\lambda &\equiv \dot{P}^\kappa_\lambda dt, \\ dQ^\kappa_\lambda &\equiv \dot{Q}^\kappa_\lambda dt, \\ dE^\kappa_\lambda &\equiv \dot{E}^\kappa_\lambda dt, \\ dT^\kappa_\lambda &\equiv \dot{T}^\kappa_\lambda dt, \end{aligned} \quad (5.13)$$

etc. The distortates are the basic entities of the kinetic theory, just as the distortions are those of the static one. It must be emphasized that, in general, one *cannot* write a distortion increment in the form

$$dD^\kappa_\lambda = \nabla_\lambda v^\kappa dt \quad (5.14)$$

as was done in [4] and [19] (p. 104). This would mean that the distortates can be derived from a well defined velocity field and therefore would exclude the creation of new defects during the distortion processes. In this sense, the treatment of [1, 2, 3, 4] is valid only for the further elastic distortion process in dislocated solids.

## VI. Stretching Tensors

The change in the state of strain can be characterized by the local time derivatives of the Eulerian metric tensors, or *metric rates*,  $\dot{G}_{\lambda\kappa}$ ,  $\dot{\mathcal{G}}_{\lambda\kappa}$ ,  $\dot{\gamma}_{\lambda\kappa}$  and  $\dot{g}_{\lambda\kappa}$ . These can be obtained by straightforward differentiation of eqs (GS 1.10):

$$\begin{aligned}\dot{G}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} G_{\lambda\kappa} = 2A_{\nu\mu} L_{(\lambda}^{\nu} \dot{L}_{\mu)\kappa}, \\ \dot{\mathcal{G}}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} \mathcal{G}_{\lambda\kappa} = 2\mathcal{A}_{\nu\mu} I_{(\lambda}^{\nu} \dot{I}_{\mu)\kappa}, \\ \dot{\gamma}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} \gamma_{\lambda\kappa} = 2\alpha_{\nu\mu} E_{(\lambda}^{\nu} \dot{E}_{\mu)\kappa}, \\ \dot{g}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} g_{\lambda\kappa} = 2a_{\nu\mu} I_{(\lambda}^{\nu} \dot{I}_{\mu)\kappa},\end{aligned}\tag{6.1}$$

Differentiating the identity

$$D_{\cdot\mu}^{\kappa} D^{\mu}_{\cdot\lambda} = I_{\cdot\lambda}^{\kappa}\tag{6.2}$$

we obtain

$$\dot{D}_{\cdot\mu}^{\kappa} D^{\mu}_{\cdot\lambda} + D_{\cdot\mu}^{\kappa} \dot{D}^{\mu}_{\cdot\lambda} = 0,\tag{6.3}$$

and hence

$$\dot{D}_{\cdot\lambda}^{\kappa} = -D_{\cdot\rho}^{\kappa} \dot{D}_{\cdot\sigma}^{\rho} D_{\lambda}^{\sigma}.\tag{6.4}$$

If (6.4) is substituted into (2.1), this becomes

$$\begin{aligned}\dot{G}_{\lambda\kappa} &= -2L_{(\lambda}^{\mu} \dot{T}_{\kappa)\mu}, \\ \dot{\mathcal{G}}_{\lambda\kappa} &= -2I_{(\lambda}^{\mu} \dot{L}_{\kappa)\mu}, \\ \dot{\gamma}_{\lambda\kappa} &= -2E_{(\lambda}^{\mu} \dot{E}_{\kappa)\mu}, \\ \dot{g}_{\lambda\kappa} &= -2I_{(\lambda}^{\mu} \dot{I}_{\kappa)\mu} = 0,\end{aligned}\tag{6.5}$$

where

$$\begin{aligned}\dot{T}_{\kappa\mu} &\equiv G_{\kappa\nu} \dot{T}_{\cdot\mu}^{\nu}, \\ \dot{L}_{\kappa\mu} &\equiv \mathcal{G}_{\kappa\nu} \dot{L}_{\cdot\mu}^{\nu}, \\ \dot{E}_{\kappa\mu} &\equiv \gamma_{\kappa\nu} \dot{E}_{\cdot\mu}^{\nu}, \\ \dot{I}_{\kappa\mu} &\equiv g_{\kappa\nu} \dot{I}_{\cdot\mu}^{\nu}.\end{aligned}\tag{6.6}$$

It is more convenient to replace the metric rates by the rates of strain, called *stretching tensors* [23]. These are defined by the equations

$$\begin{aligned}\dot{\pi}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} \pi_{\lambda\kappa} = \frac{1}{2}(\dot{\mathcal{G}}_{\lambda\kappa} - \dot{G}_{\lambda\kappa}), \\ \dot{q}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} q_{\lambda\kappa} = \frac{1}{2}(\dot{\mathcal{J}}_{\lambda\kappa} - \dot{\mathcal{G}}_{\lambda\kappa}), \\ \dot{\epsilon}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} \epsilon_{\lambda\kappa} = \frac{1}{2}(\dot{g}_{\lambda\kappa} - \dot{\mathcal{G}}_{\lambda\kappa}), \\ \dot{\tau}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} \tau_{\lambda\kappa} = \frac{1}{2}(\dot{g}_{\lambda\kappa} - \dot{G}_{\lambda\kappa}), \\ \dot{\lambda}_{\lambda\kappa} &\equiv \frac{\partial}{\partial t} \lambda_{\lambda\kappa} = \frac{1}{2}(\dot{g}_{\lambda\kappa} - \dot{\mathcal{G}}_{\lambda\kappa}),\end{aligned}\tag{6.7}$$

The stretching tensors can be expressed in terms of their respective distortions and distorates, as follows:

$$\begin{aligned}\dot{\pi}_{\lambda\kappa} &= D^\mu_{(\lambda} \dot{P}_{\kappa)\mu}, \\ \dot{q}_{\lambda\kappa} &= D^\mu_{(\lambda} \dot{Q}_{\kappa)\mu}, \\ \dot{\epsilon}_{\lambda\kappa} &= D^\mu_{(\lambda} \dot{E}_{\kappa)\mu}, \\ \dot{\tau}_{\lambda\kappa} &= D^\mu_{(\lambda} \dot{T}_{\kappa)\mu}, \\ \dot{\lambda}_{\lambda\kappa} &= D^\mu_{(\lambda} \dot{L}_{\kappa)\mu}.\end{aligned}\tag{6.8}$$

For  $\dot{\epsilon}_{\lambda\kappa}$ ,  $\dot{\tau}_{\lambda\kappa}$  and  $\dot{\lambda}_{\lambda\kappa}$  this result trivially follows from (6.5), (6.6), and (6.7), while for  $\dot{\pi}_{\lambda\kappa}$  and  $\dot{q}_{\lambda\kappa}$  it can be easily proved, using (5.5), (5.6), and taking into account that distortion and distorates of different kinds always commute.

## VII. Connexion Rates and Fluxions

The connexions involved in the geometry of CDD were defined by eqs (GS 1.14). The rate of change of a connexion, the *connexion rate*, is defined as the local time derivative of the connexion. The connexion rates, expressed in terms of distortions and distorates, become:

$$\dot{B}_{\mu\lambda}^{\kappa} \equiv \frac{\partial}{\partial t} B_{\mu\lambda}^{\kappa} = \dot{I}_{\sigma}^{\kappa} \partial_{\mu} I_{\sigma\lambda}^{\kappa} + I_{\sigma}^{\kappa} \partial_{\mu} \dot{I}_{\sigma\lambda}^{\kappa},$$

$$\dot{\mathcal{B}}_{\mu\lambda}^{\kappa} \equiv \frac{\partial}{\partial t} \mathcal{B}_{\mu\lambda}^{\kappa} = \dot{d}_{\sigma}^{\kappa} \partial_{\mu} P_{\sigma\lambda}^{\kappa} + d_{\sigma}^{\kappa} \partial_{\mu} \dot{P}_{\sigma\lambda}^{\kappa},$$

$$\dot{\mathcal{L}}_{\mu\lambda}^{\kappa} \equiv \frac{\partial}{\partial t} \mathcal{L}_{\mu\lambda}^{\kappa} = \dot{\underline{E}}_{\sigma}^{\kappa} \partial_{\mu} \bar{E}_{\sigma\lambda}^{\kappa} + \underline{E}_{\sigma}^{\kappa} \partial_{\mu} \dot{\bar{E}}_{\sigma\lambda}^{\kappa}, \quad (7.1)$$

$$\dot{b}_{\mu\lambda}^{\kappa} \equiv \frac{\partial}{\partial t} b_{\mu\lambda}^{\kappa} = \dot{L}_{\sigma}^{\kappa} \partial_{\mu} T_{\sigma\lambda}^{\kappa} + \bar{L}_{\sigma}^{\kappa} \partial_{\mu} \dot{T}_{\sigma\lambda}^{\kappa}.$$

In view of (2.4) this becomes

$$\dot{B}_{\mu\lambda}^{\kappa} = I_{\sigma}^{\kappa} (\partial_{\mu} \dot{I}_{\sigma\lambda}^{\kappa} - B_{\mu\lambda}^{\kappa} \dot{I}_{\sigma\rho}^{\kappa}) = 0.$$

$$\begin{aligned} \dot{\mathcal{B}}_{\mu\lambda}^{\kappa} &= d_{\sigma}^{\kappa} (\partial_{\mu} \dot{P}_{\sigma\lambda}^{\kappa} - \mathcal{B}_{\mu\lambda}^{\kappa} \dot{P}_{\sigma\rho}^{\kappa}), \\ \dot{\mathcal{L}}_{\mu\lambda}^{\kappa} &= \underline{E}_{\sigma}^{\kappa} (\partial_{\mu} \dot{\bar{E}}_{\sigma\lambda}^{\kappa} - \mathcal{L}_{\mu\lambda}^{\kappa} \dot{\bar{E}}_{\sigma\rho}^{\kappa}), \\ \dot{b}_{\mu\lambda}^{\kappa} &= L_{\sigma}^{\kappa} (\partial_{\mu} \dot{T}_{\sigma\lambda}^{\kappa} - b_{\mu\lambda}^{\kappa} \dot{\bar{T}}_{\sigma\rho}^{\kappa}). \end{aligned} \quad (7.2)$$

These equations have a clear physical interpretation. The first term represents the rate of creation of new defects due to the involved distorates, whereas the second term describes the rate of change in the distribution of old defects by the convection connected with the distorates.

In analogy with the connexions (GS 1.14), we shall define the following tensors:

$$\begin{aligned} \dot{B}_{\lambda}^{\kappa} &\equiv I_{\sigma}^{\kappa} \frac{\partial}{\partial t} I_{\sigma\lambda}^{\kappa} = I_{\sigma}^{\kappa} \dot{I}_{\sigma\lambda}^{\kappa} = 0, \\ \dot{\mathcal{B}}_{\lambda}^{\kappa} &\equiv d_{\sigma}^{\kappa} \frac{\partial}{\partial t} P_{\sigma\lambda}^{\kappa} = d_{\sigma}^{\kappa} \dot{P}_{\sigma\lambda}^{\kappa}, \\ \dot{\mathcal{L}}_{\lambda}^{\kappa} &\equiv \underline{E}_{\sigma}^{\kappa} \frac{\partial}{\partial t} \bar{E}_{\sigma\lambda}^{\kappa} = \underline{E}_{\sigma}^{\kappa} \dot{\bar{E}}_{\sigma\lambda}^{\kappa}, \\ \dot{b}_{\lambda}^{\kappa} &\equiv L_{\sigma}^{\kappa} \frac{\partial}{\partial t} L_{\sigma\lambda}^{\kappa} = L_{\sigma}^{\kappa} \dot{L}_{\sigma\lambda}^{\kappa}. \end{aligned} \quad (7.3)$$

The tensors will be called *fluxion* tensors, the name reminding us of “flow” and “connexion.” The fluxions describe essentially the same physical entities as the distorates. However, the fluxions have the ad-

vantage that they express the time changes of the distortions in terms of quantities referring to the solid in the ideal state [A].

### VIII. Kinematic Law

The equation

$$\dot{b}^\kappa_\lambda = \mathbf{L}^\kappa_\sigma \dot{T}^\sigma_\lambda \quad (8.1)$$

is, in fact, already a possible formulation of the *fundamental kinematic law*.

Since at any time  $t$  the solid in the final state [a] fits into the euclidian space, the fluxion  $\dot{b}^\kappa_\lambda$  must be a gradient tensor

$$\dot{b}^\kappa_\lambda = \nabla_\lambda v^\kappa, \quad (8.2)$$

where

$$v^\kappa \equiv \dot{x}^\kappa \quad (8.3)$$

is the velocity field in the solid.

According to (5.5), (5.6) the total distortate  $\dot{T}^\kappa_\lambda$  can be expressed in terms of the plastic, plastic and elastic distortates  $\dot{P}^\kappa_\lambda$ ,  $\dot{Q}^\kappa_\lambda$ ,  $\dot{E}^\kappa_\lambda$ :

$$\dot{T}^\kappa_\lambda = \dot{E}^\kappa_\sigma \bar{E}^\sigma_\lambda + \dot{Q}^\kappa_\sigma \bar{Q}^\sigma_\lambda + \dot{P}^\kappa_\sigma \bar{P}^\sigma_\lambda. \quad (8.4)$$

After transvection of (8.1) with  $T^\nu_\kappa$  and substitution of (8.2) and (8.4) we obtain the fundamental kinematic law in the form

$$\dot{T}^\kappa_\sigma \nabla_\lambda v^\sigma = \dot{E}^\kappa_\sigma \bar{E}^\sigma_\lambda + \dot{Q}^\kappa_\sigma \bar{Q}^\sigma_\lambda + \dot{P}^\kappa_\sigma \bar{P}^\sigma_\lambda. \quad (8.5)$$

In the linearized version this becomes

$$\nabla_\lambda v^\kappa - \dot{E}^\kappa_\lambda = \dot{\bar{E}}^\kappa_\lambda \quad (8.6)$$

If the plastic distortion is neglected, (8.6) simplifies to

$$\nabla_\lambda v^\kappa - \dot{E}^\kappa_\lambda = \dot{P}^\kappa_\lambda \quad (8.7)$$

which is identical with equation (III.18) of [3] as corrected in [4].

At this point we can give a physical interpretation of the fluxions. The meaning of the total fluxion  $\dot{b}^\kappa_\lambda$  is made clear by eq (8.2) and does not need additional comment. The plastic fluxion  $\dot{B}^\kappa_\lambda$  must be identified with the dislocation current, as defined in [2] and [4] (there denoted by  $J_{\lambda}^\kappa$ ). In [4] it was wrongly claimed that the dislocation current is

$$J_{\lambda}^\kappa = 2s_{\lambda\sigma}^\kappa v^\sigma. \quad (8.8)$$

This expression, however, represents only the convective part of the dislocation current due to the local velocity field  $v^\kappa$ . A correct physical definition of the dislocation current  $\dot{\mathcal{B}}_{\lambda}{}^\kappa$  is as follows: Consider a given volume element. Measure the tensors  $\overset{i}{\mathcal{S}}_{\mu\lambda}{}^\kappa$  corresponding to dislocations of all kinds (labeled by  $i$ ) that are possible in the given solid and their velocities  $\overset{i}{v}{}^\kappa$ . Then the dislocation current tensor  $\dot{\mathcal{B}}_{\lambda}{}^\kappa$  is given by

$$\dot{\mathcal{B}}_{\lambda}{}^\kappa \equiv 2 \sum_i \overset{i}{\mathcal{S}}_{\lambda\sigma} \overset{i}{v}{}^\sigma \quad (8.9)$$

The fluxion  $\dot{\lambda}{}^\kappa$  represents the total defect current, including the motion of both dislocations and point defects. We introduce the *vacancy current*

$$\dot{\mathcal{E}}_{\lambda}{}^\kappa \equiv \dot{\lambda}{}^\kappa - \dot{\mathcal{B}}_{\lambda}{}^\kappa, \quad (8.10)$$

which, of course, describes the motion of point defects of all kinds. In analogy to eq (8.9) we have the working definition

$$\dot{\mathcal{E}}_{\lambda}{}^\kappa \equiv -2 \sum_k \overset{k}{\mathcal{S}}_{\lambda\sigma} \overset{k}{v}{}^\sigma, \quad (8.11)$$

indicating that in a given volume element one has to measure the velocities  $\overset{k}{v}{}^\kappa$  with which the gradients of the point defect densities of various kinds (labeled by  $k$ ) are transported. The total *defect current* becomes

$$\dot{\lambda}{}^\kappa = \dot{\mathcal{B}}_{\lambda}{}^\kappa + \dot{\mathcal{E}}_{\lambda}{}^\kappa = 2 \sum_i \overset{i}{\mathcal{S}}_{\lambda\sigma} \overset{i}{v}{}^\sigma - 2 \sum_k \overset{k}{\mathcal{S}}_{\lambda\sigma} \overset{k}{v}{}^\sigma. \quad (8.12)$$

## IX. Continuity Equations

One can also formulate the fundamental kinematic law in a form analogous to what was called in [1, 2, 3, 4] the equation of continuity.

One way to do this is the following: Starting from the definition (GS 1.21) of the curvature tensor and differentiating it with respect to time, one obtains

$$\frac{1}{2} \dot{c}_{\nu\mu\lambda}{}^\kappa = \partial_{[\nu} \dot{b}_{\mu]\lambda}{}^\kappa + b_{[\nu}{}^\kappa \dot{b}_{\mu]\lambda}{}^\rho + \dot{b}_{[\nu}{}^\kappa b_{\mu]\lambda}{}^\rho. \quad (9.1)$$

We now take the alternated covariant derivative of  $\dot{b}_{\mu\lambda}{}^\kappa$ , which obviously is a tensor

$$\begin{aligned}\nabla_{[\nu} \dot{b}_{\mu]}^{\lambda} &\equiv \partial_{[\nu} \dot{b}_{\mu]}^{\lambda} + b_{[\nu|}{}^{\kappa} \dot{b}_{\mu]}^{\rho} - b_{[\nu|}{}^{\rho} \dot{b}_{\mu]}^{\kappa} - b_{[\nu|}{}^{\rho} b_{\mu]}{}^{\kappa} \\ &= \partial_{[\nu} \dot{b}_{\mu]}^{\lambda} + b_{[\nu|}{}^{\kappa} \dot{b}_{\mu]}^{\rho} + \dot{b}_{[\nu|}{}^{\kappa} b_{\mu]}{}^{\rho} - s_{\nu\mu}{}^{\rho} \dot{b}_{\rho\lambda}^{\kappa}.\end{aligned}\quad (9.2)$$

Hence

$$\nabla_{[\nu} \dot{b}_{\mu]}^{\lambda} = \frac{1}{2} \dot{c}_{\nu\mu\lambda}{}^{\kappa} = s_{\nu\mu}{}^{\rho} \dot{b}_{\rho\lambda}^{\kappa}. \quad (9.3)$$

The fundamental geometric equation (GS 1.22) must hold for any time, and hence follows the *kinematic compatibility condition*

$$\dot{c}_{\mu\nu\lambda}{}^{\kappa} = 0. \quad (9.4)$$

From (9.3) and (9.4) we obtain the fundamental kinematic equation in the form

$$\nabla_{[\nu} \dot{b}_{\mu]}^{\lambda} + s_{\nu\mu}{}^{\rho} \dot{b}_{\rho\lambda}^{\kappa} = 0. \quad (9.5)$$

An alternative derivation of (9.5) is as follows: Let us extend the definition (GS 1.21) of the curvature tensor and the geometric law (GS 1.22) to include time derivatives. We have for the "time curvature"

$$\partial_{\mu} \dot{b}_{\lambda}{}^{\kappa} - \dot{b}_{\lambda\mu}{}^{\kappa} - \dot{b}_{\rho}{}^{\kappa} b_{\mu\lambda}^{\rho} + b_{\nu\rho}^{\kappa} \dot{b}_{\lambda}{}^{\rho} = 0. \quad (9.6)$$

The covariant derivative of  $\dot{b}_{\lambda}{}^{\kappa}$  is

$$\nabla_{\mu} \dot{b}_{\lambda}{}^{\kappa} = \partial_{\mu} \dot{b}_{\lambda}{}^{\kappa} + b_{\mu\rho}^{\kappa} \dot{b}_{\lambda}{}^{\rho} - b_{\mu\lambda}{}^{\rho} \dot{b}_{\rho}{}^{\kappa}. \quad (9.7)$$

From (9.6) and (9.7) we obtain immediately

$$\dot{b}_{\mu\lambda}{}^{\kappa} = \nabla_{\mu} \dot{b}_{\lambda}{}^{\kappa}, \quad (9.8)$$

which is again a possible formulation of the kinematic law. Taking the alternated covariant derivative of (9.8) we have, in view of (GS 1.22):

$$\nabla_{[\nu} \nabla_{\mu]} \dot{b}_{\lambda}{}^{\kappa} + s_{\nu\mu}{}^{\rho} \nabla_{\rho} \dot{b}_{\lambda}{}^{\kappa} = 0. \quad (9.9)$$

Substituting again (9.8) we finally arrive at (9.5).

To derive a continuity equation for the dislocation current one has to start from the last one of eqs (GS 1.15). Differentiating with respect to time and using the last one of eqs (6.5) one obtains

$$\dot{b}_{\mu\lambda}{}^{\kappa} = \mathcal{S}^{\kappa\sigma} (-\dot{s}_{\{\mu\sigma\lambda\}} + \dot{q}_{\{\mu\sigma\lambda\}}). \quad (9.10)$$

Upon substitution of (9.10), eq (9.8) becomes

$$g_{\nu\sigma} \nabla_\mu \dot{b}^{\lambda\sigma} + \dot{s}_{\{\mu\nu\lambda\}} - \dot{q}_{\{\mu\nu\lambda\}} = 0. \quad (9.11)$$

## X. Conclusion

We have outlined the present state of the kinematics of continuously distributed dislocations in crystals or rather lattice defects in general. The theory appears now to be well established. Future work should advisably concentrate on dislocations in noncrystalline bodies. This might be achieved by some relaxation of the fundamental geometric conditions.

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## **Discussion on Paper by S. I. Ben-Abraham.**

SIMMONS: I see in this formulation there were a number of, as you say, useless terms. In a paper I did in 1961 — which I never published except as a report — on a dynamic theory for imperfect continua, the formulation I gave required no metric at all and had no extraneous quantities whatsoever. This formulation was completely general and included curvature also, which I interpret to mean that grain boundaries — or rather sub-grain boundaries — are free to move through the body. There was also no attempt to make the theory look like relativity theory, which I think is a spurious analogy in this context.

BEN-ABRAHAM: I could not agree more with the chairman. Relativity was good once, as a heuristic method, and it was based on physical analogies such as the so-called relativistic behavior of fast dislocations. But it only yields valid physical results when both the strains and the velocities are kept small. Then it does not matter at all what the limiting velocity is. Otherwise I believe the problem is so different that one should not involve relativity at all. I presented this review as I did because I felt this presentation was the fullest, but I prefer the three dimensional representation where all the terms are meaningful.



# **A MICROMORPHIC APPROACH TO DISLOCATION THEORY AND ITS RELATION TO SEVERAL EXISTING THEORIES**

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Two separate continuum dislocation theories are presented; one dealing with static, incompatible, micropolar dislocations and disclinations, as encountered in initial stress problems, and the other with a dynamical theory of micromorphic solids containing continuous distributions of dislocations.

Relationships between several continuum dislocation theories and micromorphic mechanics are established by providing extensions and new interpretations of the micromorphic theory. First both micromorphic and micropolar theories of elastic solids are summarized, and then the theories of Kröner, Fox, and Berdichevskii and Sedov are discussed in some detail within this framework. In the last section, by use of micromorphic kinematics, dislocation density, strain, and microstrain tensors are introduced and constitutive equations are constructed. Together with the balance laws this constitutes a complete dynamical theory. The theory is intended for predictions of motions and micromotions of a solid containing dislocations undergoing elastic deformations. From the micromotion, the dislocation density and first stress moments can be calculated.

**Key words:** Continuum mechanics; dislocation distributions; micromorphic dislocations; micropolar dislocations.

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## **I. Summary of Micromorphic Mechanics**

In this paper we present two distinct theories of dislocations. The first one (section II) constitutes an extension of the initial stress problem, as

Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough, Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

treated by Kröner, Bilby, and others, to the micropolar couple stress theory, and the second (section III) introduces a dynamical theory for microelastic solids containing continuous distributions of dislocations. The initial stress-couple stress problem treated here may be called an incompatible micropolar theory. In this theory the determination of stress and couple stress requires the solution of a set of field equations in which the dislocation and disclination densities are the prescribed source terms. This is in accord with current practice in solid-state physics. It seems to us that the specification of two second order tensors (dislocation density and disclination density) throughout a body at each state of the body is unreasonable and perhaps impractical for the determination of two other second order tensors (stress and couple stress). Our hope is that ultimately these requirements can be relaxed and replaced by simpler initial and boundary conditions. Motivated by this, in section III we present a dynamical theory of microelastic solids containing continuous distributions of dislocations. Upon the determination of the motion and micromotion by solving a boundary value problem, the dislocation density, stress, and stress moments can be calculated. Clearly for the treatment of yielding and plastic deformation further work is necessary.

As Professor Nabarro [1] has pointed out, not the least of our problems as mechanicians and solid-state physicists is terminology. In this paper, the phrase "continuum dislocation theory" is used to mean the theory of a continuous distribution of infinitesimal dislocations in the spirit of modern continuum mechanics, which includes balance laws, properly invariant constitutive equations, and associated boundary and initial conditions. We begin with a summary of the basic equations of micromorphic mechanics, and then examine aspects of various theories within that framework.

### A. MICROMORPHIC EQUATIONS

The basic equations of micromorphic mechanics were given originally by Eringen and Suhubi [2] and by Eringen [3, 4], and contacts with various other microstructure theories were provided in [5]. The balance laws are:

$$\frac{\partial \rho}{\partial t} + (\rho v_k)_{,k} = 0 \quad (\text{mass}) \quad (1.1)$$

$$\frac{\partial i_{kl}}{\partial t} + i_{kl,m} v_m - i_{lm} v_{km} - i_{km} v_{lm} = 0 \quad (\text{microinertia}) \quad (1.2)$$

$$t_{kl,k} + \rho f_l = \rho \dot{v}_l \quad (\text{momentum}) \quad (1.3)$$

$$\lambda_{klm,k} + t_{ml} - s_{ml} + \rho l_{lm} = \rho \dot{\sigma}_{lm} \quad (\text{moment of momentum}) \quad (1.4)$$

$$\rho \dot{\epsilon} = t_{kl} v_{l,k} + (s_{kl} - t_{kl}) v_{lk} + \lambda_{klm} v_{lm,k} + q_{k,k} + \rho h \quad (\text{energy}) \quad (1.5)$$

where

- $\rho$  = mass density
- $f_l$  = body force/mass
- $i_{km}$  = microinertia tensor
- $s_{lm}$  = microstress average tensor
- $l_{lm}$  = first body moment tensor/mass
- $\dot{\sigma}_{lm}$  = inertial spin tensor
- $\epsilon$  = internal energy/mass
- $q_k$  = heat flux vector
- $h$  = heat source/mass
- $t_{kl}$  = stress tensor
- $v_k$  = velocity vector
- $\nu_{kl}$  = gyration tensor
- $\lambda_{klm}$  = first stress moment tensor.

Throughout the paper all vectors and tensors are referred to rectangular coordinates  $x_k$ . We employ the usual summation convention on repeated indices, indicate material differentiation by a superposed dot, and denote partial differentiation by an index following a comma, e.g.,

$$\dot{v}_k = \frac{\partial v_k}{\partial t} + v_{k,l} v_l, \quad v_{k,l} = \frac{\partial v_k}{\partial x_l}.$$

The inertial spin tensor  $\dot{\sigma}$  is related to the gyration tensor  $\nu$  by

$$\dot{\sigma}_{lk} = i_{mk} (\dot{\nu}_{lm} + \nu_{ln} \nu_{nm}). \quad (1.6)$$

In addition to the above balance laws, constitutive relations are needed to describe the particular material under consideration. Anisotropic fluids

and microviscoelastic solids were treated in [4] and simple microfluids in [3]. For the present purpose, we employ the linear theory of *microelastic* solids.<sup>1</sup> In this case the strain measures are:

$$\begin{aligned} e_{kl} &= u_{(k, l)} = \frac{1}{2} (u_{k, l} + u_{l, k}) \\ \epsilon_{kl} &= u_{l, k} + \phi_{kl}, \quad \gamma_{klm} = -\phi_{kl, m} \end{aligned} \quad (1.7)$$

where  $e_{kl}$  is the classical strain tensor,  $\epsilon_{kl}$  and  $\gamma_{klm}$  are microstrain tensors,  $u_k$  is the displacement vector, and  $\phi_{kl}$  is the microdisplacement tensor. Constitutive equations are of the form

$$\begin{aligned} t_{kl} &= t_{kl}(e_{ij}, \epsilon_{ij}, \gamma_{ijk}) \\ s_{kl} &= s_{kl}(e_{ij}, \epsilon_{ij}, \gamma_{ijk}) \\ \lambda_{klm} &= \lambda_{klm}(e_{ij}, \epsilon_{ij}, \gamma_{ijk}). \end{aligned} \quad (1.8)$$

For explicit representations see [2]. The strain measures satisfy the following forty-two compatibility conditions [6]:

$$\begin{aligned} e_{kmp}e_{lnq}e_{mn, pq} &= 0 \\ e_{kmn}(\epsilon_{ml, n} + \gamma_{mln}) &= 0 \\ e_{kpq}\gamma_{lmp, q} &= 0. \end{aligned} \quad (1.9)$$

Appropriate boundary and initial conditions are given in [2].

The theories of Berdichevskii and Sedov and Fox are related to this microelastic theory with twelve generalized displacement degrees of freedom (three for  $u_k$  and nine for  $\phi_{kl}$ ). However, for clarity we proceed from a simpler point to this complicated situation. For this we need the the basic equations of the theory of a *micropolar solid*, as given in [2] and [7]. This will be shown to be related to Kröner's dislocation theory.

## B. MICROPOLAR EQUATIONS

The micropolar solid is obtained as a special case of the microelastic solid by setting  $\phi_{kl} = -\phi_{lk}$ , which means that the nine independent quantities  $\phi_{kl}$  are reduced to three quantities  $\phi_k$  by  $\phi_k = \frac{1}{2}e_{klm}\phi_{ml}$ .

<sup>1</sup> For the finite deformation theory see [2].

$\phi_{kl} = -e_{klm}\phi_m$ , where  $\phi_k$  is called the microrotation vector. In this case, the balance laws take the forms

$$t_{kl,k} + \rho f_l = \rho \ddot{u}_l \quad (1.10)$$

$$m_{kl,k} + e_{lmn}t_{mn} + \rho l_l = \rho j \ddot{\phi}_l \quad (1.11)$$

$$\rho \dot{\epsilon} = t_{kl}\dot{\epsilon}_{kl} + m_{kl}\dot{\kappa}_{kl} + q_{k,k} + \rho h \quad (1.12)$$

and the linear constitutive equations are, explicitly,

$$\begin{aligned} t_{kl} &= \lambda \epsilon_{mm} \delta_{kl} + (\mu + \kappa) \epsilon_{kl} + \mu \epsilon_{lk} \\ m_{kl} &= \alpha \kappa_{mm} \delta_{kl} + \beta \kappa_{lk} + \gamma \kappa_{kl} \end{aligned} \quad (1.13)$$

where

$$\epsilon_{kl} = u_{l,k} - e_{klm}\phi_m, \quad \kappa_{kl} = \phi_{l,k} \quad (1.14)$$

are the micropolar strain tensors, and  $m_{kl}$  is the couple stress tensor. From (1.13)<sub>2</sub> it is evident that the couple stresses are caused by the independent microrotation gradients in the elastic, micropolar theory. The micropolar compatibility conditions are [6]

$$\begin{aligned} e_{kmn}\epsilon_{nl,m} - \kappa_{lk} + \kappa_{mm}\delta_{kl} &= 0 \\ e_{kmn}\kappa_{nl,m} &= 0. \end{aligned} \quad (1.15)$$

Appropriate boundary and initial conditions are given in [2] and [7].

## II. Comparisons With Continuum Dislocation Theories

The dislocation theories discussed in this section range from the initial stress problem in which the dislocation density is specified to the elastic-plastic deformation problem in which the dislocation density results as part of the boundary value problem. The distinction between these different problems is relevant and important since frequently in the literature the work "plastic" is ambiguous. We begin with the theory of Kröner [8, 9] and then discuss the work of Fox [10, 11] and Berdichevskii and Sedov [12]. A continuum theory includes kinematics, balance laws, constructive relations, and boundary and initial conditions. It is these points on which the following discussion is based.

### A. GERMAN SCHOOL

Kröner's theory is divided into two parts, one with couple stress [9] and one without [8]. The fundamental equation of the theory without couple stresses is an incompatibility relation between a strain tensor and a dislocation density tensor. The balance laws and stress-strain rela-

tions are the classical elastic ones. Günther [13] pointed out that this model could be referred to as an incompatible Cosserat medium. Günther's results pertain to only the static, geometric aspects of the Cosserat medium. Examination of the micropolar solid equations (1.10)–(1.15) leads to the conclusion that the kinematics of micropolar elasticity is identical with the Cosserat model used by Günther. However, micropolar elasticity supplies the dynamical terms and thermodynamics missing in [13]. Based on these observations, one can use Günther's arguments and show that Kröner's model [8] could also be called an incompatible micropolar medium.

It should be pointed out that Günther's term *incompatibility* means the following: any second-order tensor  $A_{kl}$  is called *incompatible* if

$$e_{ikm}e_{jln}A_{kl, mn} \neq 0. \quad (2.1)$$

This is a natural definition in the context of Kröner's theory without couple stresses [8], since in the compatible case the strains satisfy *second-order* equations. However in polar mechanics, the strains satisfy *first-order* partial differential equations. This leads us to propose first-order incompatibility relations for the polar strains as follows. The total linear micropolar strains in (1.14), now denoted by  $\epsilon_{kl}^T$  and  $\kappa_{kl}^T$ , may be considered to be the sum of elastic and plastic parts,  $\epsilon_{kl}$  and  $\epsilon_{kl}^P$ , i.e.,

$$\epsilon_{kl}^T = u_{l, k} - e_{klm}\phi_m = \epsilon_{kl} + \epsilon_{kl}^P \quad (2.2)$$

$$\kappa_{kl}^T = \phi_{l, k} = \kappa_{kl} + \kappa_{kl}^P. \quad (2.3)$$

Compatibility conditions on the strains are obtained by differentiating (2.2) and (2.3) and eliminating  $u_k$  and  $\phi_k$ . Thus

$$e_{kmn}\epsilon_{nl, m} - \kappa_{lk} + \kappa_{mm}\delta_{kl} = \pi_{kl} \quad (2.4)$$

$$e_{kmn}\kappa_{nl, m} = \theta_{kl} \quad (2.5)$$

where

$$\pi_{kl} \equiv -e_{kmn}\epsilon_{nl, m}^P + \kappa_{lk}^P - \kappa_{mm}^P\delta_{kl} \quad (2.6)$$

$$\theta_{kl} \equiv -e_{kmn}\kappa_{nl, m}^P. \quad (2.7)$$

We refer to  $\pi_{kl}$  as the *micropolar dislocation density* and  $\theta_{kl}$  as the *disclination<sup>2</sup> density* [14].

<sup>2</sup> See also Anthony, deWit, Mura, and Nabarro in these Proceedings.

By differentiating (2.4) and (2.5) we obtain

$$\pi_{kl, k} + e_{lmn} \theta_{mn} = 0 \quad (2.8)$$

$$\theta_{kl, k} = 0 \quad (2.9)$$

which are identities that must be satisfied by  $\boldsymbol{\pi}$  and  $\boldsymbol{\theta}$ . Equations (2.6) may be stated as:  $\boldsymbol{\epsilon}^P$  and  $\boldsymbol{\kappa}^P$  are the sources of the micropolar dislocations. Equations (2.7) state that the disclinations arise from  $\boldsymbol{\kappa}^P$ . By differentiating (2.4) with respect to a free index yields

$$e_{kmp} e_{lnq} \epsilon_{mn, pq} + e_{klm} \kappa_{rr, m} = e_{lmn} \pi_{kn, m} + \theta_{lk} \quad (2.10)$$

The symmetric part of this equation is

$$e_{kmp} e_{lnq} \epsilon_{(mn), pq} = -e_{(k|m n|} \pi_{l)m, n} + \theta_{(kl)}. \quad (2.11)$$

When  $\theta_{(kl)}$  vanishes, (2.11) is formally the same (with a minus sign) as Kröner's incompatibility equations in [9].

The skew-symmetric part of (2.10) gives the incompatibility equations for the skew part of the micropolar strain tensor

$$e_{mnp} \epsilon_{[np], km} + 2\kappa_{mm, k} = \pi_{mm, k}. \quad (2.12)$$

Equations (2.12) appear to be new; they reflect the fact that the micropolar theory is based on non-symmetric strain and stress tensors.

With the incompatible micropolar theory presented above, the static initial stress-couple stress problem can be formulated. That is, one considers the sources of internal stress to be given (the dislocation density  $\boldsymbol{\pi}$  and disclination density  $\boldsymbol{\theta}$ ), and the problem is to determine the initial stresses and couple stresses in the body. The basic system of equation to be solved is then

$$t_{kl, k} = 0 \quad (2.13)$$

$$m_{kl, k} + e_{lmn} t_{mn} = 0 \quad (2.14)$$

$$t_{kl} n_k = 0, \quad m_{kl} n_k = 0 \quad \text{on } S \quad (2.15)$$

with the incompatibility equations

$$e_{kmn} \epsilon_{nl, m} - \kappa_{lk} + \kappa_{mm} \delta_{kl} = \pi_{kl} \quad (2.16)$$

$$e_{kmn} \kappa_{nl, m} = \theta_{kl}. \quad (2.17)$$

Here  $\pi$  and  $\theta$  cannot be specified arbitrarily but must satisfy

$$\pi_{kl, k} + e_{lmn}\theta_{mn} = 0, \quad \theta_{kl, k} = 0. \quad (2.18)$$

The constitutive equations to be used in the isotropic case are

$$t_{kl} = \lambda \epsilon_{mm} \delta_{kl} + (\mu + \kappa) \epsilon_{kl} + \mu \epsilon_{lk} \quad (2.19)$$

$$m_{kl} = \alpha \kappa_{mm} \delta_{kl} + \beta \kappa_{lk} + \gamma \kappa_{kl}. \quad (2.20)$$

The couple stress model in [9] uses the kinematics described above and combines it with the static balance laws of a Cosserat medium [18]. Kröner then proposes a constitutive relation between the couple stress and lattice curvature (or the dislocation density via the Nye relation) and retains Hook's law for the symmetric part of the stress. In this theory, once the dislocation density is given, the couple stress is known through its constitutive equation, and the skew part of the stress is known through the moment balance law. It seems to us that this theory is incomplete. There should be a constitutive relation for the entire stress tensor independent of the balance laws. Eringen [7] has demonstrated the unsoundness of using the moment balance law as a constitutive relation in the case of the "indeterminate couple stress theory."

Kröner's theory with couple stresses [9] is more explicitly compared with the incompatible micropolar theory in the following table.

TABLE 1

Kröner (with couple stresses)	Micropolar
$\sigma_{kl}, t_{kl}$ $F_k, D_k$ $e_{kmp}e_{lnq}\epsilon_{(mn)}, p, q = e_{(k mn \alpha_l)m, n}$ <hr/> $\alpha_{kl} = \kappa_{lk} - \kappa_{mm} \delta_{kl}$	$t_{kl}, m_{kl}$ $\rho f_k, \rho l_k$ $e_{kmp}e_{lnq}\epsilon_{(mn)}, p, q = -e_{(k mn \pi_l)m, n} + \theta_{(kl)}$ $e_{mnp}\epsilon_{(np), km} + 2\kappa_{mm}, k = \pi_{mm}, m$ $\theta_{kl} = -e_{kmn}\kappa_{nl, m}^P$ $\pi_{kl} = \kappa_{lk}^P - \kappa_{mm}^P \delta_{kl} - e_{kmn}\epsilon_{nl, m}^P$

This is one possible reinterpretation of incompatible micropolar mechanics. Other dislocation considerations are discussed in section III.

## B. ORIENTED MATERIALS

An approach to continuum dislocation theory utilizing the methods and ideas of multipolar mechanics and the theory of oriented materials has been suggested by Fox [10]. In his theory, an oriented medium with three

directors  $d_k^\alpha$  associated with each particle is employed. Thus Fox has nine generalized displacement degrees of freedom  $d_k^\alpha(\mathbf{X}, t)$  in addition to the classical motion  $x_k = x_k(\mathbf{X}, t)$ . For a determinate problem, twelve differential equations of motion are required. Since Fox uses energy invariance under translations and rotations, he obtains only six such equations; six are missing. Therefore an indeterminacy exists. In fact his balance laws can be shown to be identical to Cauchy's first law of motion and the micropolar moment of momentum equations (1.11), with the correspondence given in the table below. This means that the symmetric part of the general balance equation (1.4) is missing. This fact leads to a hybrid comparison between his theory and the kinematical variables of micromorphic mechanics. The functions  $x_k(\mathbf{X}, t)$  and  $d_k^\alpha(\mathbf{X}, t)$  are sufficient to correspond to the constitutive variables in micromorphic mechanics, but the equations of motion are only six (instead of twelve) and correspond to the micropolar case.

TABLE 2

Balance equation variables	
Fox	Micropolar
$\sigma_{kl}$	$t_{kl}$
$F_l$	$\rho f_l$
$v_l$	$v_l$
$e_{lmn}\pi_{km}^\alpha d_n^\alpha$	$-m_{kl}$
$e_{lmn}L_m^\alpha d_n^\alpha$	$-l_l$
$e_{lmn}\dot{w}_m^\alpha d_n^\alpha$	$-\dot{\sigma}_l$

Fox shows a relationship with dislocation theories by introducing an affine connection and defining a dislocation density by

$$a_{kl} = e_{lmn}d_k^\alpha e_{m,n}^\alpha \quad (2.21)$$

where  $e_m^\alpha$  are reciprocal directors satisfying the relations

$$d_k^\alpha e_l^\alpha = \delta_{kl}, \quad d_k^\alpha e_k^\beta = \delta^{\alpha\beta}. \quad (2.22)$$

### C. RUSSIAN SCHOOL

The recent work of Berdichevskii and Sedov [12] is also closely related to micromorphic mechanics in that they also introduce nine new generalized displacement degrees of freedom in addition to the classical three. These authors construct rather general balance equations from a variational principle, and then they proceed to show how the classical

elastic, plastic, and fluid constitutive relations can be constructed within their framework. In their final section, they choose appropriate variational variables and obtain an infinitesimal dislocation-plasticity theory which utilizes the concepts of dislocation density, plastic yield function, strain-rate, and entropy production. For comparison purposes, their theory is summarized as follows:

$$p_{kl,k} + F_l = \rho \dot{v}_l \quad (2.23)$$

$$\frac{1}{2} e_{lmn} (R_{mk} + \Sigma_{mk})_{,n} + p_{kl} - Q_{kl} = 0 \quad (2.24)$$

$$\rho \theta \frac{dn}{dt} = -\theta \left( \frac{q_k}{\theta} \right)_{,k} + \sigma_1 (\nabla \theta) + \sigma_2 (\dot{\epsilon}^{(p)}, \dot{S}). \quad (2.25)$$

No names are given to the new quantities appearing in the balance laws, but they can be identified from their constitutive relations:

$$p_{kl} = \frac{\partial u}{\partial \epsilon_{kl}^{(e)}}, \quad \Sigma_{kl} = \frac{\partial u}{\partial S_{kl}} \} \text{reversible part} \quad (2.26)$$

$$Q_{kl} = Q_{lk} = \frac{\partial \sigma_2}{\partial \dot{\epsilon}_{kl}^{(p)}}, \quad R_{kl} = \frac{\partial \sigma_2}{\partial \dot{S}_{kl}} \} \text{dissipative part} \quad (2.27)$$

$$q_k = -\frac{\partial \sigma_1}{\partial \theta_{,k}}.$$

Also a yield function is postulated in the form

$$f(Q_{kl}, R_{kl}) = 0. \quad (2.28)$$

In the above equations,  $S_{kl}$  is the dislocation density, and the superscripts on the strains denote the elastic and plastic parts.

In (2.24) the contribution to the kinetic energy in the Lagrangian from the dislocations has been neglected; hence there is no inertia term on the right-hand side. Since this is a dislocation-plasticity theory, the only point of contact with the original micromorphic theory seems to be the generalized moment of momentum equation (2.24) which Berdichevskii and Sedov refer to as the "internal parameters" equation. The skew part of (2.24) can be interpreted as an angular momentum equation. The interpretation of their symmetric part is not made clear. Their use of the entropy production equation in constructing constitutive equations is quite different from the current practice in continuum mechanics, cf. [15].

### III. A Dislocation Theory Based on Micromorphic Mechanics

Most of the existing continuum theories of dislocations appear to be either intended for initial stress problems, hence static in nature, or are incomplete for the treatment of dynamical boundary value problems in the same sense of completeness to which we are accustomed in classical elasticity. In this section we present a dynamical theory within the framework of micromorphic mechanics with the following objectives: (a) to treat dynamical motions of elastic bodies containing continuously distributed dislocations and (b) to provide a unifying framework from which some of the existing theories can be viewed. The present theory excludes macroplasticity and effects attributable to nonmetric connections, and should be considered an initial report on a larger program.

First the micromorphic kinematics is given a dislocation interpretation, and then balance and constitutive equations are derived using the dislocation density. For simplicity we employ cartesian coordinates, but sometimes for convenience retain indices in raised positions.

#### A. DISLOCATIONS AND MICROMORPHIC KINEMATICS

In micromorphic kinematics there are twelve generalized displacement degrees of freedom:  $x_k = x_k(\mathbf{X}, t)$  the classical motion, and  $\chi^k_\kappa = \chi^k_\kappa(\mathbf{X}, t)$  the micromotion. This micromotion provides the necessary mechanism for the treatment of dislocations in the solid. An average Burgers vector can be defined by

$$\Delta b^k = b^k \Delta A = \oint_C \chi^k_\kappa dX^\kappa = \int \int_S e_{LMN} \chi^k_{N, M} dA_L \quad (3.1)$$

where  $S$  is a small area element bounded by the closed circuit  $C$ . In the limit when  $S \rightarrow 0$  this gives

$$b^k = \alpha^k_L n_L, \quad \alpha^k_L(\mathbf{X}, t) = e_{LMN} \chi^k_{N, M} \quad (3.2)$$

Since Bilby, Kröner, and others have shown the relationship between the dislocation density and the torsion tensor of an appropriately defined affinely connected space, we introduce the connection

$$\Gamma^K_{LM} = \mathcal{X}^\kappa_k \chi^k_{L, M} \quad (3.3)$$

where  $\mathcal{X}^\kappa$  are three vectors reciprocal to  $\chi_\kappa$ , i.e.,

$$\chi^k_\kappa \mathcal{X}^\kappa_l = \delta^k_l, \quad \mathcal{X}^\kappa_k \chi^k_l = \delta^k_l. \quad (3.4)$$

The *material dislocation density* tensor is defined by

$$\alpha^K_L = e_{LMN} \Gamma^K_{NM} = X^K_k \alpha^k_L. \quad (3.5)$$

It is readily verified that  $\Gamma$  transforms as a connection under the coordinate transformations  $X'^K = X'^K(\mathbf{X})$ , i.e.,

$$\Gamma'^K_{LM} = \frac{\partial X'^K}{\partial X^R} \frac{\partial X^S}{\partial X'^L} \frac{\partial X^T}{\partial X'^M} \Gamma^R_{ST} + \frac{\partial X'^K}{\partial X^R} \frac{\partial^2 X^R}{\partial X'^L \partial X'^M}.$$

In Bilby's terminology, this space possesses distant parallelism since the Riemann curvature tensor based on this connection vanishes identically

$$R^K_{LMN} = \Gamma^K_{LN, M} - \Gamma^K_{LM, N} + \Gamma^R_{LN} \Gamma^K_{RM} - \Gamma^R_{LM} \Gamma^K_{RN} = 0. \quad (3.6)$$

As pointed out by Kondo, this is not the most general procedure possible, and this restriction will be lifted in a later work.

The relations presented above are in the material frame; in order to construct constitutive equations in a later section the analogous spatial form of these results is needed. Thus an average Burgers vector may be defined by

$$\Delta B^K = B^K \Delta a = \oint_C \mathcal{X}^K_k dx_k = \int_S \int e_{lmn} \mathcal{X}^K_{n, m} da_l \quad (3.7)$$

$$B^K = \alpha^K_l n_l, \quad \alpha^K_l = e_{lmn} \mathcal{X}^K_{n, m} \quad (3.8)$$

Again based on the ideas of affinely connected spaces we introduce the connection.

$$\Gamma^k_{lm} = \chi^k_K \mathcal{X}^K_{l, m} \quad (3.9)$$

The *spatial dislocation density* tensor is then given by

$$\alpha^k_l = e_{lmn} \Gamma^k_{nm} = \chi^k_K \alpha^K_l. \quad (3.10)$$

The spatial dislocation density (3.10) corresponds also to that introduced by Fox. In fact if we recognize the correspondence of our  $\chi_K$  with his  $\mathbf{d}^\alpha$  and  $\mathcal{X}^K = \mathcal{X}^K_l \mathbf{i}_l$  (where  $\mathbf{i}_l$  are the spatial cartesian base vectors) with his  $\mathbf{e}^\alpha$  then (3.10) is identical with (2.21).

It can be verified that  $\Gamma^k_{lm}$  transforms as a connection under the transformation  $x'^k = x'^k(\mathbf{x})$ , and that the space possesses *teleparallelism*.

$$R^k_{lmn} = 0. \quad (3.11)$$

In the terminology of Bilby, Bullough, and Smith [16], this is *distant parallelism*. In this respect, the present theory is more restricted than that of Kondo [17]. Contact can now be provided with the incompatibility equation of Kröner by introducing the connection

$$\bar{\Gamma}_{lm}^k = \{_{lm}^k\} + S_{lm}^{::k} - S_{m\cdot l}^{::k} + S_{\cdot lm}^k \quad (3.12)$$

where

$$S_{lm}^{::k} \equiv \Gamma_{[lm]}^k = -\frac{1}{2} e_{lmn} \alpha_n^k \quad (3.13)$$

is the torsion tensor and the Christoffel symbols are given in terms of the deformation tensor  $c_{kl}$  or the Eulerian strain tensor  $e_{kl}$ , i.e.,

$$\{_{lm}^k\} = \frac{1}{2} c_{kr}^{-1} (c_{lr, m} + c_{mr, l} - c_{lm, r})$$

$$c_{kl} = \delta_{kl} - 2e_{kl}.$$

If now we require that the Riemann-Christoffel tensor  $R^k_{lmn}$  based on  $\bar{\Gamma}_{lm}^k$  vanishes and linearize the resulting expression, we obtain Kröner's incompatibility equation

$$2e_{kmp}e_{lnq}e_{(mn), pq} = e_{kmn}\alpha_{lm, n} + e_{lmn}\alpha_{km, n}. \quad (3.14)$$

Incidentally if we do not linearize the equation  $R^k_{lmn} = 0$ , based on  $\bar{\Gamma}_{lm}^k$  we obtain a nonlinear incompatibility equation for the nonlinear strain tensor  $e_{kl}$ . We further note that

$$\bar{\Gamma}_{[lm]}^k = S_{lm}^{::k} = \Gamma_{[lm]}^k. \quad (3.15)$$

Therefore the torsion tensor in the present theory is identical to those of Kröner and Bilby. However  $\Gamma_{(lm)}^k \neq \bar{\Gamma}_{(lm)}^k$  in general. Since in micromorphic mechanics three different strain measures are used, the foregoing approach is no longer suitable. This provides basic reasons why additional incompatibility tensors may be introduced, as was done in the first part of the paper, to account for other physical phenomena.

## B. BALANCE LAWS

The balance laws used here are those of the general micromorphic theory summarized in (1.1) to (1.5).

## C. CONSTITUTIVE RELATIONS

The nonlinear, anisotropic constitutive equations for the micromorphic theory are [2]:

$$t_{kl} = \frac{\rho}{\rho_0} \left[ 2 \frac{\partial \Sigma}{\partial C_{KL}} x_{k,\kappa} x_{l,L} + \left( \frac{\partial \Sigma}{\partial \Psi_{KL}} \chi_{lL} + \frac{\partial \Sigma}{\partial \hat{\Gamma}_{KLM}} \chi_{lL,M} \right) x_{k,\kappa} \right] \quad (3.16)$$

$$s_{kl} = \frac{2\rho}{\rho_0} \left[ \frac{\partial \Sigma}{\partial C_{KL}} x_{k,\kappa} x_{l,L} + \frac{\partial \Sigma}{\partial \Psi_{KL}} x_{(k,\kappa} \chi_{l)L} + \frac{\partial \Sigma}{\partial \hat{\Gamma}_{KLM}} x_{(k,\kappa} \chi_{l)L,M} \right] \quad (3.17)$$

$$\lambda_{klm} = \frac{\rho}{\rho_0} \frac{\partial \Sigma}{\partial \hat{\Gamma}_{KLM}} x_{k,M} x_{l,\kappa} x_{m,L} \quad (3.18)$$

where

$$\Sigma = \Sigma (\mathbf{X}, C_{KL}, \Psi_{KL}, \hat{\Gamma}_{KLM}) \quad (3.19)$$

$$C_{KL} = x_{k,\kappa} x_{k,L}, \quad \Psi_{KL} = x_{k,\kappa} \chi_{KL}, \quad \hat{\Gamma}_{KLM} = x_{k,\kappa} \chi_{KL,M}. \quad (3.20)$$

The gamma hat used here is a strain tensor and should not be confused with the connection in (3.3). The gamma hat in (3.16)–(3.20) corresponds to Eringen and Suhubi's gamma.

Let  $\mathbf{P}$  and  $\mathbf{A}$  be defined by

$$P_{KLM} = \hat{\Gamma}_{K(LM)} = \frac{1}{2} (\hat{\Gamma}_{KLM} + \hat{\Gamma}_{KML}) \quad (3.21)$$

$$A_{KLM} = \hat{\Gamma}_{K[L]M} = \frac{1}{2} (\hat{\Gamma}_{KLM} - \hat{\Gamma}_{KML}). \quad (3.22)$$

Using (3.2) we see that  $A_{KLM}$  can be written as

$$A_{KLM} = -\frac{1}{2} e_{LMN} x_{k,\kappa} \alpha_{kN}. \quad (3.23)$$

Hence the dislocations in the body manifest themselves through the skew-symmetric part of  $\hat{\Gamma}$ . This leads us to call  $\mathbf{A}$  the *dislocation strain tensor*. We conjecture that  $\mathbf{P}$  is due to other types of defects, e.g., point defects. This interpretation will be elaborated on in a later paper. For the nonlinear case, we see that the dislocation tensor  $\alpha^k_L$  is not an appropriate constitutive variable, rather  $\mathbf{A}$  is. Only in the linear theory does the dislocation density tensor become an admissible constitutive variable.

To arrive at the linear theory, the analogous spatial forms of (3.16)–(3.18) must be used. They are given explicitly as eqs. (6.15) in [2]. The spatial micromorphic strain tensors are

$$c_{kl} = X_{K,k} X_{K,l}, \quad \Psi_{kl} = X_{K,k} \mathcal{X}_{kl}, \quad \gamma_{klm} = X_{K,k} \mathcal{X}_{kl,m}. \quad (3.24)$$

Again we see that the dislocation tensor  $\alpha_{kl}$  in (3.8) contributes only to  $\gamma_{klm}$ . In fact, by defining  $\mathbf{p}$  and  $\mathbf{a}$  by

$$p_{klm} = \gamma_{k(lm)}, \quad a_{klm} = \gamma_{k[lm]} \quad (3.25)$$

and using (3.8)  $\mathbf{a}$  can be written as

$$a_{klm} = -\frac{1}{2} e_{lmn} X_{K,k} \alpha_{Kn} \quad (3.26)$$

in the nonlinear case. This motivates the name *spatial dislocation strain tensor* for  $a_{klm}$ .

Passage to the infinitesimal theory requires the introduction of displacement gradients  $u_{r,k}$  and microdisplacements  $\phi_{rk}$  through

$$\begin{aligned} X_{K,k} &= \delta_{Kk} - \delta_{Kr} u_{r,k} \\ \mathcal{X}_{kk} &= \delta_{Kk} - \delta_{Ks} \phi_{sk}. \end{aligned} \quad (3.27)$$

The linearized forms of the dislocation strain tensor  $a_{klm}$  (obtained from (3.26)) and the dislocation density tensor  $\alpha_{kl}$  (obtained from (3.10)) are

$$a_{klm} = -\frac{1}{2} e_{lmn} \alpha_{kn} = \gamma_{k[lm]} = -\phi_{k[l,m]} \quad (3.28)$$

$$\alpha_{kl} = -e_{lmn} \phi_{kn,m}. \quad (3.29)$$

For later use we record the inverse of (3.28)

$$\alpha_{kl} = e_{lmn} a_{knm} = e_{lmn} \gamma_{knm} \quad (3.30)$$

The linear, isotropic constitutive equations which were written symbolically in (1.8) are explicitly eqs (6.15) of [2]. For this dislocation model we neglect contributions to the strain energy from other defects and take

$$\Sigma = \Sigma(\mathbf{e}, \boldsymbol{\epsilon}, \mathbf{a}) \quad (3.31)$$

In this case (6.15) of [2] becomes

$$t_{kl} = (\lambda + \tau) e_{mm} \delta_{kl} + 2(\mu + \sigma) e_{kl} + \eta \epsilon_{mm} \delta_{kl} + \nu \epsilon_{lk} + \kappa \epsilon_{kl} \quad (3.32)$$

$$s_{kl} = (\lambda + 2\tau)e_{mm}\delta_{kl} + 2(\mu + 2\sigma)e_{kl} + (2\eta - \tau)\epsilon_{mm}\delta_{kl} + (\nu + \kappa - \sigma)(\epsilon_{kl} + \epsilon_{lk}) \quad (3.33)$$

$$\lambda_{klm} = a_1\alpha_{rn}(e_{krn}\delta_{ml} - e_{mrn}\delta_{kl}) + a_2e_{mkn}\alpha_{ln} + a_3(e_{klm}\alpha_{mn} - e_{mln}\alpha_{kr}) \quad (3.34)$$

where

$$2a_1 \equiv \tau_2 - \tau_6, 2a_2 \equiv \tau_7 - \tau_9, 2a_3 \equiv \tau_8 - \tau_{11}, \tau_1 = \tau_5, \tau_3 = \tau_6, \tau_{10} = \tau_{11}. \quad (3.35)$$

The  $\tau_k$ 's are Eringen and Suhubi's [2] original constitutive constants.

#### D. FIELD EQUATIONS

Substitution of (3.32)–(3.34) into the equilibrium equations (1.3) and (1.4) gives 12 partial differential equations for the 12 unknowns  $u_k$  and  $\phi_{kl}$ . The field equations are

$$(\lambda + \mu + \tau + \sigma + \nu + \eta)u_{k,kl} + (\mu + \sigma + \kappa)u_{l,kk} + \eta\phi_{kk,l} + \nu\phi_{lk,k} + \kappa\phi_{kl,k} + \rho_0f_l = \rho_0 \frac{\partial^2 u_l}{\partial t^2} \quad (3.36)$$

$$\begin{aligned} & a_1(\phi_{rk,rk} - \phi_{rr,kk})\delta_{ml} - (a_1 + a_3)\phi_{km,kl} + a_1\phi_{kk,ml} \\ & + a_2(\phi_{lm,kk} - \phi_{lk,mk}) + a_3(\phi_{mk,lk} - \phi_{ml,kk} + \phi_{kl,mk}) \\ & - \eta u_{r,r}\delta_{ml} - \kappa u_{m,l} - \nu u_{l,m} + (\tau - \eta)\phi_{rr}\delta_{ml} \\ & + (\sigma - \nu)\phi_{ml} + (\sigma - \kappa)\phi_{lm} + \rho_0l_{lm} = \rho_0I_0 \frac{\partial^2 \phi_{lm}}{\partial t^2}. \end{aligned} \quad (3.37)$$

The boundary conditions to be satisfied on the surface  $S$  of a body are

$$t_{km}n_k = t_{(n)l}, \lambda_{klm}n_k = \lambda_{(n)lm} \text{ on } S_t$$

$$u_k = U_k, \phi_{kl} = \Phi_{kl} \quad \text{on } S_u = S - S_t \quad (3.38)$$

where  $t_{(n)l}$  and  $\lambda_{(n)lm}$  are prescribed surface tractions and moments on a part of the boundary  $S_t$  and  $U_k$  and  $\Phi_{kl}$  are prescribed surface displacements and microdisplacements on the remaining part of the boundary  $S_u$ . Other mixed boundary value problems are also possible, but in each case uniqueness theorems must be proved.

We notice that from (3.34)  $\lambda_{klm} = -\lambda_{mlk}$  so that eq (1.4) can also be written as

$$e_{kmn}m_{nl,k} + t_{ml} - s_{ml} + \rho l_{lm} = \rho I_0 \frac{\partial^2 \phi_{lm}}{\partial t^2} \quad (3.39)$$

where

$$\lambda_{klm} = e_{kmn}m_{nl}, \quad m_{kl} = \frac{1}{2} e_{kmn}\lambda_{mln} \quad (3.40)$$

and

$$m_{kl} = -a_3\alpha_{mm}\delta_{kl} - a_1\alpha_{kl} + (a_1 - a_2 + a_3)\alpha_{lk}. \quad (3.41)$$

The twelve partial differential equations (3.36) and (3.37) constitute the field equations of the dynamical theory of dislocations presented here. A set of initial conditions may be of the form

$$\begin{aligned} u_k &= u_k^0(\mathbf{x}) & \dot{u}_k &= v_k^0(\mathbf{x}) \\ \phi_{kl} &= \phi_{kl}^0(\mathbf{x}), & \dot{\phi}_{kl} &= v_{kl}^0(\mathbf{x}) \text{ in } V, \quad t = 0 \end{aligned} \quad (3.42)$$

where  $\mathbf{u}^0$ ,  $\mathbf{v}^0$ ,  $\phi^0$ , and  $\mathbf{v}^0$  are the prescribed initial fields. The field equations (3.36) and (3.37) subject to conditions of the type (3.38) and (3.42) constitute a well-posed set of equations for boundary and initial value problems of the theory. Once  $u_k$  and  $\phi_{kl}$  are so determined, the strains are calculated through (1.7), the dislocation strain from (3.28) and the dislocation density from (3.29). The stresses and stress moments follow from (3.32) to (3.34).

#### IV. Concluding Remarks

In this paper we have shown how the incompatible dislocation approach can be viewed in the context of micromorphic mechanics. In the last section a dislocation theory was developed for the treatment of dynamical boundary and initial value problems. The theory supplies a determinate mechanism for the prediction of the motion and deformation of elastic solids with dislocations.

#### V. Acknowledgement

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# ON THE CONTINUUM THEORY OF DISLOCATIONS

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The kinematics of an oriented medium is discussed with reference to the continuum theory of dislocations. The concepts of dislocation density, dislocation flux and slip velocity are introduced and a corresponding constitutive theory is developed.

Key words: Continuum mechanics; dislocation kinematics; dislocations; constitutive relations; oriented media; thermodynamics and dislocation motion.

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## I. Introduction

During the last ten years considerable advances have been made in the development of various generalizations of classical continuum mechanics. And it is our purpose here to reexamine the continuum theory of dislocations in the light of these advances. (For reviews by the originators of research in this area see Kondo [1], Bilby [2] and Kröner [3]).

Motivated by the geometry of dislocated crystals, we show how the concepts of dislocation density, slip velocity, dislocation diffusion, and dislocation flux may be introduced into a continuum theory without recourse to non-euclidean geometry and without making a transition from a theory of dense distributions of discrete dislocations. This is made possible by adapting the theories of oriented media which are now available. (For a review of these theories see for example Truesdell and Noll [4] p. 389). Moreover, generalizing the theory of internal state variables given by Coleman and Gurtin [5], the thermodynamic background to the subject may also be developed.

Most of the significant work on the continuum theory of dislocations is summarised, or referred to, in the Proceedings [6] of the recent IUTAM Symposium on the subject. It appears that authors who seek a basis for this theory within the framework of general continuum mechanics adopt, broadly speaking, one of two possible starting points. In the first, some kind of oriented medium is defined by introducing new kinematic variables which are variously called directors, multipolar displacement fields or

microdisplacements. Then either static or dynamic theories are derived which provide a model for a dislocated crystalline material. The other starting point was suggested by Noll [7]. He showed how the idea of dislocation density or inhomogeneity emerges from the properties of the constitutive equation for a simple material using the concept of local reference configurations. And these ideas have been carried further by Wang [8, 9]. However, these two approaches are not entirely distinct. Toupin [6] has shown that, although directors may be introduced as new kinematic variables defining an oriented medium, they may also be related to Noll's analysis of a simple material.

We do not consider further the relationship between these approaches. However, we note that Noll's theory starts by defining over the body a set of local reference configurations which does not vary in time. Consequently the theory gives rise to a time-independent dislocation density. And although it seems possible to extend this theory to allow the local reference configurations to vary with time (see Fox [10]), the idea of dislocation flux appears to be clearer if approached from the standpoint of director kinematics. For this reason, we adopt the terminology of the oriented medium.

We introduce dislocation density and slip velocity using simple vector and tensor analysis in euclidean three-space. We show how the transport of dislocation density may be separated into a diffusive part and a convective part. This leads us to a definition of dislocation diffusion vectors which we then relate to dislocation flux vectors. We postulate constitutive equations, including one for the dislocation flux vectors and analyse the restrictions on these equations arising from the laws of thermodynamics and the principle of material indifference. And finally we arrive at a complete set of equations governing the deformation of an oriented medium in which slip processes arise from dislocation flux.

## II. Preliminaries

We use fixed rectangular cartesian axes. The position vector of a generic particle of the body in a reference configuration  $\mathcal{C}_0$  is denoted by  $\mathbf{X} \equiv (X_A)$ . Its position vector in the configuration  $\mathcal{C}_t$  at the current time  $t$  is denoted by  $\mathbf{x} \equiv (x_i)$ . All upper and lower case suffixes take the values 1, 2, and 3.

The motion of the body is given by the time-dependent mappings

$$\mathbf{x} = \chi(\mathbf{X}, t); \quad x_i = \chi_i(X_A, t). \quad (2.1)$$

We assume that all functions used are differentiable as many times as required and we denote the deformation gradient tensor by

$$\mathbf{F} \equiv (x_{i,A}), \quad (2.2)$$

where a comma followed by an upper or lower case suffix denotes partial differentiation with respect to  $X_A$  or  $x_i$  respectively. As usual, we assume that

$$J \equiv \det \mathbf{F} > 0. \quad (2.3)$$

And so (2.1) has the unique inverse

$$\mathbf{X} = \chi^{-1}(\mathbf{x}, t). \quad (2.4)$$

We denote the velocity of a particle by

$$\mathbf{v} = \frac{\partial}{\partial t} \chi(\mathbf{X}, t) \quad (2.5)$$

and in virtue of (2.4) we may also regard  $\mathbf{v}$  as a function of the spatial coordinates  $x_i, t$ . As no confusion arises we normally omit the explicit dependence on  $x_i$  and  $t$ . Then  $(\partial/\partial t)$  is used to denote the time derivative keeping  $x_i$  fixed and  $(D/Dt)$  to denote the material time derivative keeping  $X_A$  fixed. For convenience we sometimes use the superposed dot in place of  $(D/Dt)$ .

Associated with each particle of the body we suppose that there are defined three vectors  $\mathbf{d}^\alpha$  known as directors. Greek indices take the values 1, 2, and 3 and serve simply as labels for the directors. A repeated index or suffix implies summation.

The motion of the directors is given by equations of the form

$$\mathbf{d}^\alpha = \delta^\alpha(\mathbf{X}, t). \quad (2.6)$$

We define the director gradient tensors  $\mathbf{D}^\alpha$  as

$$\mathbf{D}^\alpha \equiv (d_{i,K}^\alpha) \quad (2.7)$$

and the director velocities by

$$\dot{\mathbf{d}}^\alpha = \frac{\partial}{\partial t} \delta^\alpha(\mathbf{X}, t). \quad (2.8)$$

Using (2.1) the directors may also be considered as functions of the spatial coordinates  $x_i, t$ .

We suppose that throughout the motion the directors associated with any given particle remain noncoplanar. Thus we may define reciprocal directors  $\mathbf{e}^\alpha$  by the relations

$$\mathbf{e}^\alpha \cdot \mathbf{d}^\beta = \delta^{\alpha\beta} \quad (2.9)$$

where  $\delta^{\alpha\beta}$  is the Krönecker symbol.

### III. Dislocation Kinematics

By analogy with Burgers circuits in real crystals, the circulation of the vectors  $\mathbf{e}^\alpha$  about any reducible circuit C of material particles in  $\mathcal{C}_t$  may be used as a continuum definition of the Burgers vector for the circuit C. This leads naturally to the definition of the dislocation density vectors  $\boldsymbol{\omega}^\alpha$  as

$$\boldsymbol{\omega}^\alpha = \operatorname{curl} \mathbf{e}^\alpha, \quad (3.1)$$

where the curl operator is defined in terms of the spatial coordinates  $x_i$ . These vectors may be resolved into components  $\omega^{\alpha\beta}$  in the triad  $\mathbf{d}^\alpha$ . That is

$$\boldsymbol{\omega}^\alpha = \omega^{\alpha\beta} \mathbf{d}^\beta \quad (3.2)$$

where

$$\omega^{\alpha\beta} = \boldsymbol{\omega}^\alpha \cdot \mathbf{e}^\beta. \quad (3.3)$$

We call  $\omega^{\alpha\beta}$  ( $\alpha \neq \beta$ ) the *edge components* of the dislocation density vectors and  $\omega^{\alpha\beta}$  ( $\alpha = \beta$ ) the *screw components*.

The time rates of change of the dislocation density vectors measured per unit area of an element of surface moving with the material are given by the convected time derivatives

$$\overset{\circ}{\omega}_i^\alpha = \dot{\omega}_i^\alpha + v_{k, k} \omega_i^\alpha - v_{i, j} \omega_j^\alpha. \quad (3.4)$$

Alternatively, we may write (3.4) in the form

$$\overset{\circ}{\omega}^\alpha = (\partial \boldsymbol{\omega}^\alpha / \partial t) + \operatorname{curl} (\boldsymbol{\omega}^\alpha \times \mathbf{v}). \quad (3.5)$$

For any smooth material surface S bounded by a smooth curve C we may write, in virtue of (3.1) and (3.4),

$$\frac{D}{Dt} \oint_C e_i^\alpha dx_i = \frac{D}{Dt} \int_S \omega_i^\alpha n_i dS = \int_S \overset{\circ}{\omega}_i^\alpha n_i dS, \quad (3.6)$$

where  $n_i$  is the unit normal to S.

The slip velocities  $\xi_i^\alpha$  are defined by

$$\xi_i^\alpha = v_{i, j} \mathbf{d}_j^\alpha - \dot{\mathbf{d}}_i^\alpha \quad (3.7)$$

and the vectors  $\mathring{\omega}^\alpha$  are related to the vectors  $\xi^\alpha$  by the formula

$$\mathring{\omega}^\alpha = \text{curl} \{ (\xi^\beta \cdot \mathbf{e}^\alpha) \mathbf{e}^\beta \}. \quad (3.8)$$

The derivation of the above relations and the physical motivation for the definitions has been given by Fox [11].

Now it is clear from (3.1) that the vector fields  $\omega^\alpha$  are solenoidal and an extensive study of such fields has been given recently by Marris and Passman [12]. They have generalized the Beltrami identity concerning vorticity transport to provide a relation governing the transport of an arbitrary solenoidal field. And they have derived a general integral of this relation which is the counterpart of Truesdell's [13] integral of the Beltrami identity. Much of this analysis has direct application to the present theory.

Applied to the vector fields  $\omega^\alpha$ , their fundamental identity gives

$$J^{-1}(D/Dt)(J\omega^\alpha) = \mathring{\omega}^\alpha + (\omega^\alpha \cdot \text{grad}) \mathbf{v}, \quad (3.9)$$

which may of course be deduced directly from (3.4). This relation shows how the time rate of change of the dislocation density vectors may be separated into what we call a diffusive part and a convective part. In particular, we see that when  $\omega^\alpha$  is zero a necessary and sufficient condition that  $\mathring{\omega}^\alpha$  be zero is that  $\mathring{\omega}^\alpha$  is zero. We call  $\mathring{\omega}^\alpha$  the (spatial) *dislocation diffusion vector*.

The integral of (3.9) may be written as

$$\omega_i^\alpha = \left\{ A_K^\alpha + \int_{t_0}^t J X_{K,j} \mathring{\omega}_j^\alpha dt \right\} x_{i,K} J^{-1} \quad (3.10)$$

where  $A_K^\alpha x_{i,K} J^{-1}$  is the value of  $\omega_i^\alpha$  at time  $t=t_0$ . The time integration in (3.10) is carried out following a material particle. And so, for example, if a dislocation diffusion vector  $\mathring{\omega}^\alpha$  is zero, the associated dislocation density vector  $\omega^\alpha$  may be said to be convected only by the velocity field  $\mathbf{v}$ . In this case

$$\omega_i^\alpha = x_{i,K} A_K^\alpha J^{-1}. \quad (3.11)$$

If all three vectors  $\mathring{\omega}^\alpha$  are zero in some region of the body, we say that, in this region, the motion is *dislocation preserving*. And we see from (3.6) that in such a region, the circulation of the vectors  $\mathbf{e}^\alpha$  about any material circuit is constant. It is also possible to discuss motions in which the strengths of the vector tubes of the fields  $\omega^\alpha$  remain constant while being

convected by distinct velocity fields  $\mathbf{V}(\alpha)$  (see Fox [11]). However, the deformation of real crystals due to the independent motions of edge and screw dislocations suggests that a more general analysis is required.

A general dislocation flux tensor has been introduced by Kröner and Rieder [14] and the associated theory has been further developed by Mura (see [6] for references). However, this approach involves a transition from a theory of densely distributed discrete dislocations and the object of the present analysis is to provide a basis for a continuum theory of dislocations using only continuum hypotheses. We therefore proceed by introducing what we call dislocation flux vectors, using the ideas of the above authors as motivation but relying only on the kinematic variables so far defined.

We assume that at each point of the body there exist nine vectors  $\mathbf{v}^{\alpha\beta}$  such that the slip velocity is given by

$$(\xi^\beta \cdot \mathbf{e}^\alpha) \mathbf{e}^\beta = \mathbf{v}^{\alpha\beta} \times \mathbf{d}^\beta. \quad (3.12)$$

An analysis of this relation in conjunction with (3.6) and (3.8) leads us to define  $\mathbf{v}^{\alpha\beta}$  to be the *dislocation flux vector* associated with the dislocation density component  $\omega^{\alpha\beta}$ . Clearly the vectors  $\mathbf{v}^{\alpha\beta}$  determine the  $\xi^\alpha$  but the  $\mathbf{v}^{\alpha\beta}$  are not uniquely determined by the  $\xi^\alpha$ . This corresponds physically to the fact that certain slip velocities may arise from the motion of distinct dislocation components. If all the vectors  $\mathbf{v}^{\alpha\beta}$  are zero the motion is necessarily dislocation preserving. But a dislocation preserving motion does not necessarily imply that all the vectors  $\mathbf{v}^{\alpha\beta}$  are zero.

From the point of view of generalized continuum mechanics, we regard  $\mathbf{v}^{\alpha\beta}$  as new primitive variables for which constitutive equations must be formulated. Once these equations have been postulated, (3.12) determine the slip vectors, which in virtue of (3.7) give rise to first order differential equations for  $\mathbf{d}^\alpha$ .

#### IV. Thermodynamics and Constitutive Equations

In order to discuss thermodynamic processes, we introduce the Cauchy stress tensor  $\mathbf{T}$ , the body force  $\mathbf{b}$  per unit mass, the internal energy  $\epsilon$  per unit mass, the heat flux vector  $\mathbf{q}$ , the heat supply function  $r$  per unit mass, the entropy  $\eta$  per unit mass and the absolute temperature  $\theta$ . The equations of motion and energy balance may be written in the forms:

$$T_{ji,j} + \rho b_i = \rho \dot{v}_i \quad (4.1)$$

$$\rho \dot{\epsilon} - T_{ij} v_{i,j} + q_{i,i} = \rho r. \quad (4.2)$$

We do not consider here the modifications of (4.2) due to director stresses and director inertia. We assume that these effects are negligible.

We now proceed using a generalization of the techniques of Coleman and Gurtin [5] and we use their terminology.

The set of eleven functions  $\{\chi, \mathbf{T}, \mathbf{b}, \epsilon, \mathbf{q}, r, \eta, \theta, \mathbf{d}^\alpha\}$  defined over the body for all time  $t$  is called a thermodynamic process if and only if it satisfies (4.1) and (4.2). Clearly any set  $\{\chi, \mathbf{T}, \epsilon, \mathbf{q}, \eta, \theta, \mathbf{d}^\alpha\}$  determines a thermodynamic process since corresponding values of  $\mathbf{b}$  and  $r$  may be calculated from (4.1) and (4.2).

The rate  $\gamma$  of production of entropy is given by

$$\rho\gamma = \rho\dot{\eta} - (\rho r/\theta) + \operatorname{div}(\mathbf{q}/\theta) \quad (4.3)$$

and the Clausius-Duhem inequality is written

$$\gamma \geq 0. \quad (4.4)$$

In virtue of (4.2), (4.3) may be written as

$$\theta\gamma = -\dot{\Psi} - \eta\dot{\theta} + S_{iA}x_{i,A} - (g_i q_i / \rho\theta), \quad (4.5)$$

where

$$T_{ij} = \rho S_{iA}x_{j,A}, \quad g_i = \theta_{,i},$$

and  $\Psi = \epsilon - \theta\eta$  denotes the Helmholtz free energy per unit mass.

We make the following constitutive assumptions:

$$\Psi = \hat{\Psi}(\mathbf{F}, \mathbf{d}^\alpha, \mathbf{D}^\alpha, \theta, \mathbf{g}), \quad (4.6)$$

$$S = \hat{S}(\mathbf{F}, \mathbf{d}^\alpha, \mathbf{D}^\alpha, \theta, \mathbf{g}), \quad (4.7)$$

$$\eta = \hat{\eta}(\mathbf{F}, \mathbf{d}^\alpha, \mathbf{D}^\alpha, \theta, \mathbf{g}), \quad (4.8)$$

$$\mathbf{q} = \hat{\mathbf{q}}(\mathbf{F}, \mathbf{d}^\alpha, \mathbf{D}^\alpha, \theta, \mathbf{g}), \quad (4.9)$$

$$\mathbf{v}^{\alpha\beta} = \hat{\mathbf{v}}^{\alpha\beta}(\mathbf{F}, \mathbf{d}^\alpha, \mathbf{D}^\alpha, \theta, \mathbf{g}). \quad (4.10)$$

And we say that a thermodynamic process is admissible if it is compatible with (4.6)–(4.10).

From (3.7) we see that

$$\dot{x}_{i,A} = (\xi_i^\alpha + \dot{d}_i^\alpha) e_j^\alpha x_{j,A}. \quad (4.11)$$

Hence, (4.5) may be written

$$\theta_\gamma = -\dot{\Psi} - \eta\dot{\theta} + S_{iA}(\xi_i^\alpha + \dot{d}_i^\alpha)e_j^\alpha x_{j,A} - (g_i q_i / \rho \theta). \quad (4.12)$$

Using (4.6) and (4.11), (4.12) becomes

$$\begin{aligned} \theta_\gamma = & -\left(\frac{\partial \Psi}{\partial \theta} + \eta\right)\dot{\theta} + \left\{\left(S_{iA} - \frac{\partial \Psi}{\partial x_{i,A}}\right)e_j^\alpha x_{j,A} - \frac{\partial \Psi}{\partial d_i^\alpha}\right\}\dot{d}_i^\alpha \\ & - \frac{\partial \Psi}{\partial d_{i,A}^\alpha}\dot{d}_{i,A}^\alpha - \frac{\partial \Psi}{\partial g_i}\dot{g}_i + \left(S_{iA} - \frac{\partial \Psi}{\partial x_{i,A}}\right)e_j^\alpha x_{j,A}\xi_i^\alpha - (g_i q_i / \rho \theta). \end{aligned} \quad (4.13)$$

And we recall that  $\xi$  is given in terms of  $\mathbf{v}^{\alpha\beta}$  by (3.12).

Now the second law of thermodynamics asserts that the inequality (4.4) must be satisfied at all points of the body for all time  $t$  by every admissible thermodynamic process. And in order to examine the consequences of this law, we select some particular processes. First we note that if  $\chi(\mathbf{X}, t)$  and  $\theta(\mathbf{X}, t)$  are specified then  $\mathbf{F}$  and  $\mathbf{g}$  may be calculated directly. Equation (4.10) then gives first order differential equations for  $\mathbf{d}^\alpha(\mathbf{X}, t)$ . Assuming that these equations have a solution for some chosen initial values  $\mathring{\mathbf{d}}^\alpha(\mathbf{X})$ , we see that, in virtue of (4.6)–(4.9) the functions  $\chi(\mathbf{X}, t)$ ,  $\theta(\mathbf{X}, t)$ ,  $\mathring{\mathbf{d}}^\alpha(\mathbf{X})$  are sufficient to determine an admissible thermodynamic process.

Let  $\{\mathring{\mathbf{F}}, \mathring{\mathbf{d}}^\alpha, \mathring{\mathbf{D}}^\alpha, \mathring{\theta}, \mathring{\mathbf{g}}\}$  be an arbitrary set of values of the independent variables in the constitutive equations at a material point  $\mathbf{X}'$  of the body. We consider the admissible thermodynamic process defined by

$$\begin{aligned} \chi_i(\mathbf{X}, t) = & X'_i + \{\mathring{F}_{iA} + (t - \mathring{t})\mathring{A}_{iA}\}(X_A - X'_A) \\ & + (1/2)B_{iAB}(t - \mathring{t})(X_A - X'_A)(X_B - X'_B), \end{aligned} \quad (4.14)$$

$$\theta(\mathbf{X}, t) = \mathring{\theta} + (t - \mathring{t})a + \{\mathring{g}_i + (t - \mathring{t})a_i\}\mathring{F}_{iA}(X_A - X'_A), \quad (4.15)$$

$$d_i^\alpha(\mathbf{X}) = \mathring{d}_i^\alpha + \mathring{D}_{iA}^\alpha(X_A - X'_A) + (1/2)C_{iAB}^\alpha(X_A - X'_A)(X_B - X'_B), \quad (4.16)$$

where time  $\mathring{t}$ , the scalar  $a$ , the vector  $\mathbf{a}$  and the tensors  $A_{iA}$ ,  $B_{iAB}$ ,  $C_{iAB}^\alpha$  are chosen arbitrarily (except for the symmetries  $B_{iAB} = B_{iBA}$ ,  $C_{iAB}^\alpha = C_{iBA}^\alpha$ ).

This process has the properties:

$$\begin{aligned}
 \mathbf{F}(\mathbf{X}', \overset{\circ}{t}) &= \overset{\circ}{\mathbf{F}}, & \mathbf{d}^\alpha(\mathbf{X}', \overset{\circ}{t}) &= \overset{\circ}{\mathbf{d}}{}^\alpha, & \mathbf{D}^\alpha(\mathbf{X}', \overset{\circ}{t}) &= \overset{\circ}{\mathbf{D}}{}^\alpha, \\
 \theta(\mathbf{X}', \overset{\circ}{t}) &= \overset{\circ}{\theta}, & \mathbf{g}(\mathbf{X}', \overset{\circ}{t}) &= \overset{\circ}{\mathbf{g}}, & \dot{x}_{i,A}(\mathbf{X}', \overset{\circ}{t}) &= A_{iA}, \\
 \dot{x}_{i,AB}(\mathbf{X}', \overset{\circ}{t}) &= B_{iAB}, & \dot{\theta}(\mathbf{X}', \overset{\circ}{t}) &= a, & \dot{g}_i(\mathbf{X}', \overset{\circ}{t}) &= a_i, \\
 d_{i,AB}^\alpha(\mathbf{X}', \overset{\circ}{t}) &= C_{iAB}^\alpha. & & & & (4.17)
 \end{aligned}$$

Now using (4.10) and (3.12) we see that  $\xi^\alpha$  may be regarded as a function of the form

$$\xi^\alpha = \hat{\xi}^\alpha(\mathbf{F}, \mathbf{d}^\alpha, \mathbf{D}^\alpha, \theta, \mathbf{g}). \quad (4.18)$$

And from (4.11)

$$\dot{d}_i^\alpha = \dot{x}_{i,A} X_{A,j} d_j^\alpha - \xi_i^\alpha. \quad (4.19)$$

Hence,

$$\dot{d}_i^\alpha(\mathbf{X}', \overset{\circ}{t}) = A_{iA} \overset{\circ}{F}_{Aj}^{-1} \overset{\circ}{d}_j^\alpha - \hat{\xi}_i^\alpha(\overset{\circ}{\mathbf{F}}, \overset{\circ}{\mathbf{d}}{}^\alpha, \overset{\circ}{\mathbf{D}}{}^\alpha, \overset{\circ}{\theta}, \overset{\circ}{\mathbf{g}}). \quad (4.20)$$

Also, using (4.19) again, we find

$$\begin{aligned}
 \dot{d}_{i,K}^\alpha(\mathbf{X}', \overset{\circ}{t}) &= B_{iAK} \overset{\circ}{F}_{Aj}^{-1} \overset{\circ}{d}_j^\alpha + \overset{\circ}{F}_{Aj}^{-1} \overset{\circ}{D}_{jK}^\alpha A_{iA} \\
 &\quad - \left. \frac{\partial \hat{\xi}_i^\alpha}{\partial d_j^\beta} \right|_0 \overset{\circ}{D}_{jK}^\beta - \left. \frac{\partial \hat{\xi}_i^\alpha}{\partial D_{jA}^\beta} \right|_0 C_{jAK}^\alpha - \left. \frac{\partial \hat{\xi}_i^\alpha}{\partial \theta} \right|_0 \overset{\circ}{g}_j \overset{\circ}{F}_{jK}, \quad (4.21)
 \end{aligned}$$

where the symbol  $|_0$  indicates that the preceding function is to be evaluated at  $(\mathbf{X}', \overset{\circ}{t})$ .

Now in (4.21)  $B_{iAK}$ ,  $C_{iAK}^\alpha$  are tensors which have been chosen arbitrarily (except for symmetry in the last two suffixes). But it does not necessarily follow that values of these tensors can be found which give an arbitrary set of values  $\dot{d}_{i,K}^\alpha(\mathbf{X}', \overset{\circ}{t})$ . Certain values of the coefficients of these tensors in (4.21) may give restrictions on the possible values of  $\dot{d}_{i,K}^\alpha(\mathbf{X}', \overset{\circ}{t})$ . However, we exclude these special cases from our consideration and assume that the form of (4.21) always permits an arbitrary choice of  $\dot{d}_{i,K}^\alpha(\mathbf{X}', \overset{\circ}{t})$ . If this assumption were not made the form of  $\Psi$  could be made slightly more general than that used below.

Using (4.17) (4.19) and (4.21), we see that for the admissible process determined by (4.16), the values of  $\dot{\theta}$ ,  $\mathbf{d}^\alpha$ ,  $\mathbf{D}^\alpha$ ,  $\mathbf{g}$  at  $(\mathbf{X}', \overset{\circ}{t})$  in eq (4.13) are arbitrary while all other terms in the equation are fixed by the choice of  $\{\overset{\circ}{\mathbf{F}}, \overset{\circ}{\mathbf{d}}{}^\alpha, \overset{\circ}{\mathbf{D}}{}^\alpha, \overset{\circ}{\theta}, \overset{\circ}{\mathbf{g}}\}$ . Hence in virtue of (4.4) we must have,

$$\eta = -\frac{\partial \Psi}{\partial \theta}, \quad S_{iA} = \frac{\partial \Psi}{\partial x_{i,A}} + \frac{\partial \Psi}{\partial d_i^\alpha} d_j^\alpha X_{A,j}, \quad \frac{\partial \Psi}{\partial D_{ik}^\alpha} = 0, \quad \frac{\partial \Psi}{\partial g_i} = 0, \quad (4.22)$$

$$\frac{\partial \Psi}{\partial d_i^\alpha} \xi_i^\alpha - \frac{g_i q_i}{\rho \theta} \geq 0. \quad (4.23)$$

And the energy equation (4.2) reduces to

$$-\rho \frac{\partial \Psi}{\partial d_i^\alpha} \dot{\xi}_i^\alpha + \rho \theta \dot{\eta} + q_{i,i} = \rho r. \quad (4.24)$$

## V. Material Indifference

In addition to the requirements of the laws of thermodynamics the constitutive equations are also subject to the restrictions of the principle of material frame indifference. (For a discussion of this principle see Truesdell and Noll [4] p. 44). To use this principle we consider a second motion of the continuum in which the particle  $\mathbf{X}$  has position vector  $\mathbf{x}^*$  at time  $t$  given by

$$x_i^* = Q_{ij}(t)x_j + c_i(t) \quad (5.1)$$

where  $Q_{ij}(t)$  is an arbitrary time-dependent proper orthogonal tensor,  $c_i(t)$  is an arbitrary time-dependent vector and  $x_i$  is given by (2.1). It follows that

$$x_{i,A}^* = Q_{ij}x_{j,A} \quad (5.2)$$

and we assume that the other variables appearing in the constitutive equations transform as follows:

$$d_i^{*\alpha} = Q_{ij}d_j^\alpha, \quad \theta^* = \theta, \quad \Psi^* = \Psi, \quad T_{ij}^* = Q_{ir}Q_{js}T_{rs},$$

$$\eta^* = \eta, \quad q_i^* = Q_{ij}q_j, \quad v_i^{*\alpha\beta} = Q_{ij}v_j^{\alpha\beta}. \quad (5.3)$$

Using these relations it can be shown that

$$\Psi = \bar{\Psi}(x_{i,A}x_{i,B}, d_i^\alpha x_{i,A}, \theta). \quad (5.4)$$

(See for example Green, Naghdi, and Rivlin [15]. Or equivalently, we may write

$$\Psi = \tilde{\Psi}(d_i^\alpha x_{i,A}, d_i^\alpha d_i^\beta, \theta). \quad (5.5)$$

Hence, using (5.5) and writing

$$f_A^\alpha = d_i^\alpha x_{i,A}, \quad g^{\alpha\beta} = d_i^\alpha d_i^\beta, \quad (5.6)$$

we see that the constitutive equations (4.22) must take the form

$$\eta = -\frac{\partial \tilde{\Psi}}{\partial \theta}, \quad (5.7)$$

$$T_{ij} = \rho (x_{j,A} d_i^\alpha + d_j^\alpha x_{i,A}) \frac{\partial \tilde{\Psi}}{\partial f_A^\alpha} + 2\rho d_i^\beta d_j^\alpha \frac{\partial \tilde{\Psi}}{\partial g^{\alpha\beta}}. \quad (5.8)$$

Applying the transformations (5.3) to (4.9) and (4.10) we find that each of the 10 vectors  $\mathbf{q}, \mathbf{v}^{\alpha\beta}$  must satisfy a relation which is most conveniently expressed in tensor notation as

$$\mathbf{f}(\mathbf{QF}, \mathbf{Qd}^\alpha, \mathbf{QD}^\alpha, \theta, \mathbf{Qg}) = \mathbf{Qf}(\mathbf{F}, \mathbf{d}^\alpha, \mathbf{D}^\alpha, \theta, \mathbf{g}). \quad (5.9)$$

Vector functions of this type could be expressed in canonical form using the theory of isotropic invariants but we do not enter into the details here.

The final forms of (4.23) and (4.24) are

$$2(\partial \Psi / \partial g^{\alpha\beta}) d_i^\beta \xi_i^\alpha - g_i q_i (\rho \theta)^{-1} \geq 0, \quad (5.10)$$

$$-2(\partial \Psi / \partial g^{\alpha\beta}) d_i^\beta \xi_i^\alpha + \rho \theta \dot{\eta} + q_{i,i} = \rho r. \quad (5.11)$$

This leads us to define an internal dissipation function

$$\sigma = 2\theta^{-1}(\partial \Psi / \partial g^{\alpha\beta}) d_i^\beta \xi_i^\alpha. \quad (5.12)$$

An interesting special case of the above theory is obtained if we assume that the constitutive equations do not depend on  $\mathbf{F}$ . In this case,

$$T_{ij} = 2\rho d_i^\alpha d_j^\beta \partial \tilde{\Psi} / \partial g^{\alpha\beta}. \quad (5.13)$$

And then incidentally, if the slip velocities were assumed to be identically zero and the directors were initially the base vectors of a coordinate

system over the body, our theory would reduce to elasticity with  $\sigma = 0$ . In any case, with the assumption (5.13) we have

$$\sigma = (\rho\theta)^{-1} T_i^\alpha \xi_i^\alpha \quad (5.14)$$

where

$$T_i^\alpha = T_{ij} e_j^\alpha \quad (5.15)$$

and we note that  $T_i^\alpha |e_i^\alpha|^{-1}$  (no sum) is the traction across the plane containing  $\mathbf{d}^\beta$ ,  $\mathbf{d}^\gamma$  ( $\alpha \neq \beta \neq \gamma \neq \alpha$ ).

Clearly in an isothermal deformation the thermodynamic restriction (5.10) becomes

$$\sigma \geq 0. \quad (5.16)$$

This ensures, for example, that if only one slip vector  $\xi^\alpha$  is non-zero, the component of the slip velocity in the direction of the resultant traction over the slip-plane must be nonnegative.

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## Discussion on Papers by A. C. Eringen and W. D. Claus, Jr., and N. Fox.

TEODOSIU: I would like to make some comments concerning the paper by Professor Eringen and Mr. Claus. As long as we are concerned with developing a theory of continuum mechanics in which new invariant kinematical and dynamical quantities are involved, we can do it in a rather elegant way, and I think we have so far two beautiful examples. One is the theory of micropolar mechanics developed by Green and Rivlin,<sup>1</sup> and the other that of micromorphic materials developed by Eringen and Suhubi.<sup>2</sup> These two theories provide a good framework for developing other general theories of physical phenomena. But if we intend to describe new physical phenomena with these theories, we must be very careful when approaching physical objects to consider the descriptions by people studying such quantities.

I would like to indicate some points which are, in my opinion, not quite clear in this paper, not in the sense of a continuum mechanical theory, but in respect to its relation with the theory of dislocations. First, they consider in the second part of their paper ordinary motion and another, micromorphic motion. It seems to me from the relations presented that this micromorphic motion is nothing but the time dependence of the so-called elastic distortion in dislocation theory. Then, there is an important point which was not presented here, which is that one can always decompose the general motion into two parts which are additive in the linear case and may be written in the non-linear case as a product of two asymmetric matrices, the plastic and elastic distortions. If this is so, then the strain measures presented are no longer correct because they are based on the assumption that the response of the material is completely determined by the elastic part of the deformation, that is by those quantities named in this paper the micromorphic displacements.

In the meantime there is another point which is not quite clear to me: It is true that in previous developments of dislocation theory no asymmetric stress appears, and there is a good reason for this. We do not have in dislocation theory, in fact, a new independent degree of freedom such as a rotation, and as long as we don't have such independent rotations, we are always able to redefine the stress tensor in order to make it symmetrical. So there is no asymmetric part of the stress tensor in dislocation

<sup>1</sup> Green, A., and Rivlin, R., *Arch. Rat. Mech. Anal.* **17**, 113 (1964).

<sup>2</sup> Eringen, A. C., and Suhubi, E. S., *Int. J. Engng. Sci.* **2**, 189 (1964); Suhubi, E. S., and Eringen, A. C., *Int. J. Engng. Sci.* **2**, 389 (1964).

theory, as long as we don't introduce a new rotation. This question has also been discussed some time ago by Professor Kröner. I should, therefore, be interested to know the opinion of the authors about the significance of their asymmetric stress.

The next point I should like to make is about both the papers up for discussion. This is that the usual law of conservation of mass is no longer complete in the theory of moving dislocations. It can be proved that it must be supplemented by the equation:  $\dot{\rho} + \rho \operatorname{Tr} I = 0$ , where  $\rho$  is the mass density in the local natural configuration and  $I$  is the dislocation flux tensor. This was already known in the linear theory and could be proved easily for the non-linear case. If we consider the case of a uniformly moving dislocation density, say, we have a simple relation between the dislocation flux, the dislocation velocity, and the dislocation density. If we specialize this relation for a singular dislocation, then it can be proved, as was shown by Kosevich in the linear case,<sup>3</sup> that one can describe the climb of edge dislocations; and this is a known fact that climb is a non-conservative motion associated with mass defects.

Concerning the paper by Dr. Fox, I have another question. That is whether the directors considered in this theory are material directors or not, because if they *are* material directors then they are completely equivalent to the components of the elastic distortions. If they are not, what significance has the independent motion of these directors with respect to the general motion of the material?

CLAUS: Let me take Dr. Teodosiu's questions in ascending order of complicatedness. First of all, we think we have been careful. As far as identifying terms and so forth, we have a continuum analogue of a body which contains a distribution of dislocations. We are not counting atoms and so forth, and we recognize this can be a tricky business so we have attempted to be careful.

The second point: The conservation of mass equation given by Dr. Teodosiu, I think, simply requires interpretation. A couple of other points needing interpretation, I think, are based not so much on dislocation ideas, but rather the method of micromorphic mechanics in general. Our mass density is an average mass density, and the conservation of mass equation is valid.

The question of asymmetric stress is one which has been frequently discussed in the literature lately. The balance of linear momentum is fine and the question is what is the moment of momentum or angular momentum equation. In the classical case the stress is symmetric. If one includes extra degrees of freedom into the angular momentum equation,

<sup>3</sup> Kosevich, A. M., J. Exptl. Theoret. Phys. **42**, 152 (1962). Usp. Fiz. Nauk **84**, 79 (1964).

we claim that the equation leads to a non-symmetric stress tensor, whether it is a couple stress or a stress moment tensor.

SIMMONS: Is there, by the way, a physical example you can give where the energy has this type of rotational dependence?

CLAUS: That is precisely the problem. Everybody these days is looking for situations in which the stress is non-symmetric. In continuum mechanics many people are trying to think along these lines. Some of the areas of promise to be pointed out are liquid crystal experiments where inherently there is a structure to the liquid which could conceivably lead to a non-symmetric stress tensor. Another area is in a body which contains a polarization, and the behavior of that body in an internal field. Many people are trying to look for asymmetries there. But I cannot quote an experimental paper where it has been demonstrated.

Concerning the question about elastic and plastic distortion, the interpretation here is that we have a body with dislocations that are deforming elastically so there is no slip in a lattice sense. There is no plastic deformation taking place; you put loads on the body and get only elastic reactions. Obviously what we are trying to construct is a plasticity theory, and we think we have the beginning of a mechanism to do that. Again the strain arises by looking at the average motion of the center of gravity of the collection we are considering. Starting off with a collection of elements, the center of gravity deforms in a way which is described in the classical fashion. It is the motion of the microelements that we are trying to describe, and through a very tedious process of looking at the motion with respect to the center of gravity and studying the appropriate kinematics we arrive at an elastic non-symmetric strain. That decomposition is a result of the kinematics and not an artificial postulate involving the division of the motion into an elastic and plastic part. Everything is elastic.

ERINGEN: I would also like to answer Dr. Teodosiu. The remarks that I am about to make will, I hope, clarify some of the main points. One of these points is concerned with the strain measures in the present theory. The present theory employs three sets of precisely defined strain measures. One of these is the classical strain tensor, the second one involves the directors, and the third one is a third order strain tensor arising from the deformation of the directors, in terms of which the dislocation density is defined. All these strains are exact; they are non-linear, possessing linear approximations. The material response is neither determined by the elastic strain nor by the microdisplacements alone.

I believe Dr. Teodosiu also missed the crucial point that the dynamical theory introduced here is not intended to be a plasticity theory. Theulti-

mate goal of the present theory is to determine the motions and micromotions by solving an initial-boundary-value problem. Once they are determined, the dislocation density can be calculated in a straightforward manner. This point of view is, perhaps, in clash with the present practices in dislocation theory. In harmony with the long-established traditions in other well-developed fields of continuum physics, I suggest that the continuum dislocation theory should offer a set of field equations subject to a set of well-posed initial and boundary conditions to predict the evolution of the motion and of the dislocations. Present practice in this field requires that the distribution of a second-order tensor (the dislocation density) be given throughout the body at all times in order that we determine another second order tensor, namely, the stress tensor. This is not only unreasonable on logical grounds, but also not feasible experimentally. After all, why not ask for the stress tensor in the first place! When a proper continuum theory is constructed, this problem, I believe, will be reduced to a boundary-initial value problem as in other branches of continuum physics. Our present work contains an attempt in this direction which is concerned only with elastic motions of a body containing dislocations.

[Written comment] Dr. Teodosiu also stated that the law of conservation of mass is not valid in dislocation theory. In this he is wrong, of course. This law is valid for all non-relativistic theories of continua.

FOX: I think my answer to Dr. Teodosiu can be very brief, actually. Your question was, "Do the directors move relative to the material?" The answer is "Yes." This is the whole point of having the slip velocities. The idea that the material can deform relative to the directors gives us a continuum analogue of slip processes.

RIVLIN: As I listened to some of these papers and remarks, I was struck by the fact that the products of research in theoretical physics are quite different from the products of activity in the field of architecture. If you build a small hut on weak foundations, it may perhaps stand. But as a building is developed by adding story after story, if the foundations are weak, it will eventually collapse. In building up a physical theory, the situation is quite different. If the foundations of the theory are weak and there is only one paper on the subject, it is quite easy to demolish the theory. However, as generation after generation of papers is added to the literature of a physical theory, it eventually becomes impossible to get rid of the theory, no matter how weak its foundations.

AUDIENCE: General laughter.

RIVLIN: Now, I will preface the comment I really intended to make by a quotation from the Hunting of the Snark:

“. . . I have said it twice: (at the IUTAM Conferences in Vienna and Freudenstadt in 1966 and 1967, respectively).

“. . . I have said it thrice: (at the conference in Rome in 1968). What I tell you three times is true.”

These remarks are not directed against anybody personally—although they may be at everybody. In my youth, about five years ago, I was myself guilty of the same errors I am about to criticize. In many of the theories of generalized continuum mechanics, there is a tendency to pass from a physical inspiration to continuum statement without any clear indication of the passage from one to the other. For example, in the so-called micropolar theory with which Dr. Claus's paper was concerned, a material is considered which consists of many structural elements, each of which undergoes deformation. Mention was made of the coordinates of the centers of mass of the deformed elements. Then, suddenly there appeared spatial derivatives of these coordinates. Now one cannot take spatial derivatives of functions defined on a discrete set of points—at least not in my kind of mathematics. So, somewhere a passage has been made from functions defined on a discrete set of points to continuous and, indeed, differentiable functions defined throughout a region of space. Now, as soon as one begins to think about the manner in which this passage might be made, one realizes that it cannot be made in a unique fashion. For example, averaging procedures might be used, interpolation procedures and so on. The spatial derivatives take on quite different meanings and values depending on how this passage is made. In some of these ways of carrying out the passage from functions defined on a discrete set of points to functions defined over a region of space, the derivatives are quite meaningless. In others they have a more limited meaning than is attached to them by their users. In all events, one cannot pass from the discrete model to a continuum by saying, “We just smooth it,” however engagingly this may be said.

ERINGEN: [Written contribution] That was a most entertaining diatribe. Since it was directed to “everybody” we should let “everybody” reply. However, reference has been made to micropolar theory with accusations that partial differentiations were carried out on functions defined at discrete points. Neither in this nor any other of our previous publications concerned with this topic has such been the case. It is true that Dr. Claus's presentation here emphasized the physical motivation of the theory in terms of discrete elements. However, the mathematics of both the present paper and the previous ones are innocent of such accusations.

With regard to the averaging procedure here questioned, I have also said several times; on one of these occasions (which took an hour at Freuden-

stadt in 1967), Professor Rivlin told me that he understood completely the points that he has raised here today—at least he then said so—and expressed his thanks. But, once again I am obliged to tell you that it is true: the micropolar theory is a rational continuum theory based on proper postulates, thermodynamics, and uniqueness theorems. Any reference to discrete elements is only motivational to exhibit its physical basis. Equations of motion of the theory were already given to us in 1962<sup>4</sup> (pp. 104, 124, 125). The theory was fully developed in 1964 at the end of a sequence of two papers,<sup>2</sup> especially Art. 6 in the second, as a special case of the theory of microelastic solids. Recapitulations of the theory based on proper postulates, thermodynamics, and uniqueness theorems are to be found in later reviews.<sup>5</sup>

The micromorphic theory—which Professor Rivlin apparently confuses with the micropolar theory—was first introduced in 1964,<sup>2</sup> and extended in a series of papers in subsequent years. We make a brief mention of one paper<sup>6</sup> where the general micromorphic theory of all grades was derived under postulates and theorems. In these works various volume and surface averages and moments are introduced through integrals defined over the surface and volume of the body. The integrands of these integrals contain piecewise continuous functions (stress, body force, etc.) which are multiplied by infinitely differentiable functions. The averages and moments generated by these integrals are continuously differentiable at all points of the body at all times, except possible at some singular surfaces, lines, and points which may be present in the body. Again I repeat, no differentiation has been carried on functions defined at discrete points. Careful and precise as they are in their definitions, these concepts are used for motivational purposes. The balance laws so motivated systematically may just as well be considered as postulates of the theory, as practiced in all other branches of continuum mechanics.

The authors of several hundred papers, which have appeared on the subject since the reception of our work in 1964, seem to have understood this point very clearly. I believe that any competent scholar who will take the time to read these papers as well as to examine the figures in the texts will find no reason to disagree with our theory.

KRÖNER: I completely agree with Professor Rivlin that we need to be as exact as possible in mathematics to make the transition from discrete

<sup>4</sup> Eringen, A. C., in *Nonlinear Theory of Continuous Media* (McGraw-Hill, New York, 1962).

<sup>5</sup> Eringen, A. C., *J. Math. and Mech.* **15**, 909 (1966). Eringen, A. C., in *Fracture II*, H. Liebowitz, Ed. (Academic Press, New York, 1968), Chapter 7, especially Arts. XVII to XXIII.

<sup>6</sup> Eringen, A. C., in *Mechanics of Generalized Continua*, E. Kröner, Ed., (Springer-Verlag, Berlin, 1968).

particles to the continuum. With regard to our work, you may recall from the previous session that we use the Euler-MacLaurin formula, although there may be other ways to do it. But, I think this is a crucial point in constructing continuum theories.

Now I would like to address a short question to Dr. Fox. Are your particles atoms or are they little crystal domains?

FOX: They are the same particles that we use throughout continuum mechanics. I am not *at this stage* giving any interpretation of them. They are points within a continuous body and associated with each point I am taking directors.

KRÖNER: When you want to apply your theory to physics you must identify your particles with something physically real, and then you must decide whether your particles are atoms or domains. And, I think you must consider domains because a single atom has no direction, so your particles can only be little crystalline domains. Is that true?

FOX: But I'm deriving a continuum theory and it must stand or fall on what it predicts at a macroscopic level. For instance, in hydrodynamics, one predicts what happens at a macroscopic level; one predicts flows. In the same sense I suggest that this theory will predict certain behavior of crystalline materials at a macroscopic level.

SIMMONS: I think we are uncovering here a fundamental difference in philosophy between the viewpoint of continuum mechanics and that of solid state physics.

KRÖNER: Well, eventually, Dr. Fox, you must construct your constitutive equations from a knowledge of the constitution of the body. And the body is made up of atoms.

FOX: No, I am *not* constructing my constitutive equations from statistical theories. And my particles are mathematical points, they are not domains. I model the structure with directors.

KRÖNER: Well, let's forget this. I would like to make clear why the skew symmetric stress does not appear in dislocated bodies. Assume particles which are little crystalline domains, for instance little cubes which build up a perfect crystal. Now imagine two of these particles to be isolated from the rest and be rotated through the same angle (fig. 1a). By this operation the atomic structure is not disturbed and the state of the crystal along the interface between the particles is not changed. So there is no statical response to this kind of deformation and that is why the skew symmetric part of the ordinary stresses vanishes in dislocation theory.

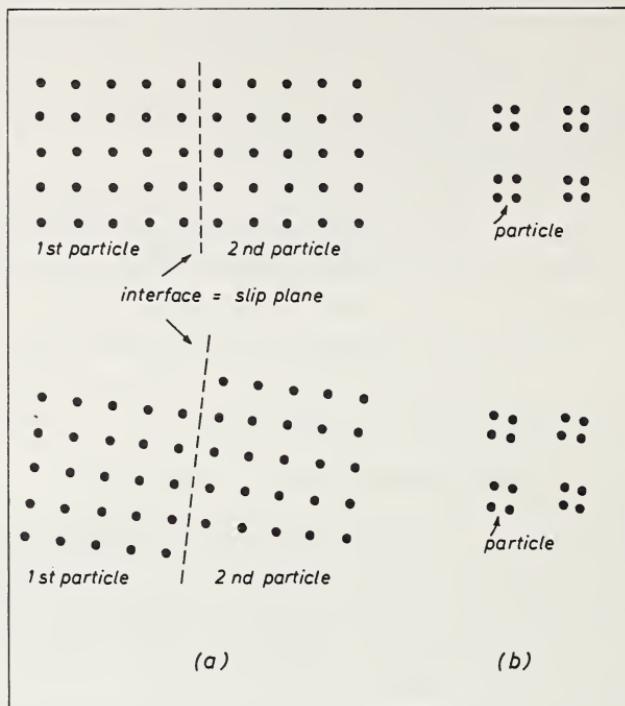


FIGURE 1. (a) Two adjacent "particles" of a crystalline body before and after a rotation through the same angle. This kind of rotation implies the slip of a dislocation along the interface. It *does not* change the *state* of the crystal. (b) Four adjacent "particles" of a Cosserat type material before and after a rotation through the same angle. This kind of rotation *does* change the *state* of the body.

It does not vanish in Cosserat type theories where one considers oriented point particles which do not possess a crystalline structure (fig. 1b). Such bodies could be, for instance, non-primitive crystal lattices where the atoms in a cell are so tightly bound that the deformation of a cell can be disregarded whereas the bonds between the cells are weak. In this example the cells are the particles of the Cosserat continuum; they possess the usual translational and rotational degrees of freedom. Now rotate these particles through the same angle and the body is in a different state. So you expect a response.

I call the body described firstly a *dislocated body* and the other a *Cosserat continuum*. In the dislocated body one observes the occurrence of slip because the above described rotation of the two crystalline domains implies the slip of a dislocation along the interface between them. Slip has no meaning in the usual Cosserat continuum.

FOX: May I just reply to that statement? I can only repeat that my particles are not domains, they are points. And on couple stresses, certainly I did not include in my energy equation possible generalizations which arise from the inertia associated with the directors or possible higher order stresses. This can be done. There is no difficulty in principle; I just omitted them for simplicity.

KRÖNER: Let me also ask this. You said you make no reference to differential geometry. Now, some of the fundamental equations of dislocation theory are the incompatibility equations which are equations of differential geometry if you formulate them in the general non-linear way. Now, if you don't have equations like these, then you can't solve actual problems with internal stresses. Do some of your equations correspond to the incompatibility conditions or is your theory still incomplete in this respect?

FOX: No, it's not incomplete in this respect. What I said was that I could formulate the theory without using the geometry of higher spaces. You can put this interpretation on the director theories if you wish; it is there as an interpretation. All I am saying is that you don't have to start with it and I don't think it's fundamental to the formulation of the theory.

KRÖNER: Yes, but I think the dislocation concept is, by definition, a differential geometric notion. So, I don't see any point in emphasizing that you don't need differential geometry. In some way it must be in your formulation.

SIMMONS: May I insert a brief remark here. In a static development done by Dr. Bullough and myself,<sup>7</sup> we used an approach which is effectively equivalent to that of Dr. Fox, although we have emphasized deformations throughout, rather than the director concepts. If you do that, you can introduce the idea of a reference connection—the Euclidean connection—in the undeformed state. When the body is deformed, one can define the deformation of the connection also. Then the incompatibility conditions come out merely from the study of the deformed connection in the deformed state. So it's possible to get the incompatibility equations from Dr. Fox's theory—at least in the static situation and, no doubt, in the dynamic one also.

FOX: Oh, you can do it all right. It's just a matter of looking at the geometry of the directors. I just don't think this is relevant to producing the constitutive equations.

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<sup>7</sup> Bullough, R., and Simmons, J. A., in *Physics of Strength and Plasticity*, A. Argon, Ed. (MIT Press, Cambridge, Mass., 1969) p. 47.

SIMMONS: I'm not sure exactly what you mean by constitutive equations, but it's necessary for solving problems, because these provide generalized continuity conditions, if you will.

KRÖNER: I did not want to criticize Dr. Fox's theory: I think it is a beautiful theory. Also it may well work just as well as other theories, or even better, if one knows the mathematics well enough. Actually, I am pleased that so many people from continuum mechanics and mathematics are now interested in dislocation theory. Their contributions may, eventually, help us to solve our problems.

Finally, you have emphasized that Noll had introduced local reference lattices, or configurations, or whatever. These also appear in papers by Kondo and by Bilby and coworkers which were published in the early fifties. .

# VIII THERMALLY ACTIVATED PROCESSES AND STATISTICAL THEORIES

*Chairman:*

A. SEEGER



# DISLOCATION DYNAMICS IN THE PRESENCE OF A MULTIPLE SPECTRUM OF THERMALLY SURMOUNTABLE BARRIERS

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A theoretical treatment is given of the thermally activated motion of dislocations in the presence of dislocation barriers with different heights. The height of a barrier is allowed to depend on an arbitrary number of characteristic parameters (multiple obstacle spectrum). Under the assumptions which are usually made for the derivation of an Arrhenius equation for the slip rate  $\dot{a}$  in the case of a uniform array of dislocation barriers,  $\dot{a}$  is calculated for a multiple spectrum of barriers. It is found that even under these conditions the validity of an Arrhenius equation  $\dot{a} = \dot{a}_0 \exp(-\Delta\overline{G}/kT)$  ( $\dot{a}_0 = \text{const.}$ ,  $\Delta\overline{G}$  = mean free enthalpy of activation) is preserved. An application of the "spectrum theory" is discussed.

Key words: Arrhenius rate theory; dislocation dynamics; statistical theory of dislocation; thermal acceleration.

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## I. Introduction

Macroscopic deformation of a crystal is connected with the properties of the individual glide dislocations by the relation

$$\dot{\epsilon} = \sum_i \Gamma_i \eta_i \dot{a}_i = \sum_i \Gamma_i \eta_i b_i \rho_i \bar{v}_i, \quad (1.1)$$

where  $\dot{\epsilon}$  is the macroscopic deformation rate,  $b_i$  the strength,  $\rho_i$  the density, and  $\bar{v}_i$  the mean velocity of mobile  $i$ -type dislocations.  $\eta_i$  is a geometrical factor which projects the resolved slip rate

$$\dot{a}_i = b_i \rho_i \bar{v}_i \quad (1.2)$$

of  $i$ -type dislocations to the direction in which the macroscopic deformation rate is measured.  $\Gamma_i$  means a relative active slip volume, i.e., the crystal fraction which is actually deformed by gliding of  $i$ -type dislocations. For sake of simplicity we assume homogeneous deformation ( $\Gamma_i = 1$ ) and

restrict ourselves to one type of glide dislocations with an  $\eta_i$ -factor equal to unity. Then eq (1.1) is reduced to

$$\dot{\epsilon} = \dot{a} = b\rho\bar{v}. \quad (1.3)$$

Moreover, we shall consider a steady state of deformation in which the production rate of mobile dislocations by sources cancels the rate of annihilation and immobilization of dislocations ( $\rho = \text{const}$ ). Consequently, the following theory cannot account for phenomena involving a change of the dislocation density, such as work-hardening. The problem which is left is the determination of the mean dislocation velocity  $\bar{v}$  from the properties of individual glide dislocations by means of statistical methods. In the present paper a solution will be presented for the case of dislocations moving through a crystal under the action of a locally constant effective stress  $\tau$  in the presence of thermally surmountable barriers with different heights. At first, however, a quasi-regular arrangement of uniform dislocation obstacles will be treated, in order to introduce the most relevant notations.

## II. Quasi-Regular Arrangement of Uniform Dislocation Obstacles

A quasi-regular arrangement is defined as an array of obstacles for which the *geometrical* activation parameters do not vary from one activation event to another. Examples for geometrical activation parameters are the separation  $l$  between neighbouring barriers along the dislocation lines, the distance  $\lambda$  covered by a dislocation between subsequent activation events, and the separation  $\delta$  of the obstacle centres from the slip planes. Even if all obstacles are uniform, the condition for quasi-regularity can be hardly fulfilled rigorously for  $l$ ,  $\lambda$ , and  $\delta$  at the same time. For a random array there are natural distribution widths of  $l$  and  $\lambda$ , whereas the distribution of  $\delta$  is determined by the range of the obstacle-dislocation interaction. In a regular array the condition for quasi-regularity is satisfied for  $l$  and  $\lambda$ ; for  $\delta$  it will be approximately fulfilled if the obstacle-dislocation interaction range is small compared with the minimum separation between the slip planes. Then, only those obstacles act as actual barriers which lie directly on the slip planes.

Pegel [1] derived a criterion which permits to decide in which cases quasi-regularity is a good approximation. If  $x$  represents an activation parameter,  $w(x)$  its distribution probability, and  $v(x)$  the velocity of an individual dislocation, the mean dislocation velocity  $\bar{v}$  as a function of  $x$  is given by

$$\bar{v} = \int v(x)w(x)dx = v(\bar{x}) + \frac{1}{2} \frac{\partial^2 v}{\partial x^2}(\bar{x}) \overline{(x - \bar{x})^2} + \dots \quad (2.1)$$

$\bar{v} \approx v(\bar{x})$ , if the mean square  $\overline{(x-\bar{x})^2}$  of the distribution width of  $x$  is sufficiently small. Thus, an array of obstacles may be called quasi-regular, if this condition is fulfilled for the *geometrical* activation parameters. If this condition holds for *all* activation parameters, we are concerned with a quasi-regular array of uniform obstacles.

Now we proceed to the calculation of  $\bar{v}$ , at first *without* the restriction to quasi-regularity and uniformity.—If the mobility of dislocations is controlled by surmountable local barriers, the mean dislocation velocity may be written as

$$\bar{v} = \bar{v}\bar{\lambda}, \quad (2.2)$$

where  $\bar{\lambda}$  is the mean value of  $\lambda$  and  $\bar{v}$  the mean jump frequency of dislocations over barriers.

The individual barriers will be described by waiting times  $t(P; \tau, T)$  for the glide dislocations:

$$t(P; \tau, T)^{-1} = \nu_0(P; \tau, T) \exp [-\Delta G(P; \tau, T)/kT] \quad (2.3)$$

( $k$  = Boltzmann's constant;  $\nu_0(P; \tau, T)$  = attempt frequency of a dislocation for overcoming an obstacle, which is characterized by a set  $P$  of parameters, at the effective stress  $\tau$  and the deformation temperature  $T$ ;  $\Delta G(P; \tau, T)$  = free enthalpy which must be supplied by thermal lattice vibrations, in order to push a dislocation over an obstacle  $P$ ). According to Schöck [2] we have

$$\Delta G(P; \tau, T) = \Delta g(P; \tau, T) - b\bar{l}(\tau, T)\Delta x(P; \tau, T)\tau. \quad (2.4)$$

Herein,  $\Delta g(P; \tau, T)$  and  $b\bar{l}(\tau, T)\Delta x(P; \tau, T)\tau$  mean the work done over the activation distance  $\Delta x(P; \tau, T)$  against the dislocation-obstacle interaction force and by the effective external stress  $\tau$ , respectively ( $\bar{l}$  = mean value of  $l$ ). At this point we have assumed that  $\overline{(l-\bar{l})^2}$  is sufficiently small, in order to replace  $\Delta G(l)$  by  $\Delta G(\bar{l})$ . This condition is less stringent than the assumption of quasi-regularity, which requires the smallness of  $\overline{(x-\bar{x})^2}$  for all geometrical activation parameters.

Within the framework of the string model for a dislocation the attempt frequency has been calculated [3, 4] to

$$\nu_0(P; \tau, T) = b\nu_D \alpha(P)/2\bar{l}(\tau, T), \quad (2.5)$$

where  $\nu_D$  is the Debye frequency and  $\alpha(P)$  a numerical factor, which depends only weakly on the properties  $P$  of the obstacles ( $1.8 \lesssim \alpha(P) < 2$ ) [3]. Therefore, we put approximately

$$\nu_0(P; \tau, T) \approx \frac{b\nu_D}{\bar{l}(\tau, T)} \equiv \bar{\nu}_0(\tau, T). \quad (2.6)$$

Thus, eq (2.3) is simplified to

$$t(P; \tau, T)^{-1} = \bar{\nu}_0(\tau, T) \exp [-\Delta G(P; \tau, T)/kT]. \quad (2.7)$$

Hence, an obstacle is characterized completely by its  $\Delta G(P; \tau, T)$ -value.

In the special case of a quasi-regular array of uniform obstacles, with which we are mainly concerned in this section, all  $t(P; \tau, T)$ -values are identical. This leads to

$$\bar{\nu}(\tau, T) = t(P; \tau, T)^{-1} = \bar{\nu}_0(\tau, T) \exp [-\Delta G(P; \tau, T)/kT]. \quad (2.8)$$

Combination of the eqs (1.3), (2.2), (2.6), and (2.8) yields

$$\dot{a} = b^2 \rho \nu_D \frac{\bar{\lambda}(\tau, T)}{\bar{l}(\tau, T)} \exp [-\Delta G(P; \tau, T)/kT]. \quad (2.9)$$

Conveniently,

$$\lambda(\tau, T) \approx \bar{l}(\tau, T) \quad (2.10)$$

is assumed. Then we are left with the Arrhenius equation

$$\dot{a} = \dot{a}_0 \exp [-\Delta G(P; \tau, T)/kT] \quad (2.11)$$

for the deformation rate  $\dot{a}$ . Therefore,  $\dot{a}_0$  means the abbreviation

$$\dot{a}_0 = b^2 \rho \nu_D, \quad (2.12)$$

which is a constant.

### III. Multiple Spectrum of Dislocation Barriers

#### III.1. Definitions and assumptions

An array of dislocation obstacles is called a *spectrum* of barriers if they differ with respect to their heights for moving dislocations. If the heights of barriers depend on a set  $P$  of parameters, namely on  $m$  continuously varying parameters  $p_1, \dots, p_m$  and on  $n$  discrete variables  $q_1, \dots, q_n$ , we denote such an arrangement a *multiple* spectrum of barriers. We shall demonstrate in the following that in the presence of a multiple spectrum

of barriers the deformation rate  $\dot{a}$  is given by an Arrhenius equation provided that the subsequent conditions are satisfied:

1. An individual activation event is characterized completely by a waiting time  $t(P; \tau, T)$  which is given by an Arrhenius-type eq (2.3).
2. It must be possible to define a mean value  $\bar{l}$  of  $l$  for which  $(l - \bar{l})^2$  is sufficiently small, in order to replace  $\Delta G(l)$  by  $\Delta G(\bar{l})$ , i.e., eq (2.4) is assumed to be valid.
3. The attempt frequency does not depend explicitly on  $P$ :

$$\nu_0(P; \tau, T) \approx \bar{\nu}_0(\tau, T) \equiv \frac{b\nu_D}{l(\tau, T)}. \quad (2.6)$$

$$4. \quad \bar{\lambda}(\tau, T) \approx \bar{l}(\tau, T). \quad (2.10)$$

These assumptions are exactly the same as those which have been made for the derivation of the Arrhenius eq (2.11) in the case of a quasi-regular array of uniform obstacles.

### III.2. Historical remarks

Thermally activated motion of dislocations in the presence of a spectrum of barriers has been treated theoretically by Wyatt [5], Basinski [6], Diehl and co-workers [7], and Kocks [8].

Wyatt and Basinski assumed the activation events at different obstacles to be alternative processes. Hence, in order to obtain the *mean jump frequency*  $\bar{\nu}$ , they added the obstacle-characteristic jump frequencies. Diehl et al. recognized that the assumption of consecutive activation events at spatially separated obstacles and thus a summation of obstacle-characteristic waiting times to a mean waiting time should be a better approach. Finally, Kocks treated the case in which the flow stress is controlled by two types of barriers by assuming that the dislocations have to go through both kinds of obstacles at the same time so that the waiting time is the same for both barriers. This model is far from reality if the dislocations behave like flexible strings, but it will be a useful description in cases where the dislocations may be regarded as stiff rods.

Besides the determination of the mean dislocation jump frequency another problem arises for a spectrum of obstacles, namely the calculation of the *mean effective separation*  $\bar{l}$  of obstacles. It has been treated in a qualitative way for a single spectrum of obstacles by Diehl et al. [7], while Kocks [8] was concerned with the special case of two types of obstacles with  $l_1 \gg l_2$ .

In the subsequent sections we shall present a general theory which permits the calculation of  $\bar{\nu}$  (sect. III.3) and  $\bar{l}$  (sect. III.4) for a multiple spectrum of barriers provided that the conditions compiled in section III.1 are satisfied.

### III.3. Mean dislocation jump frequency $\bar{\nu}(\tau, T)$

#### A. DISTINCTION BETWEEN "SOFT" AND "HARD" OBSTACLES

In the following it turns out to be useful to distinguish between "soft" and "hard" obstacles which are defined by

$$t(P; \tau, T)^{-1} \geq \bar{\nu}(\tau, T), \quad (3.1)$$

respectively. For "intermediate" obstacles we may put

$$t(P; \tau, T)^{-1} = \bar{\nu}(\tau, T). \quad (3.2)$$

Under the assumptions 1 to 4 in section III.1, eq (3.2) is equivalent to

$$\Delta G(P; \tau, T) = kT \ln \frac{\dot{a}_0}{\dot{a}} \quad (3.3)$$

with

$$\dot{a}_0 = b^2 \rho \nu_D. \quad (3.4)$$

Correspondingly, the conditions (3.1) for soft and hard obstacles are reformulated:

$$\Delta G(P; \tau, T) \leq kT \ln \frac{\dot{a}_0}{\dot{a}}. \quad (3.5)$$

Now we shall have a look at the physical meaning of the distinction between soft and hard obstacles. In a steady state of plastic flow, segments of a mobile dislocation which are stopped at hard obstacles lag behind the mean dislocation front, while segments at soft obstacles are ahead of it (fig. 1). Thus overcoming of a hard obstacle is an alternative process to the passing of spatially neighbouring barriers. Surmounting of

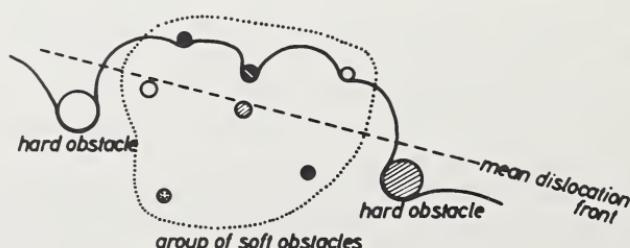


FIGURE 1. Distinction between "soft" and "hard" dislocation barriers.

a group of soft obstacles, however, is mainly controlled by the relatively hardest obstacles of the group, since the activation events within the group are consecutive processes. Therefore, the mean waiting time  $t_s(\tau, T)$  at a "soft" group has to be calculated by a summation over the waiting times characterizing the individual events within the group.  $\bar{\nu}(\tau, T)$  itself is obtained by addition of the  $t_s(\tau, T)^{-1}$ -values of the soft groups and the  $t(P; \tau, T)^{-1}$ -values of the various hard obstacles.

### B. MEAN WAITING TIME $t_s(\tau, T)$ AT A SOFT GROUP

According to the qualitative considerations in the preceding section, the mean waiting time at a soft group is given by

$$t_s(\tau, T) = \frac{\sum_{q_1} \cdots \sum_{q_n} \int_{p_1=0}^{\infty} \cdots \int_{p_{m-1}=0}^{\infty} \int_{p_m=0}^{p_m^*} t(P; \tau, T) N(P; \tau, T) dp_1 \dots dp_m}{\sum_{q_1} \cdots \sum_{q_n} \int_{p_1=0}^{\infty} \cdots \int_{p_{m-1}=0}^{\infty} \int_{p_m=0}^{p_m^*} N(P; \tau, T) dp_1 \dots dp_m}, \quad (3.6)$$

where  $N(P; \tau, T) dp_1 \dots dp_m$  is the effective differential obstacle density per unit area of the slip planes in the intervals  $(p_1, p_1 + dp_1), \dots, (p_m, p_m + dp_m)$  of the continuous parameters  $p_i$  and at the values  $q_1, \dots, q_n$  of the discrete variables  $q_j$ . In eq (3.6) it is assumed that the "hardness"  $\Delta G(P; \tau, T)$  of the obstacles increases monotonously with increasing values of  $p_m$ . The upper limit  $p_m^*$  of the integral over  $p_m$  is the solution of eq (3.3) for  $p_m$  and therefore depends on  $p_1, \dots, p_{m-1}, q_1, \dots, q_n, \tau$ , and  $T$ . Thus, the cutting-off of the integration over  $p_m$  at  $p_m = p_m^*$  ensures that only soft obstacles are taken into account in the calculation of  $t_s(\tau, T)$ .

### C. CALCULATION OF $\bar{\nu}(\tau, T)$

If the effective integral densities per unit area of the slip planes for soft obstacles, hard obstacles, and soft groups are

$$N_s(\tau, T) = \sum_{q_1} \cdots \sum_{q_n} \int_{p_1=0}^{\infty} \cdots \int_{p_{m-1}=0}^{\infty} \int_{p_m=0}^{p_m^*} N(P; \tau, T) dp_1 \dots dp_m, \quad (3.7)$$

$$N_h(\tau, T) = \sum_{q_1} \cdots \sum_{q_n} \int_{p_1=0}^{\infty} \cdots \int_{p_{m-1}=0}^{\infty} \int_{p_m=p_m^*}^{\infty} N(P; \tau, T) dp_1 \dots dp_m, \quad (3.8)$$

and

$$G_s(\tau, T) = \frac{N_s(\tau, T) \cdot N_h(\tau, T)}{N_s(\tau, T) + N_h(\tau, T)}, \quad (3.9)$$

respectively,  $\bar{\nu}(\tau, T)$  may be expressed as

$$\begin{aligned}\bar{\nu}(\tau, T) = & \frac{1}{G_s(\tau, T) + N_h(\tau, T)} \left[ t_s(\tau, T)^{-1} G_s(\tau, T) \right. \\ & + \sum_{q_1} \cdots \sum_{q_n} \int_{p_1=0}^{\infty} \cdots \int_{p_{m-1}=0}^{\infty} \int_{p_m=p_m^*}^{\infty} \\ & \left. t(P; \tau, T)^{-1} N(P; \tau, T) dp_1 \cdots dp_m \right].\end{aligned}\quad (3.10)$$

By these equations the calculation of  $\bar{\nu}(\tau, T)$  is reduced to a computation of  $N(P; \tau, T) dp_1 \cdots dp_m$ , which is performed in the subsequent section.

### III.4. Mean effective separation $\bar{l}(\tau, T)$ between obstacles

The relation between  $\bar{l}(\tau, T)$  and the total effective integral density

$$N(\tau, T) = N_s(\tau, T) + N_h(\tau, T) \quad (3.11)$$

of obstacles is rather complex even in the case of uniform obstacles [9, 10, 11, 12]. As discussed elsewhere [13], for a multiple spectrum of obstacles it is completely hopeless neither to derive an exact analytical expression connecting  $\bar{l}(\tau, T)$  and  $N(\tau, T)$  nor to give an approximate relation which is better than the conveniently used formula

$$\bar{l}(\tau, T) \approx 1/\sqrt{N(\tau, T)}. \quad (3.12)$$

Therefore, for applications of the theory the use of eq (3.12) is proposed. It has been successfully applied to an example, which will be discussed in section IV. It should be emphasized, however, that the validity of an Arrhenius equation for the deformation rate  $\dot{a}$ , as demonstrated in the following section, does not depend on the assumption made about the relation between  $\bar{l}(\tau, T)$  and  $N(\tau, T)$ .

By the eqs (3.12), (3.7), and (3.8) the calculation of  $\bar{l}(\tau, T)$  is reduced to that of the effective differential obstacle density  $N(P; \tau, T) dp_1 \cdots dp_m$ . If  $D(P) dp_1 \cdots dp_m$  denotes the actual differential obstacle density and if  $\kappa(P; \tau, T)$  is the probability that a potential obstacle of the type  $P$  is not transparent for dislocations moving at the effective stress  $\tau$  and the temperature  $T$ , we may put

$$N(P; \tau, T) dp_1 \cdots dp_m = 2 \kappa(P; \tau, T) D(P) dp_1 \cdots dp_m. \quad (3.13)$$

The factor of two accounts for the fact that obstacles are located on both sides of the slip planes. The nontransparency factor  $\kappa(P; \tau, T)$  is simply given by

$$\kappa(P; \tau, T) = \frac{\int_{u=0}^{\Delta G(P; \tau, T)} e^{-u/kT} du}{\int_{u=0}^{\infty} e^{-u/kT} du} = 1 - \exp \left[ -\frac{\Delta G(P; \tau, T)}{kT} \right] \quad (3.14)$$

for  $\Delta G(P; \tau, T) \geq 0$ . For  $\Delta G(P; \tau, T) < 0$   $\kappa(P; \tau, T)$  has to be taken equal to zero.

### III.5. Validity of the Arrhenius equation

Since the attempt frequency  $\bar{\nu}_0(\tau, T)$  does not depend explicitly on the properties  $P$  of the obstacles (see eq (2.6)),  $\bar{\nu}(\tau, T)$  may be brought into the form

$$\bar{\nu}(\tau, T) = \bar{\nu}_0(\tau, T) \exp \left[ -\frac{\bar{\Delta G}(\tau, T)}{kT} \right] \quad (3.15)$$

with

$$\exp \left[ -\frac{\bar{\Delta G}(\tau, T)}{kT} \right] = \frac{t'_s(\tau, T)^{-1} G_s(\tau, T) + h(\tau, T)}{G_s(\tau, T) + N_h(\tau, T)}, \quad (3.16)$$

$$t'_s(\tau, T) = N_s(\tau, T)^{-1} \sum_{q_1} \dots \sum_{q_n} \int_{p_1=0}^{\infty} \dots \int_{p_{m-1}=0}^{\infty} \int_{p_m=0}^{p_m^*} \exp \left[ \frac{\Delta G(P; \tau, T)}{kT} \right] \times N(P; \tau, T) dp_1 \dots dp_m, \quad (3.17)$$

and

$$h(\tau, T) = \sum_{q_1} \dots \sum_{q_n} \int_{p_1=0}^{\infty} \dots \int_{p_{m-1}=0}^{\infty} \int_{p_m=p_m^*}^{\infty} \exp [-\Delta G(P; \tau, T)/kT] \times N(P; \tau, T) dp_1 \dots dp_m. \quad (3.18)$$

Under the assumptions of section III.1 a comparison between the eqs (1.3), (2.2), and (3.15) yields

$$\dot{a} = \dot{a}_0 \exp \left[ -\frac{\bar{\Delta G}(\tau, T)}{kT} \right], \quad (3.19)$$

where  $\dot{a}_0$  is the constant defined by (3.4). Hence, even in the presence of a multiple spectrum of dislocation obstacles an Arrhenius equation for the deformation rate  $\dot{a}$  remains valid. It should be noted that the mean free enthalpy  $\overline{\Delta G}(\tau, T)$  of activation which enters this equation is just equal to  $\Delta G(P; \tau, T)$  of those obstacles which were defined as "intermediate" ones at these  $\tau, T$ -values (compare eq (3.19) to (3.3)).

#### IV. Application of the Spectrum Theory

We shall not enter a discussion of the variety of examples to which the spectrum theory is applicable in principle, but shall report on a problem to which it *has* been applied successfully. This is plastic flow of neutron-irradiated copper single crystals [13, 14].

By means of stereo-electron-microscopy the dislocation barriers in copper after neutron irradiation at 80°C were found to be preferentially vacancy dislocation loops of the Frank type on {111} -planes [15]. These loops represent a triple spectrum of barriers, which is characterized by the loop radius  $r$ , the distance  $\delta$  of the centre of a loop from the slip planes, and the discrete orientation parameter  $i$  which distinguishes between the four different types of {111} -planes on which a loop may be located. Obviously, the differential density  $D(r, \delta, i)drd\delta$  of the loops does not depend on  $\delta$  and  $i$ . However, it is a function of the loop radius  $r$ , which has been determined by means of electron microscopy on neutron-irradiated copper foils [16, 17].

Using the  $D(r, \delta, i)drd\delta$ -law obtained in this way and  $\Delta G(r, \delta, i; \tau, T)$ -values calculated by Saxlová [18],  $\dot{a}(\tau, T)$  has been computed from experimental  $\tau, T$ -values [14] according to the spectrum theory [19]. In figure 2 the results are shown for a crystal which has been irradiated with  $4 \cdot 10^{17}$  neutrons/cm<sup>2</sup> (neutron energy  $> 0.1$  MeV,  $\dot{\epsilon} = 3 \cdot 10^{-6}$  s<sup>-1</sup>). The variation of  $\dot{a}/\dot{a}_0$  with the deformation temperature for a constant  $\dot{\epsilon}$ -value is due to the inhomogeneity of the deformation process: A neutron-irradiated copper single crystal shows the expansion of a Lüders band along the crystal length during deformation. This may be described mathematically by eq (1.1) specialized to one type of mobile dislocations,

$$\dot{\epsilon} = \Gamma \dot{a}, \quad (4.1)$$

with a temperature-dependent relative active slip volume  $\Gamma(T)$ , which obviously leads to a temperature dependence of  $\dot{a}(T)$  for a constant macroscopic deformation rate  $\dot{\epsilon}$ .

From the  $\dot{a}/\dot{a}_0$ -values of figure 2 the mean free enthalpy  $\overline{\Delta G}$  of activation was calculated as a function of the deformation temperature with the aid of eq (3.19) (solid curve through the open circles in fig. 3). On the other, the mean enthalpy  $\overline{\Delta H}$  of activation could be determined experimentally

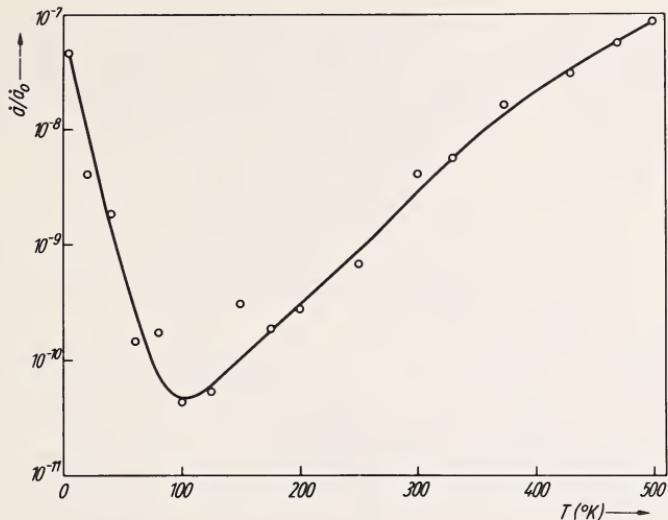


FIGURE 2. Logarithm of  $\dot{\alpha}/\dot{\alpha}_0$  versus deformation temperature  $T$  for  $\dot{\epsilon} = 3.10^{-6} \text{ s}^{-1}$ , calculated by means of the spectrum theory from the temperature dependence of the critical shear stress of copper single crystals after neutron-irradiation [14].

from change-in-strain-rate and change-in-temperature tests [14] (full circles in fig. 3). Since the contribution  $-T\bar{\Delta S}$  by the mean entropy  $\bar{\Delta S}$  of activation is small compared to  $\bar{\Delta H}$  ( $\bar{\Delta S} = (5 \pm 4)k$ ) [13], the "theoretical"  $\bar{\Delta G}$ -values may be directly compared to the "experimental"  $\bar{\Delta H}$ -values (fig. 3). The excellent agreement appears to be particularly noteworthy, since no adjustable parameter enters into the calculations.

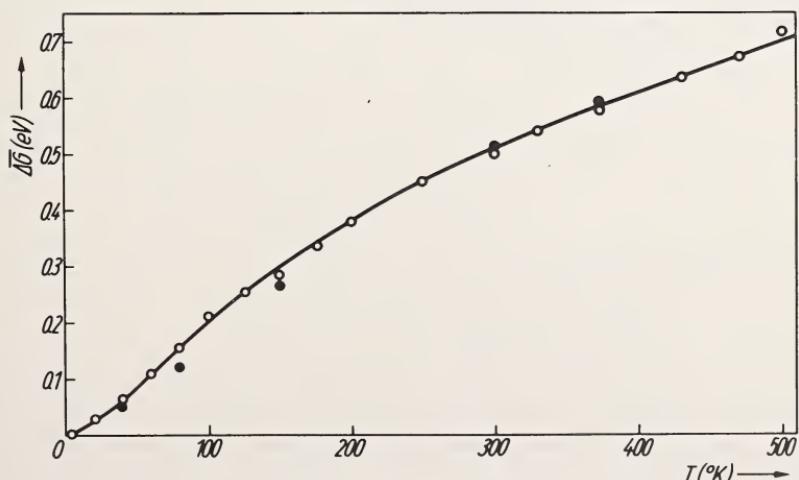


FIGURE 3. Comparison of the "theoretical"  $\bar{\Delta G}$ - $T$  curve obtained from data in figure 2 by means of eq (3.19) (solid curve through the open circles) with "experimental"  $\bar{\Delta H}$ -values determined from change-in-strain-rate and change-in-temperature tests [14] (full circles).

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# FLOW AND THE ARRHENIUS EQUATION IN THE STATISTICAL FRAMEWORK

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The rate equation of plastic flow and a general work-hardening law are combined into a single equation of flow. It degenerates into the Arrhenius law only under certain specified conditions. A single Arrhenius term with temperature insensitive pre-exponential (and entropy) terms adequately describes the rate dependence of dislocation motion through a slip plane studded with obstacles of any spectrum of strengths and spacings. In this case, the mobile dislocation density in the slip plane generally does not enter the flow equation; only the density of slip planes does.

Key words: Arrhenius law; mechanical properties; precipitation hardening; thermal activation.

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## I. The General Equation of Flow

The rate equation of plastic flow, linking strain rate or dislocation velocity to stress and structure, and the work-hardening law, linking flow stress increments to strain increments, are often treated independently of each other. They may be combined into a single equation of flow, with a gain in generality especially for applications to large plastic strains. The general equation of flow to be derived below is similar to a "mechanical equation of state" except that the strain enters only in differential form, and the (dislocation) structure enters explicitly.

The rate determining factor in plastic flow problems is generally thermal activation rather than, say, phonon drag. Dislocation motion then consists of spurts between positions at which some waiting time is spent. The spurts may be, for example, from one Peierls valley to the next, or from one series of obstacles to the next, or from a pinned dislocation source to the surface. If there are  $N$  potentially mobile segments per unit volume (i.e., those waiting plus those in transit) and a fraction  $dP$  of these actually gets free for some reason, they can clear a number of further obstacles without further cause and sweep out an average area  $a$  in the process.

Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough,  
Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

For time increments larger than the time of flight between waiting positions [1], the macroscopic shear rate is then<sup>1</sup> [2-5]

$$d\gamma/dt = baN dP/dt \quad (1)$$

(b: Burgers vector). The fraction  $dP$  may become unstable not only through thermal activation after an average waiting time  $t_w$ , but also through an increase  $d\sigma$  in applied stress:

$$dP = dt/t_w + p d\sigma - h d\sigma. \quad (2)$$

Equation (2) allows for a decrease in the activation probability through work hardening, which we describe by an increase  $d\rho$  in the density of those dislocations that influence the flow stress. It may increase through storage of some mobile dislocation lengths after they have traversed a "mean free path" [2, 9]  $L$ , and it may decrease through (stress aided) thermal recovery at a rate  $r$  [10, 5]:

$$d\rho = \frac{1}{bL} d\gamma - r dt \quad (3)$$

For the average inverse waiting time, we explicitly assume an Arrhenius term, as shall be justified in the next section. Combining eqs (1) through (3), we thus get the general equation of flow:<sup>2</sup>

$$\dot{\gamma} = baN \left\{ \nu^* \exp \left( -\frac{H^*}{kT} \right) + p(\dot{\sigma} - \theta \dot{\gamma}) \right\}, \quad (4)$$

where the work-hardening rate

$$\theta = \frac{h}{p} \left( \frac{1}{Lb} - \frac{r}{\gamma} \right). \quad (5)$$

$N$ ,  $a$ ,  $\nu^*$ ,  $H^*$ ,  $p$ ,  $\theta$ ,  $h$ ,  $L$ , and  $r$  may all depend on the applied stress as well as on the structure and on the temperature. We again emphasize that eq (4) holds only after transient times of the order of the spurt length.

<sup>1</sup> For an application to linear problems such as etch pit propagation, one may prefer to replace  $(aN)$  by  $(\rho x)$ , where  $\rho$  is the total length of essentially straight mobile dislocations and  $x$  the average distance they move forward per spurt. One may then interpret  $(x dP/dt)$  as the average dislocation velocity, or conversely  $(\rho dP/dt)$  as the dislocation generation rate. This distinction [6, 7] is arbitrary for spurt-like motion [8].

<sup>2</sup> By  $\dot{\gamma}$  we mean the plastic shear rate only; to include elastic (and machine) strains, a term  $\dot{\sigma}/G$  has to be added to the right-hand side. To obtain the relevant shear component of the tensorial strain, the entire equation has to be divided by 2.

Equation (4) shows that the Arrhenius equation for plastic flow holds only if

$$\dot{\sigma} = \theta \dot{\gamma}. \quad (6)$$

This is the equation of the stress strain curve after the initial transition region: The stress is continuously raised to compensate for structural changes. Thus the Arrhenius law holds for the asymptotic flow stress.

The Arrhenius equation holds in a creep experiment ( $\dot{\sigma} = 0$ ) only if  $\theta = 0$ , i.e., when there is no structural change, as in steady state creep. In transient creep, the term  $\theta \dot{\gamma}$  is finite (although it is often negligible with respect to the Arrhenius term). Similarly, stress relaxation experiments involve all three terms in eq (4).

In a strain rate change experiment, the Arrhenius law holds again for the asymptotic flow stress as mentioned before. The existence of transients such as yield drops suggests slow movement of dislocations between waiting positions. This may be either due to a high drag or lattice friction stress, when one considers spurt-like activation over discrete obstacles; or it may be due to a quasi-viscous propagation through obstacles, but spurt-like generation at sources.

One may be tempted to apply the Arrhenius equation also at the top of the yield point (or properly where eq (6) is fulfilled). However, this would presuppose that the velocity of dislocations in transit is itself controlled by thermal activation, such as in the quasi-viscous model discussed above, and that elastic effects of machine and specimen may be neglected. The latter is grossly untrue during transients. The situation gets worse if one back-extrapolates the transient itself to zero strain [11].

## II. Statistics and Geometry in the Slip Plane

Detailed models of spurt-like slip have been developed for the case in which the flow stress is controlled by the difficulty of propagation through a slip plane studded with point-like obstacles, i.e., obstacles that are of limited extent in both dimensions in the plane. Such obstacles may vary in strength, spacing, and angular arrangement with respect to each other. The waiting time for thermal activation of a dislocation segment at an obstacle depends on all of these parameters. While each one of these waiting times may be described by an Arrhenius term, the macroscopic strain rate depends on some average of these, and the question is, what average?

For the simple case of a square lattice of obstacles of varying strength, Frank [12] has recently written out the averaging procedure in elaborate

form, considering soft spots in series and hard spots in parallel.<sup>3</sup> The case of identical obstacles in random spacial arrangement had been treated analytically by Kocks [2-5] and numerically by Foreman and Makin [14, 15].

Formally, the two cases may be transformed into each other by a simple strength-to-inverse-spacing transformation. However, some of the geometrical implications may be easier to see, and were derived, in Kocks's model.

The important observation is that, independent of the temperature, dislocation loops sweeping over the same area of the slip plane have to overcome the same set of obstacles in the same sequence: they pass through weak obstacles in series until they get to a critical "gateway," and all "gateways" in the slip plane have to be overcome in parallel before the entire slip plane has been swept out. For this reason, the weight attributable to the various obstacles in the averaging procedure does not depend on temperature and, as a consequence, neither does the configurational entropy of activation (into which Frank [12] has put the effect); there is no "thermal front" [16]. Only when the pre-exponential factor in the Arrhenius equation, including the activation entropy, depends on temperature to a degree much smaller than that described by the exponential does a phenomenological description of rate processes in terms of an Arrhenius law make any sense.

There is one case in which the critical path, and therefore the activation entropy, can change with temperature; namely, when the activation *depth* differs widely from obstacle to obstacle, so that those obstacles that are the harder ones at low temperature may become the weaker ones at high temperature. As Diehl et al. [17] have shown, this leads to an inverse square-root dependence of the pre-exponential factor on temperature, in first approximation.<sup>4</sup>

The average waiting time per spurt, which consists of the sum of the waiting times at all "soft" obstacles and at the critical one, may be approximated by the waiting time at the critical obstacle only [4, 5]. All soft obstacles are overcome so much faster, particularly because of the "zipper" effect. Thus, a single Arrhenius term adequately describes activation in eq (4).

In a specific case, Kocks [4, 5] has shown that the waiting times at different critical obstacles along the same dislocation line arrange them-

<sup>3</sup> He neglects the interaction between various obstacles along the same dislocation line, which makes the waiting time at one obstacle depend on whether the dislocation has already overcome the next one ("zipper effect" [13]).

<sup>4</sup> Their specific reason for assuming such an inversion, which was not based on a spectrum of obstacle depths, was, however erroneous [3, 4].

selves to be equal at the flow stress; this applies when many weak obstacles and few strong ones are both randomly distributed in the slip plane.

### III. The Number of Mobile Segments

Another consequence of the geometric conditions in the slip plane is that, at least in many cases, the number of mobile dislocations enters as an independent parameter only through the slip plane spacing (or the “active glide volume” [18]). This may be seen by separating the volume density of mobile segments  $N$  into an area density  $N_p$  on the slip plane and a slip plane density  $1/d$ :

$$N = N_p/d \quad (7)$$

and then considering the product  $(aN_p)$  which enters into the general equation of flow (4). This product must be a constant of order 1 if the whole slip plane has to be swept out, and that was shown to be necessary at the flow stress [2]: otherwise back stresses will build up that prevent any further flow. If there were just one source per slip plane, it would have to cover the entire slip plane. If there are  $N_p$  sources, each has to cover an area roughly equal to the average area per source, so that dislocations of opposite sign can annihilate each other or form low-stress arrangements.

The pre-exponential term then becomes

$$b a N = b/d. \quad (8)$$

Dislocations on different slip planes are truly independent of each other. The strain rate contributions from different slip planes are additive, and a “thermal front” may develop. Whether a description of macroscopic rate processes by the Arrhenius equation is then still helpful, can only be decided by experiments that do not presume a temperature independent pre-exponential.

### IV. Acknowledgement

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# MOVEMENT OF A DISLOCATION THROUGH RANDOM ARRAYS OF POINT AND PARALLEL LINE OBSTACLES

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The motion of a dislocation through random arrays of impenetrable point and parallel line obstacles is considered. For impenetrable point obstacles the difference in line tension for edges and screws, and the elliptical equilibrium shape of the bowing-out loop are taken into account, and the yield stress for screws and edges is found to be the same. The results of a calculation of the effect of interaction between neighboring segments of the dislocation on the critical breaking angle and on the yield stress are presented. Computer calculations on the motion of dislocations through random arrays of parallel line obstacles show that the dislocations move by the generation and motion of large "kinks." The yield stress is found to increase approximately linearly with the obstacle length. These calculations are relevant to and are compared with the hardening in the early stages of the work hardening curve of dispersion hardened alloys containing small particles, in which rows of prismatic loops are formed at the particles, which act as linear obstacles to the gliding dislocations.

**Key words:** Computer simulation; dislocation motion; mechanical properties; precipitation hardening.

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## I. Introduction

Foreman and Makin [1] and Kocks [2] have considered the problem of the flow stress for a dislocation passing through a random array of im-

Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough, Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

penetrable point obstacles on a slip plane assuming that the line tension is independent of dislocation character, and that the dislocations bow out into circular arcs. It is found that the yield stress  $\tau$  is related to the line tension  $T$  and the mean planar obstacle spacing  $D_s$  ( $D_s = (1/N_s)^{1/2}$ ) by the relation

$$\tau = k \frac{2T}{bD_s} \quad (1)$$

where  $\mathbf{b}$  is the Burgers vector and  $k$  is a constant (the statistical factor). If the assumption is made that dislocations pass through the obstacle when the breaking angle ( $\phi$ ) between the two arms of the dislocation at the obstacle is zero then  $k=0.8$  and 0.842 on the two treatments respectively.

Equation (1) has been applied to the yield stress of dispersion hardened materials by Ashby [3].

It has been suggested that since the line tension of the edges and screws are different, the yield stress for these two types of dislocations will differ by a factor equal to the ratio of the line tensions, that consequently edge dislocations will move more easily, and that ribbon slip will be produced (Ashby [4], Kocks [5]).

However in this argument the noncircular shape of the bowing dislocation loop is not taken into account. In this paper we shall consider two problems related to the passage of dislocations through random arrays of impenetrable point obstacles.

(1) The effect of the shape of the loop if the dependence of line tension on dislocation character is taken into account.

(2) The effect of the interaction between neighbouring segments of the dislocations on the critical breaking angle and on the yield stress.

After small deformations dislocations passing through dispersion hardened alloys containing impenetrable particles generate rows of prismatic loops behind these particles by a process of cross-slip (Hirsch [6], Humphreys and Martin [7], Hirsch and Humphreys [8]). Screw dislocations interact with these rows of loops, forming helices which act as parallel line obstacles. The second part of this paper presents computer calculations on the movement of dislocations through arrays of parallel line obstacles, as a function of length of obstacle and breaking angle.

## II. Movement of Dislocation Through Random Arrays of Point Obstacles

### II.1. Effect of dependence of line tension on dislocation character

If this factor is taken into account, the shape of the noncircular loop must also be considered.

To a first approximation the equilibrium shape of a bowed out loop is elliptical (deWit and Koehler [9]).

For an elliptical loop the critical configuration of the dislocations passing through a random array of point obstacles can be obtained from that for circular loops by a suitable shear transformation, which transforms the circles into the appropriate ellipses, and the lattice into another random lattice with the same density of points. It follows that the statistical factor for ellipses is the same as for circular loops of the same area. The major (screw  $\lambda_s$ ) and minor (edge  $\lambda_E$ ) axes of the ellipse are related to the line energies of screw and edge dislocations ( $E_s, E_E$ ) by

$$\frac{\lambda_s}{\lambda_E} = \frac{E_E}{E_s} \quad (2)$$

(deWit and Koehler [9]), and for isotropic elasticity

$$\frac{\lambda_s}{\lambda_E} = (1 - \nu)^{-1} \quad (3)$$

where  $\nu$  is Poisson's ratio. This means that the average spacing between obstacles along the screw is larger than along the edge direction by the factors given in eqs (2) or (3). Furthermore, since the circular and elliptical loops (related by shear) have the same area,  $\lambda_s \lambda_E = \lambda^2$  where  $\lambda$  is the diameter of the equivalent circle.

$\lambda$  is the effective spacing appropriate to circular loops; i.e., in the notation of equation (1)  $\lambda = D_s/k$ .

The yield stress  $\tau$  is given by

$$\tau = \frac{2E_s}{b\lambda_E} = \frac{2E_E}{b\lambda_s} = \frac{2}{b\lambda} \sqrt{E_s E_E} = k_2 \frac{\sqrt{E_s E_E}}{bD_s} \quad (4)$$

It is clear therefore that there is only one yield stress for dislocations passing through a random lattice of point obstacles, that the yield stress for edges and screws are equal, and that "ribbon slip" does not occur.

This result holds in general for elliptical loops, irrespective of whether the ellipticity is due to the dependence of line tension on dislocation character, elastic anisotropy, or interaction between neighbouring dislocation segments; or stating the result in another way, if dislocation interaction results in loops becoming elliptical the yield stress is given by (4), where  $E_s$ ,  $E_E$  are the appropriate line energies. The yield stresses of dispersion hardened crystals are in reasonable agreement with (4) (Ebeling and Ashby [10], Jones [11], Hirsch and Humphreys [8], Ashby [12]).

It should be noted that the result for a random lattice that the yield stresses for screws and edges are equal holds more generally for loop shapes which can be derived by shear from loops with four fold symmetry.

However in the more general case the statistical factor will have a different value.

## II. 2. Interaction of Dislocation Segments

Ashby [3] has pointed out that when considering the by-passing of particles by dislocations, the interaction between the arms on opposite sides of the particle should be taken into account. As a first approximation this interaction is taken into account by considering the line tension to be that of a dipole of spacing equal to the particle diameter.

However, it is inevitable that as a result of this interaction, the critical breaking angle at which the dislocation loop becomes unstable is greater than zero. This problem has been considered for the case of a screw dislocation cutting a forest dislocation by Foreman [13], and Ashby [12] has considered qualitatively its relevance to the by-passing of a particle.

In principle, in order to determine the yield stress, the interaction of the various segments of dislocations passing through a random lattice must be taken into account; such a calculation has not been attempted. Instead, in order to obtain an estimate of the importance of the interaction both on the yield stress and critical breaking angle the model shown in figure 1 has been adopted.

The interaction of two neighbouring loops bowing out around a particle of diameter  $x$  has been fully taken into account within the framework of isotropic elasticity, following the method of Foreman [13]. The pinning points are taken along the screw direction, and the particles are spaced at a distance  $(L+x)$ . In the calculations the equilibrium configuration of the loops is determined for a given stress  $\tau$ , each element being in equilibrium under the combined forces of the applied stress and the self stress, including the interaction. Detailed interactions with the particle however are not taken into account.

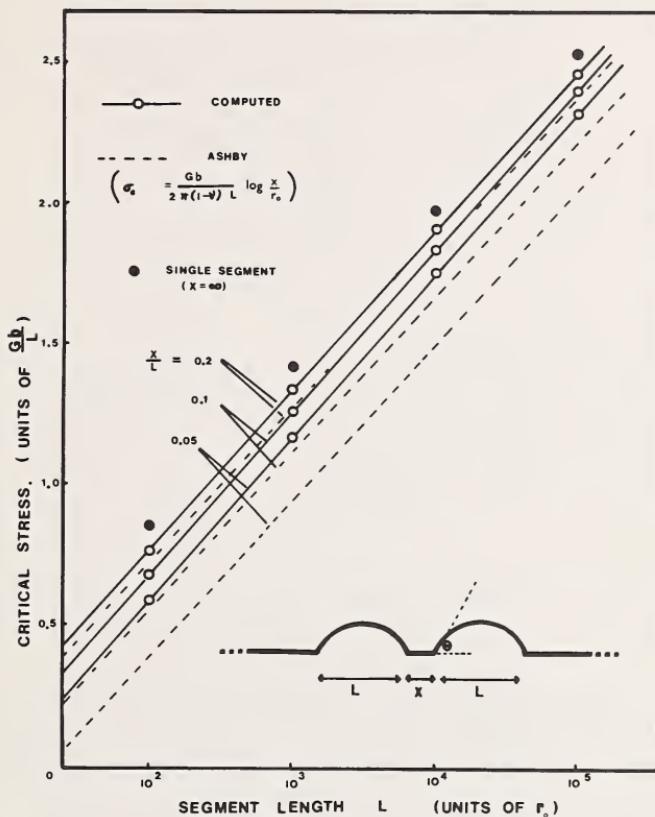


FIGURE 1. Stress to bow a pair of screw dislocation segments at a finite obstacle.

Above a particular value of stress, and inclination  $\theta$ , the loop becomes unstable, no solution being possible, and this corresponds to the critical by-passing configuration, and the yield stress. (The breaking angle  $\phi$  is given by  $(\pi - 2\theta)$ .)

Figure 1 shows the yield stress as a function of  $L$  for three values of  $x/L$  typical of dispersion hardened alloys. The curves show that the yield stress is in fact rather greater than that predicted by Ashby's [3] formula; for values typical of dispersion hardened alloys, say  $L = 10^4 r_0$  (where  $r_0$  is the cutoff radius) and  $x/L = 0.1$ , the yield stress is larger by about 10 percent. At the same time the critical values of  $\theta$  are considerably less than  $90^\circ$ ; table 1 gives typical values; the instability occurs at angles of  $\theta$  varying between about  $65^\circ$  and  $85^\circ$  for the cases considered.

Table 1. Inclination ( $\theta$ ) of critical segment

$x/L$	$L/r_0$			
	$10^2$	$10^3$	$10^4$	$10^5$
0.05	65°	69°	73°	74°
0.10	74°	75°	78°	80°
0.20	87°	84°	86°	84°

In these results,  $\theta$  is the inclination of the last stable segment obtained, and the values in table 1 show some scatter due to the finite stress increments used. Because the statistical factor  $k$  is dependent on  $\theta$  (ref [1] fig. 3) the raising of the critical stress predicted by figure 2 will be partly compensated by a lowering of  $k$  in the final expression for the Orowan stress.

### III. Movement of Dislocations Through Random Arrays of Parallel Line Obstacles

After small deformations, dislocations moving through alloys containing small impenetrable particles generate rows of prismatic loops parallel to the primary Burgers vector, behind the particles (Humphreys and Martin [7], Hirsch and Humphreys [8]).

Figure 2 shows an example of such rows of loops in a single crystal of copper containing alumina particles, deformed at 77 K and observed by electron microscopy at room temperature. Screw dislocations interact with the rows of loops forming helices (A in fig. 2).

It is thought that the helix will compress like a spring as a result of the bowing out of a free length of screw (see fig. 3). However, when the pitch of the helix becomes of the order of the diameter, the interaction between the turns rises rapidly (Hirth and Lothe [14]) and the spring compresses no further. The dislocation then bows out through the gap until at a critical stress it becomes unstable, and the particle and the loops therefore act effectively as parallel linear obstacles.

Edge dislocations on the same slip plane as one of the sides of the loop also repel the loops and force them together to a critical spacing which will again be of the order of the loop diameter. The edge dislocations must therefore bow out between the rows of loops which act again as parallel linear obstacles.

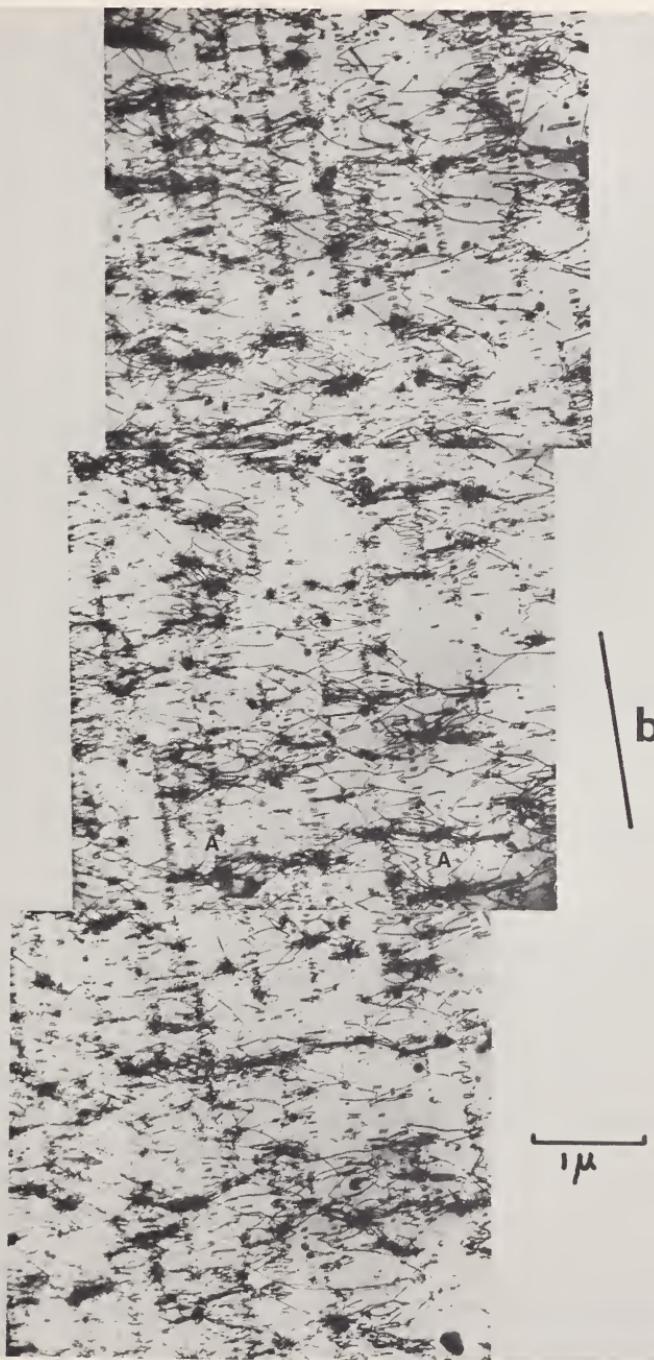


FIGURE 2. Parallel linear obstacles consisting of precipitates with rows of primary prismatic dislocation loops in a Cu-Al<sub>2</sub>O<sub>3</sub> crystal deformed at 77 K to a strain of 0.15 (section parallel to primary slip plane (111)).

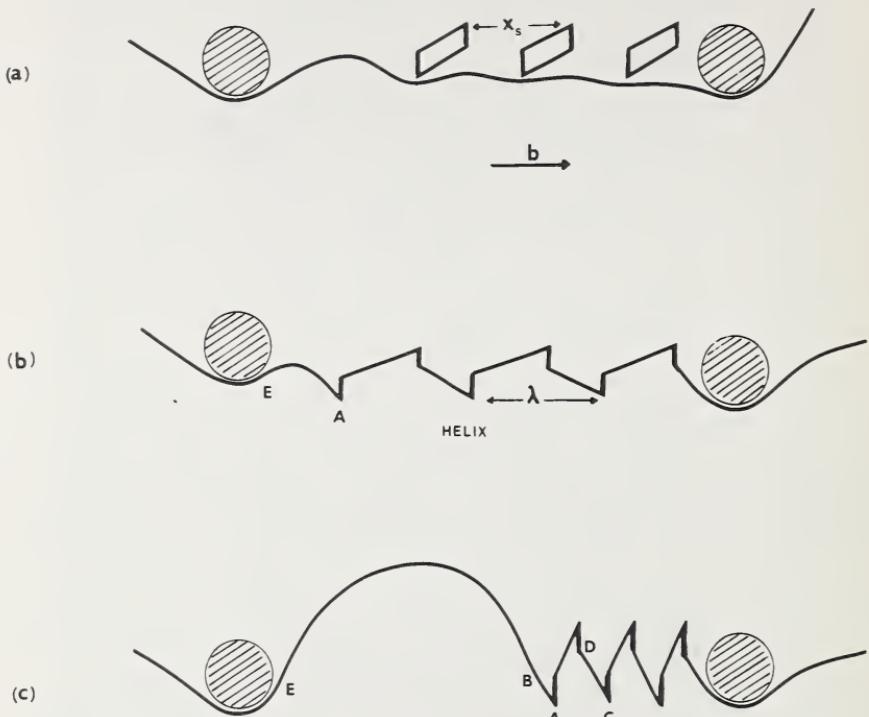


FIGURE 3. The interaction of a screw dislocation with a row of prismatic loops to form a helix.

The motion of screw dislocations through such an array has been described qualitatively elsewhere (Hirsch and Humphreys [8]), and the dislocation effectively moves by the generation and propagation of a super double kink between the rows (fig. 4).

Computer calculations have now been carried out on an IBM 360/65 computer for the movement of dislocations through random arrays of linear obstacles of various lengths, represented by closely spaced points. It was found that a spacing of these points of  $D_s/10$  was sufficiently small to simulate a linear obstacle for the range of stresses encountered.

In order to avoid the clustering of obstacles which is found in a truly random array and which does not occur in a real precipitation hardened system, obstacles which were closer than  $D_s/2$  were excluded.

Figures 5a and 5b show critical configurations for screws in two such arrays, assuming a breaking angle of zero. It is clear that for the longer obstacles the screws tend to remain straighter, and propagate indeed by the generation and movement of kinks.

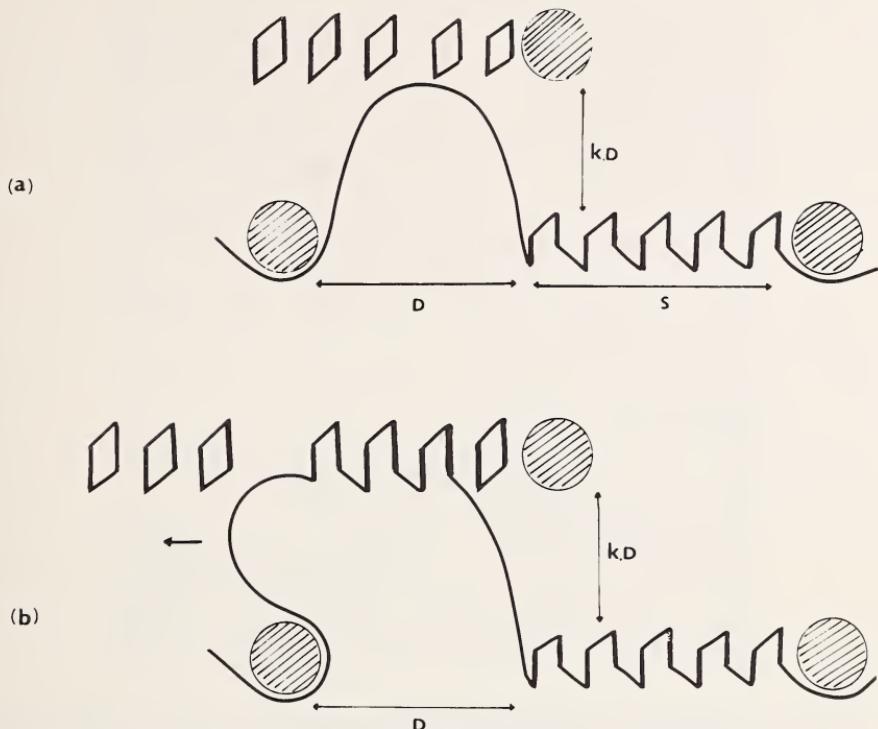


FIGURE 4. Formation and propagation of an edge kink.

Figure 6 shows part of the configuration for the case when the breaking angle for the obstacle is  $90^\circ$ , except for the "particle" at one end at which the breaking angle is zero. This figure shows a dislocation passing through the obstacle at  $A$ ; examples of such configurations in practice are seen in figure 7, and also in Hirsch and Humphreys [8] figure 9.

It is assumed that the yield stress is reached when a screw dislocation starting at the bottom of the diagram reaches the top. Figure 8 shows the yield stress as a function of obstacle length(s) for three cases corresponding to breaking angle:

- (a) zero
- (b)  $90^\circ$
- (c)  $90^\circ$  except at one end where there is a "hard" particle.<sup>1</sup>

<sup>1</sup> Similar calculations for a completely random array showed values lower by 5 percent to 10 percent.

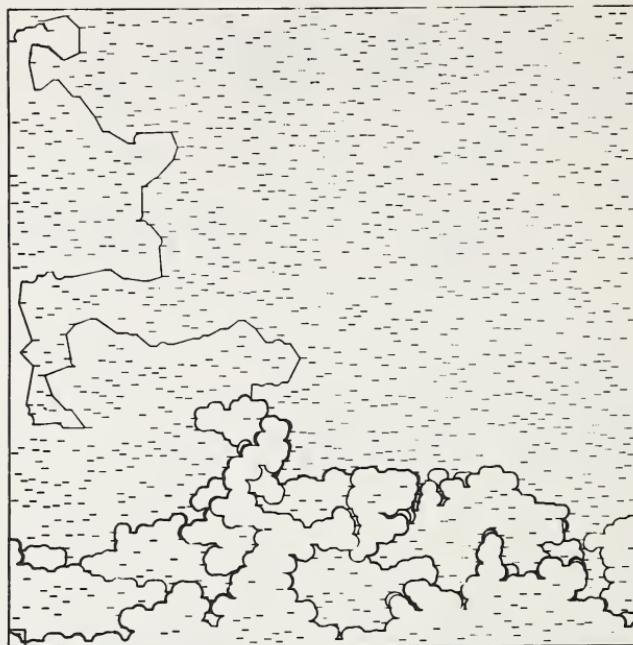


FIGURE 5(a). Diagram obtained directly from the computer by a Stromberg-Carlson 4060 graph plotter for the movement of a "screw" dislocation through an array of linear obstacles of length  $s$ . The dislocation moves from the bottom of the array and its position is shown for successive stress increments. The straight parts of the dislocation at the top are nonequilibrium positions which occurred when the dislocation broke out of the top of the array. Infinitely hard obstacles  $s = 0.4D_s$ .

Curves (a), (b) are linear in  $s$ , curve (c) is linear except for a region for small  $s$ .

For impenetrable linear obstacles the yield stress  $\tau$  is

$$\tau = \tau_0 + \frac{2Ts}{bD_s^2} \quad (5)$$

$\tau_0$  is the yield stress for point obstacles

$T$  is the line tension

$D_s$  is the mean planar spacing of the obstacles.

The slopes of the other curves are somewhat smaller.

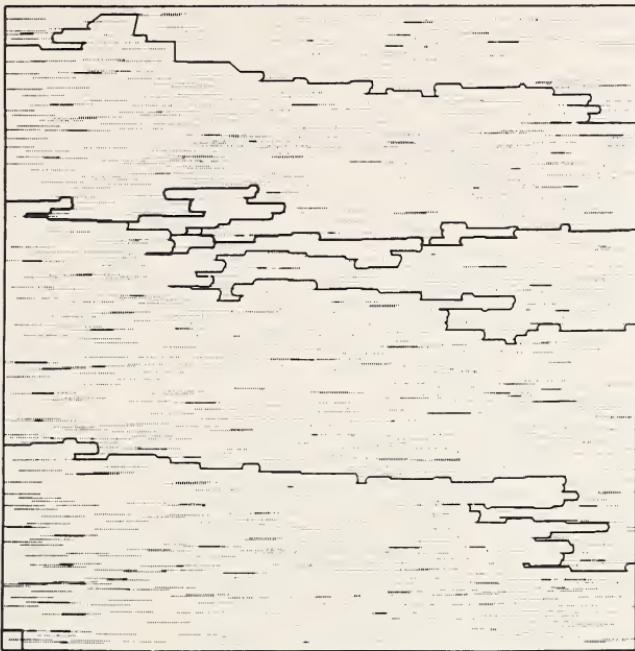


FIGURE 5(b). Diagram obtained directly from the computer by a Stromberg-Carlson 4060 graft plotter for the movement of a "screw" dislocation through an array of linear obstacles of length  $s$ . The dislocation moves from the bottom of the array and its position is shown for successive stress increments. The straight parts of the dislocation at the top are non-equilibrium positions which occurred when the dislocation broke out of the top of the array. Infinitely hard obstacles  $s = 2D_s$ .

An approximate calculation based on the idea that kink generation is the critical step, gave a linear variation with small  $s/D_s$  with a smaller slope (see Hirsch and Humphreys [8]). If kink movement is the critical step, it is easily shown that for long obstacles, assuming zero breaking angle,

$$\tau \sim \frac{2Ts}{bD_s^2} \quad (6)$$

which agrees with equation (5) for large values of  $s/D_s$ .

Similar calculations were carried out for edge dislocations passing through the array (fig. 9). It is found that ribbons of edge dislocation can find easy paths through the lattice but that these generally terminate after some distance, which may however be of the order of the size of the array.

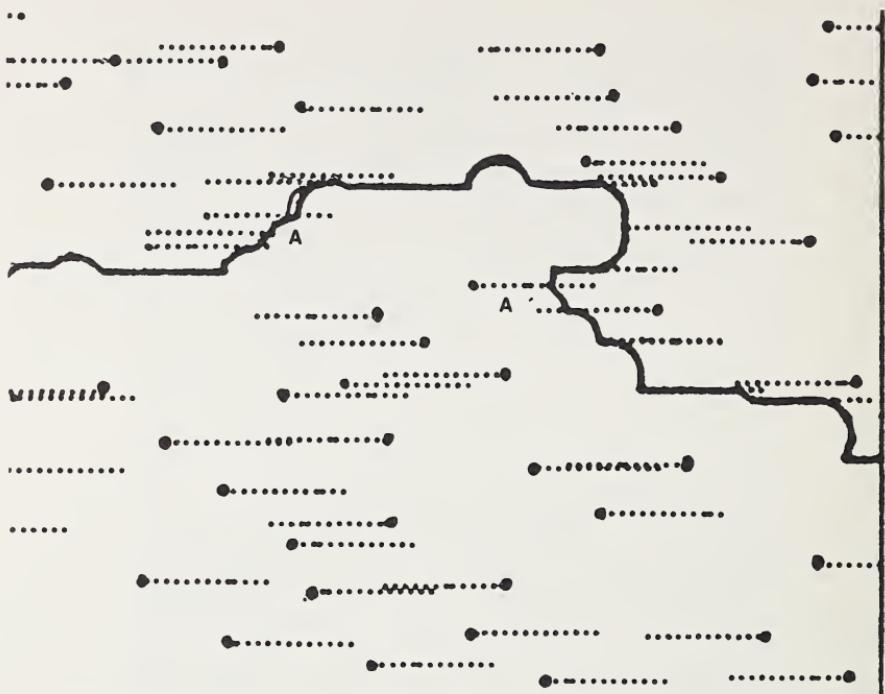


FIGURE 6. Detail of a computer diagram for hard particles with soft loops ( $90^\circ$  breaking angle). Note how the dislocation can break through the obstacles.

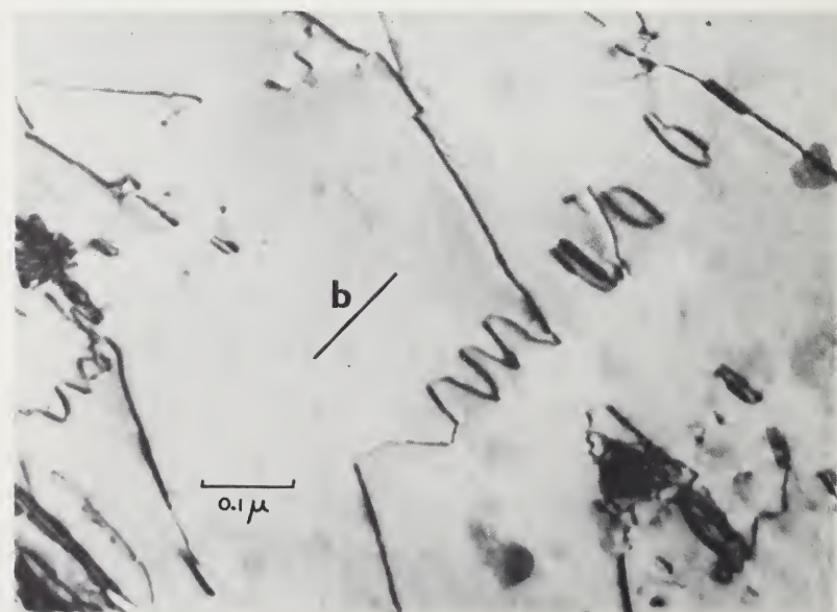


FIGURE 7. As figure 2, showing a similar configuration to figure 6.

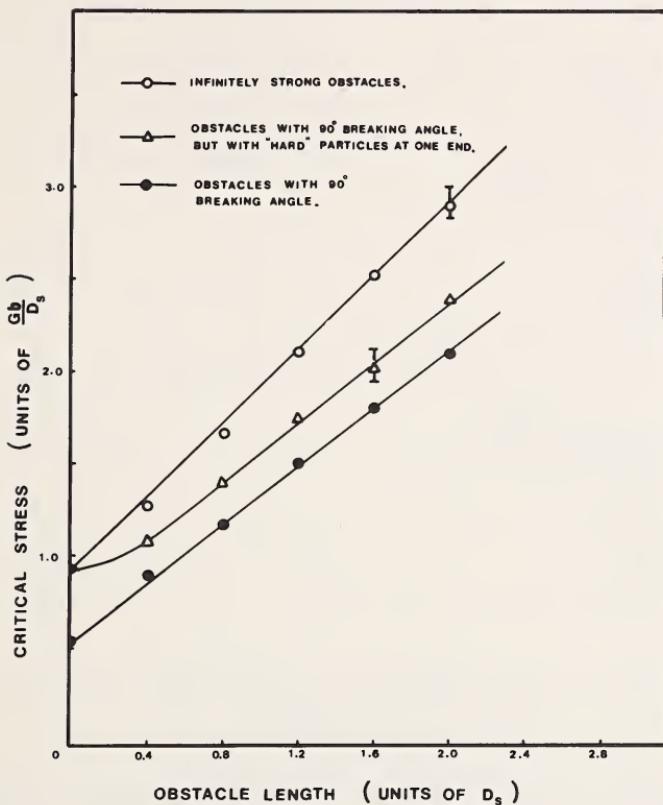


FIGURE 8. The stress to move a screw dislocation with line tension  $T = \frac{Gb^2}{2}$  through an array of parallel linear obstacles as a function of obstacle length ( $s$ ).

In effect this means that the flow stress (as defined by the stress at which the edge dislocation crosses the array) is lower than for screws.

However the total area of slip plane swept out in this case is very small, and macroscopic slip can not be said to have occurred; and thus it appears that our model is too small. Calculations with different sized arrays suggest that as the size is increased, so the yield stress approaches that for screws.

Thus if we consider a dislocation loop expanding in this array, it will be elongated considerably in the screw direction, but the macroscopic flow stress will be that as calculated in our array for screws. Thus in contrast to an array of point obstacles, a type of ribbon slip will occur for a set of parallel linear obstacles.

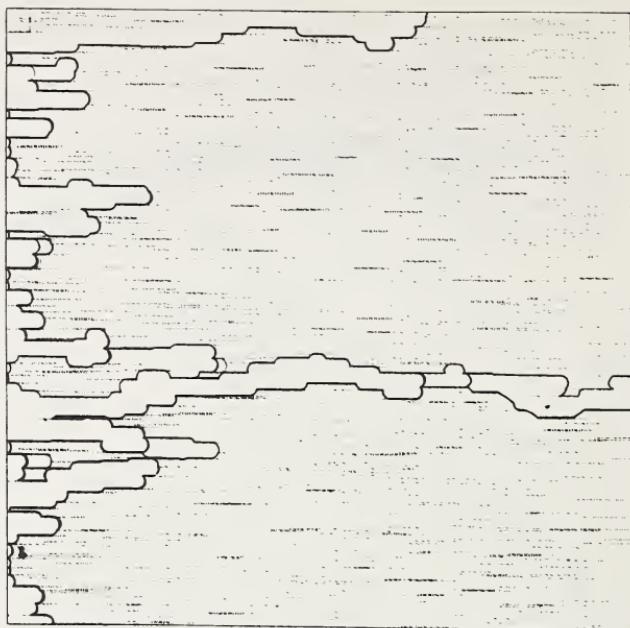


FIGURE 9. Computer diagram for the movement of an edge dislocation through an obstacle array. Infinitely hard obstacles,  $s = 2D_s$ .

An attempt has been made to correlate the computer results with a real metal. Single crystals of copper containing a dispersion of  $\text{Al}_2\text{O}_3$  particles of diameter  $\sim 500 \text{ \AA}$  were deformed into stage I (see fig. 2) at 77 K, and the flow stress at a given strain was measured and compared with the microstructure of that specimen. Such an alloy shows considerable recovery (Jones [11], Hirsch and Humphreys [8]) and up to 60 percent of the work hardening may be lost if the crystal is warmed up to room temperature. Thus the observed microstructure corresponds to the recovered flow stress, and it was this parameter which was measured. The results are shown in figure 10 (open circles). However the obstacles will expand when the stress is removed, and we will observe a longer obstacle length than the true one. In order to correct for this, the number of loops at the obstacles was counted, and a new obstacle length was calculated assuming that the loops under stress could approach to a diameter (full circles).

These results indicate an agreement with the computer calculation, and with the evidence that the obstacles are cut, e.g., figure 7 and reference [8] figure 9, suggest that this type of crystal shows the behaviour of the middle curve in figure 8, i.e., hard particles and soft loops.

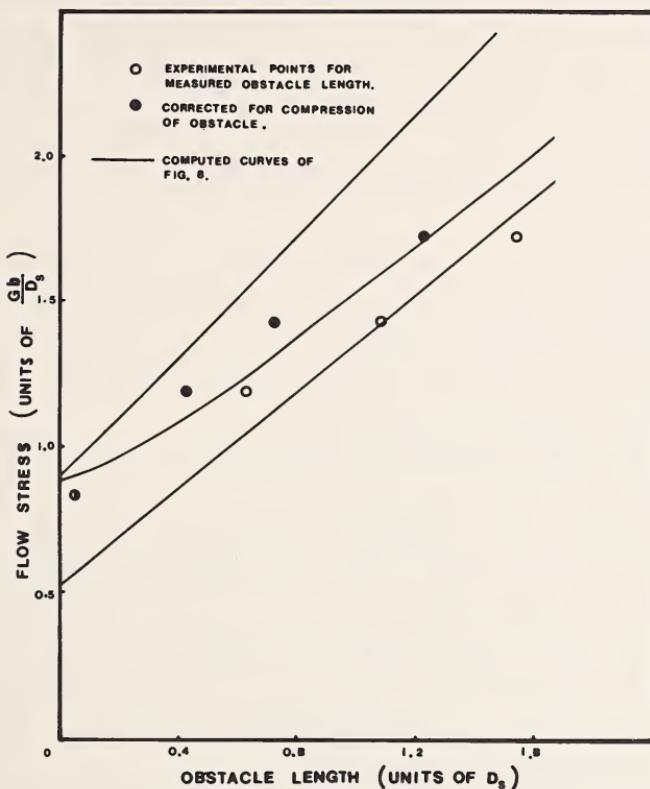


FIGURE 10. Experimental points for a Cu-Al<sub>2</sub>O<sub>3</sub> crystal, compared with the computed results of figure 8.

The application of this type of analysis to the prediction of a stress-strain curve is complicated as it will depend on how the loops are distributed with strain. There is evidence, see [8], that all the loops are not in the rows, but that some are swept away, thus reducing the build up of the linear obstacles to below that predicted by a simple model.

#### IV. Conclusions

- (1) For a random array of infinitely hard point obstacles there is only one yield stress for both edges and screws, and "Ribbon Slip" does not occur.
- (2) Computer calculations on the bowing of pairs of interacting dislocation segments separated by a "particle," show that the critical by-pass stress is a little greater than that calculated by Ashby [3] and the breaking angle may be considerably greater than zero.

(3) Computer calculations on the movement of a dislocation through an array of linear obstacles parallel to the screw direction show that as the obstacle length increases, the dislocation moves by the generation and propagation of edge kinks, and a type of ribbon slip occurs.

The hardening increases linearly with obstacle length.

(4) Experimental results on a dispersion-hardened copper alloy show a satisfactory agreement with the computer calculations.

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# STRAIN RATES IN DISLOCATION DYNAMICS

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Since the success by Johnston and Gilman in relating yield phenomena in LiF to direct measurements of dislocation velocities and densities, the  $\Lambda bv$  expression for the strain rate has been used almost exclusively, where  $\Lambda$  is the mobile dislocation density,  $b$  the Burgers vector, and  $v$  is the average dislocation velocity. We note that there are cases for which the strain rate is independent of dislocation velocity. When the velocity is large enough the strain rate is given in a simplified model by  $\Lambda b\bar{x}$ , where  $\bar{x}$  is the average distance traveled by a dislocation. The strain rate is eventually determined, then, by the rate at which new dislocations are created and not necessarily by the rate at which old dislocations expand or by the dislocation velocity.

Key words: Dislocation kinetics; mobile dislocations, stress rates.

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The shear strain  $\epsilon$  produced by  $N$  dislocation loops which sweep out an average area  $A$  is given by

$$\epsilon = N\mathbf{b}\bar{A}, \quad (1)$$

where  $\mathbf{b}$  is the Burgers vector. It is often simpler in discussions of mechanisms to consider straight dislocations, for which case eq 1 may be written as

$$\epsilon = \Lambda b\bar{x}, \quad (2)$$

where  $\Lambda$  is the total length of mobile dislocations per unit volume, and  $\bar{x}$  is the average distance moved. This relation, and others depending on it, can be easily generalized to the case of curved dislocations.

In early discussions of strain rate formulas for dislocation dynamics by Orowan [1] and by Seitz and Read [2], it was appreciated that there were two limiting possibilities. The strain rate  $\dot{\epsilon}$  might be given as

$$\dot{\epsilon} = \Lambda b\bar{v}, \quad (3)$$

or by

$$\dot{\epsilon} = \dot{\Lambda} b \bar{x} \quad (4)$$

where  $\bar{v}$  is the average velocity of the dislocations, and  $\bar{x}$  is the average distance traveled by a dislocation before it is stopped or annihilated. Although a clear decision between these possibilities was not possible at that time, the available evidence seemed to favor the  $\Lambda b \bar{v}$  mode of description.

Since the success by Johnston and Gilman [3] in relating yield phenomena in LiF to direct measurements of dislocation densities and velocities, the  $\Lambda b \bar{v}$  expression has been used almost exclusively, and is usually taken as the fundamental equation of dislocation dynamics [4]. We wish to show that there exist cases for which the average velocity  $\bar{v}$  is not necessarily relevant to a description of strain rates. In such cases, dislocation generation, and not the overcoming of obstacles, becomes the rate limiting step in plastic deformation.

Recently, comparisons [5] of ultrasonic measurements with etch pit measurements have led to a realization of the fact that in many materials there are several important time constants relevant to the description of dislocation velocities and strain rates. The first of these is the time of flight  $\tau_F$  between obstacles which is determined normally by the dislocation-phonon interaction. The second is the time of waiting  $\tau_W$  to overcome obstacles; the ratio of the first two determines the average dislocation velocity  $\bar{v}$  as measured by etch pit techniques. The third is the lifetime of a movable dislocation, which is related to  $\bar{x}$  through

$$\bar{x} = \bar{v}\tau. \quad (5)$$

The fourth is a time determined by the rate of production of dislocations  $\tau_D$ , and the fifth is the experiment time  $\tau_E$ . These times are all distinct. The time  $\tau$  is particularly relevant in a discussion of strain rates. The distinction between these times can be appreciated from a detailed consideration of the dependence of dislocation velocity on stress.

Velocities as a function of stress in NaCl as derived from etch pit and ultrasonic data are shown in figure 1. The etch pit data were obtained by Gutmanas et al. [6]. The two curves on the left represent average velocities as a function of stress for relatively pure ( $< 10^{-3}$  % Ca) NaCl. The upper curve of each pair is for the faster moving edge dislocations, while the lower curve is for screws. For relatively impure NaCl ( $\sim 10^{-2}$  % Ca) the dislocations are much slower at a given stress, as shown by the pair of curves on the right. For high speeds, the dependence of the velocities on

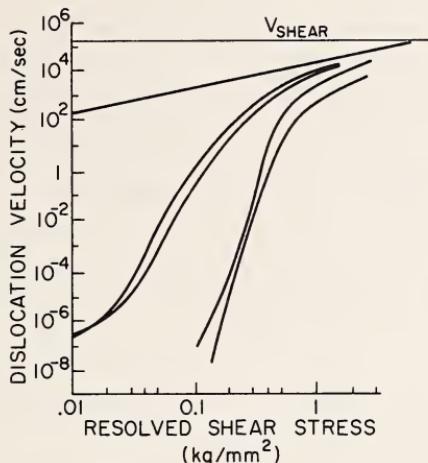


FIGURE 1. Dislocation velocities as a function of stress in NaCl. The etch pit data is from Gutmanas, et al. The ultrasonic data is from Fanti, et al.

stress becomes weak, and the difference between the velocities of edges and screws at a given stress is reduced greatly. The effect of hardening and of radiation damage is qualitatively similar to that of impurity addition.

There are evidently three regimes in the velocity-stress curve, for which different physical mechanisms limit the velocity. At the highest stresses, the velocities are limited by relativistic effects to the velocity of sound. There is also a structure insensitive domain where the velocity is linear in stress. At the lowest stresses, the velocities are structure sensitive, depending on the defect content of the specimen. It was suggested by Mason [7] that it should be possible to determine the strength of the dislocation-phonon interaction from the velocity measurements in the linear regime by equating the drag force per unit length of dislocation to the applied force per unit length:

$$Bv = b\sigma, \quad (6)$$

where  $B$  is the drag force constant and  $\sigma$  is the applied resolved shear stress.

The three-regime interpretation is supported by measurements of the temperature dependence of the velocities and by ultrasonic measurements. It has been found that the velocities as low stress increase strongly with temperature, while the velocities in the phonon-drag limited region decrease weakly [8]. This behavior is as would be expected if thermally activated processes operate at low stresses, leading to an exponential

dependence on temperature. At higher stresses, where the velocities are limited by phonon scattering, increasing temperature should lead to increased drag as a consequence of the increased phonon density. Using ultrasonic measurements, Baker [9] showed that the etch pit velocities at low stresses were not instantaneous velocities, but only average velocities. He found that velocities of dislocations between pinning points were orders of magnitude greater than the average velocities measured by etch pit observations at the same stress. Instantaneous dislocation velocities can be determined ultrasonically by making attenuation measurements at high frequencies, where the motion is again limited by the phonon drag [10]. The linear curve shown in figure 1 represents an extrapolation (above  $\sim 10^2$  cm/s) of velocities deduced from ultrasonic measurements by Fanti et al. [5]. It is easily seen that the same mechanism limiting dislocation motion in high frequency ultrasonic measurements does indeed also limit the velocities of the unidirectional motion of dislocations over longer distances. This correspondence has also been found for pure Cu, Zn and Al by Vreeland and his co-workers [11].

The corresponding displacements, velocities, and time constants of a given dislocation under the action of a stress are shown schematically in figure 2. It is supposed that a shear stress, of amplitude  $\sigma_0$  and relatively long duration ( $\tau_E$ ) is applied at a given time. The velocity  $v_i$  of the  $i$ th dislocation then quickly achieves its limit velocity  $v_{iL}$ . The limit velocity is given by the sound velocity at high stresses or low temperatures, but in the intermediate range (phonon limited) is given by  $b\sigma/B$ . The dislocation travels a time  $\tau_F$  until it becomes stuck at an obstacle. After a wait time  $\tau_W$ , with the help of thermal fluctuations, the process is repeated. After having traveled a distance  $\bar{x}_i$ , the dislocation becomes permanently stopped, and moves no more even though the stress is still applied. In an impure specimen where there are many obstacles, the average velocity  $\bar{v}_i$ , indicated by the dashed line, is small compared to the limit velocity. The magnitude of the average velocity is determined by the limit velocity and the ratio of the free-flight time  $\tau_F$  to the wait time  $\tau_W$ . The motion is discontinuous, but is quasi-continuous on a macroscopic scale.

It has been pointed out by Argon [12] and by Kocks [13] that the strain rate can be described equally well by either eq (3) or (4) for sputtlke motion, the distinction being arbitrary. This is true for times  $\tau_E$  long compared to  $\tau_F$  and  $\tau_W$ , but short compared to  $\tau$ . We are primarily concerned here with cases for which  $\tau_E$  is long compared to  $\tau$ , and will use subsequently the smoothed-out (dashed) curves shown in the time interval  $\tau$ . For the latter case, we believe the distinction not to be arbitrary. We thus regard the average velocity  $\bar{v}_i$  (that observed in etch pit experiments) to be zero before the stress is applied, to have the value  $\bar{v}_i$  during the time interval  $\tau$ , and then to be zero again subsequently. The behavior described

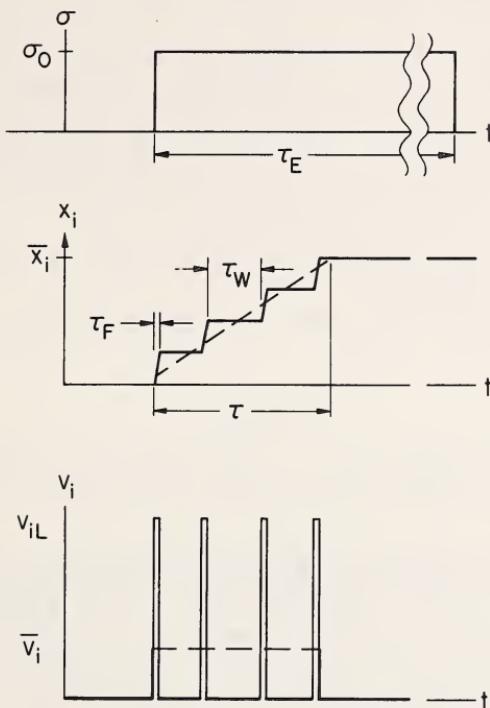


FIGURE 2. Schematic sketch of dislocation displacement  $x_i$  and velocity  $v_i$  for an applied stress  $\sigma_0$  of duration  $\tau_E$ .

in figure 2 is idealized and simplified. The average velocity  $\bar{v}_i$  is likely to decrease with time. However, we believe this description is a useful first approximation which already contains much of the important physical behavior and which can be easily generalized later to a more realistic description.

As an example of a specific physical system to discuss, we have in mind the recent results found by Vreeland [11] and Suzuki [14] for high purity, low dislocation density copper. It has already been mentioned that the dislocation velocities were found to be linear in stress, with a drag coefficient agreeing well with that determined ultrasonically for phonon drag. This means that  $\tau_W$  is negligible and  $\tau$  is extremely short. Suzuki applied stress pulses of amplitude near  $20 \text{ g/mm}^2$  and durations as low as  $5 \times 10^{-4} \text{ s}$ . He found that if successive pulses are used, then most of the dislocations which are stopped after the first pulse do not move again unless the stress amplitude is increased significantly, even if the pulse time is lengthened. Also he found that the average distance of motion  $\bar{x}$  is independent of the length of the pulse and the testing temperature.

Some representative values from his data are  $\bar{x} \sim 4 \times 10^{-2}$  cm and  $\bar{v} \sim 4 \times 10^2$  cm/s from which we find  $\tau \sim 10^{-4}$  s from eq (5). Also, using eq (3) and the values of  $v$  and  $\dot{\epsilon}$  observed by Suzuki, one obtains  $\Lambda \sim 40 \text{ cm}^{-2}$ , showing that very few dislocations move simultaneously. It is then apparent that after a time  $t = \Lambda_0 \tau / \Lambda$ , where  $\Lambda_0$  is the initial dislocation density, the old dislocations will have already made their contribution to the strain and new dislocations have to be created to support the strain rate. With  $\Lambda_0 \sim 4 \times 10^4$ , this time is then  $\sim 10^{-1}$  s.

A simplified model, stimulated by these data, can then be based upon the following assumptions.

1. The dislocation velocities are large (phonon or relativistically limited).
2.  $\bar{x} = \text{const.}$
3.  $\dot{\epsilon} = \text{const.}$

These assumptions are used to simplify the discussion. They are sufficient but not necessary, and can be relaxed somewhat for a more general treatment.

Assumption (1) has been verified for some low dislocation density, high purity metals. At finite temperatures the velocity is given by  $b\sigma/B$ , and so depends weakly (1st power) on stress and temperature. As the velocity depends exponentially on stress and temperature in the low stress regime, it is a reasonable approximation to neglect by comparison the weak dependence entirely in a first approximation.

Assumption (2) is derived from the experimental results. Presumably  $\bar{x}$  depends upon the dislocation forest density  $\Lambda_F$  and also weakly on impurity content, stress and temperature. The lowest value of  $\bar{x}$  observed in etch pit measurements is of order  $10^{-3}$  cm while the largest value is limited by the specimen size. A typical value would seem to be  $\sim 3 \times 10^{-2}$  cm, and the maximum variation of about a factor of 30 is in any case small compared to the range of velocities (a factor of  $10^{12}$ ) which can enter eq (5). It is therefore reasonable to suppose that  $\tau$  is determined primarily by  $\bar{v}$ .

The total strain at time  $t$  is given by the sum over all dislocations

$$\epsilon(t) = \sum_i b \bar{x}_i(t), \quad (7)$$

and the strain rate by the corresponding sum

$$\dot{\epsilon}(t) = \sum_i b \bar{v}_i(t). \quad (8)$$

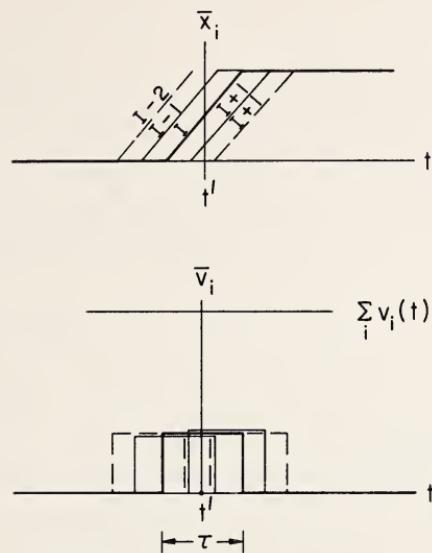


FIGURE 3. Schematic sketch of dislocation average displacements  $\bar{x}_i$  and average velocities  $\bar{v}_i$  at a time  $t'$  in a time interval  $\tau$ .  $\sum_i v_i(t)$  is the sum of the velocities of dislocations moving simultaneously.

The terms in the sum of eq (8) are step functions of time, each of which is zero most of the time. To evaluate the strain rate at a time  $t'$ , we must know which of the  $i$  dislocations are moving at that time and the velocity of each. This sum is easily evaluated with assumptions (1)–(3) as indicated in figure 3. The displacement and velocity of the  $I$ th dislocation are indicated with a heavy line. For a constant strain rate, the stress level presumably increases at a slow rate. However, in this range of high velocities, the velocity is only a weak function of stress, and to a first approximation the velocities can be taken to be constant or independent of  $i$  in the time interval  $\tau$ . But constant strain rate then implies that dislocations become available at a constant rate, so that the spacing of the curves for different  $i$  must be uniform. Only those dislocations in motion at time  $t'$  contribute to the strain rate  $\dot{\epsilon}(t')$ . For example, in figure 3, dislocations  $I-2$  and  $I+2$  do not contribute to  $\dot{\epsilon}(t')$ . Thus the mobile dislocation density  $\Lambda$  at time  $t'$  is given by

$$\Lambda = \dot{L}\tau, \quad (9)$$

where  $\dot{\Lambda}$  is the rate at which mobile dislocations become available. The sum of eq (8) then becomes

$$\dot{\epsilon} = \Lambda bv = \dot{\Lambda} \tau bv.$$

Using eq (5), the velocity dependence then cancels out to give eq (4). Thus, for the conditions described here, the strain rate is independent of dislocation velocity.

Since the mobile dislocation density required, for example under the conditions of Suzuki's measurements, is so low ( $\sim 40 \text{ cm}^{-2}$ ), the strain rate could be sustained for a period with the pre-existing dislocation density ( $\Lambda_0 \sim 4 \times 10^4 \text{ cm}^{-2}$ ). However, the time constant  $\tau$  is so small ( $\sim 10^{-4} \text{ s}$ ), that even these are insufficient to maintain the strain rate for reasonable experiment times  $\tau_E$ . From eq 5, using values given by Suzuki, we find  $\dot{\Lambda} = 4 \times 10^5 \text{ cm}^{-2} \text{ s}^{-1}$ . This defines a critical time  $\tau_c$  through the relation  $\Lambda_0 = \dot{\Lambda} \tau_c$  to be  $\tau_c \sim 10^{-1} \text{ s}$ . For times greater than  $\tau_c = \Lambda_0 / \dot{\Lambda} = \Lambda_0 \tau / \Lambda_m$ , new dislocations must be produced. Even if dislocations are able to move again as the stress is raised,  $\bar{x}$  is still limited by the specimen size, so that  $\tau_c$  is still small compared to reasonable experiment times. Also, if not all the old dislocations move,  $\tau_c$  will be reduced. Under these conditions the rate limiting step in deformation is determined by the dislocation production rate and not by the rate at which obstacles are overcome.

*Note added proof:* It has come to our attention that a similar argument has been given independently by Mecking and Lücke. It appears in Mecking, H., Thesis, Aachen (1967), is sketched in Mecking, H., and Lücke, K., *Acta Mat.* **17**, 279 (1969), and will be published separately.

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## Discussion on Papers by W. Frank and U. F. Kocks.

SCHOECK: If you have a spectrum of two different types of obstacles, hard ones and soft ones, is it not correct that the effective distance for penetrating the hard obstacles is given, not by the average spacing between obstacles, but by the spacing of the hard obstacles?

FRANK: No, it is given by the distance between the so-called effective obstacles, the hardnesses of which are high enough to be not overcome at a given stress level.

SEEGER: If there is a bunch of small obstacles, they also count. The isolated soft obstacle will not count, but if there are enough to be effective, then they count just as much as the hard obstacles.

ARSENAULT: One question I would like to ask Professor Schoeck is whether the appropriate quantity to use in such activation calculations is the Gibbs free energy, the activation free energy or the free enthalpy.

SCHOECK: When you formulate the equation for a rate process you have to make certain assumptions. In describing the movement of a dislocation which intersects other dislocations or a dispersion of fixed obstacles by thermal activation one generally uses the so-called transition state model which was first developed by Zener<sup>1</sup> for atomic diffusion, later generalized by Vineyard,<sup>2</sup> and applied to dislocations by Granato et al.<sup>3</sup> The rate of overcoming the obstacles in this model is given by the ratio of the partition functions in the saddle point configuration and in the equilibrium position in front of the obstacle. From this formulation it follows then that the quantity which occurs in the exponent of the rate equation and which is called activation energy is really the difference in the Gibbs free energy between the configuration in the activated state in the saddle point and in the ground state in front of the obstacle.

ARSENAULT: I would like to introduce a different name, if possible. Instead of worrying about whether it's the Gibbs free energy or not, call it reversible work.

SEEGER: That, of course, is the same thing. Reversible work under conditions of constant temperature and constant pressure, as you are told in thermodynamics, is the Gibbs free energy.

ARSENAULT: Yes, but Gibbs didn't consider a shear stress.

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<sup>1</sup> Zener, C., in *Imperfections in Nearly Perfect Crystals* (Wiley and Sons, 1952) p. 259.

<sup>2</sup> Vineyard, H., *J. Phys. Chem. Solids* **3**, 121 (1957).

<sup>3</sup> Granato, A. V., Lücke, K., Schlipf, J., and Teutonico, L. J., *J. Appl. Phys.*, **35**, 2732 (1964).

SEEGER: If you look up Zener<sup>4</sup> you will find this very point made there. He says that it's the reversible work to be done, and this is equal to change in Gibbs free energy.

KOCKS: If I may first say something on this same topic which actually links to Dr. Frank's talk. I think we are all agreed that there are fundamental principles that put the free enthalpy<sup>5</sup> in the exponent of an Arrhenius equation, but there is the other half of that and that is the operational procedure. If one does experiments and plots the logarithm of the strain rate against  $1/T$ , of course the slope of the line is not  $G$  but  $H$ . So the problem that complicates this activation process in plastic flow is that the activation entropy, which you may put into the pre-exponential factor, is then not distinguishable from other parameters that enter into this pre-exponential factor. It is, then, not possible in principle to measure the activation entropy despite whatever Dr. Frank may have said, because you have to make assumptions about  $a_0$  in his terminology. That brings me to a discussion of Dr. Frank's work. When one has a complicated problem there are two approaches: One is to try and write down the general solution, and the other is to try and find what sounds like the most plausible approximation. From what we can gather from the slides, Dr. Frank has tried to write down a general equation. Firstly, his result that the Arrhenius equation formally still holds has meaning only to a limited extent. It is specifically assumed, and generally true, that the spectrum of obstacles that is important may depend on the temperature, so that therefore, the activation entropy may be very much stronger than what we would expect merely from the temperature dependence of the elastic constants. Now whenever that is the case, the Arrhenius equation becomes a formalism that has very little meaning left. You might as well describe it by a Fourier series or something else. The Arrhenius equation means something *only* if the major temperature dependence is described by the  $1/T$  term in the exponent and if one knows independently something about the other terms in front. I have discussed this problem with Dr. Frank and if I may give my summary of that discussion, he takes the perfectly valid approach that some of the properties that go into  $a_0$  can be found independently by microscopic means—not by making stress-strain tests, but by microscopic techniques. One can try to measure the distribution spectrum of spacings or strengths, for example. On the other hand, one thing that I don't think one has any handle on measuring microscopically is the mobile dislocation density, and since that

<sup>4</sup> Zener, C., Trans. AIME 147, 361 (1942).

<sup>5</sup> In the American literature "free enthalpy" is usually referred to as the Gibbs free energy.

does enter into his equation, I think there is a parameter that I cannot quite see being called a non-adjustable parameter.

If I may be allowed one more word on the evaluation of his term "quasi-regularity," I have not been able to see how it can really deviate from regularity without very much disturbing the procedure that he uses. For example, the picture he had on the board showing obstacles was very far away from regularity, and he stated that the distance between obstacles may change a little. One of the most important things in my opinion about non-regular arrangements of obstacles is not only that the spacing changes, but also that the angle between them changes. If you want to write a general equation the angle is one of the most important parameters. It does not even enter into this general summary of all possible interesting parameters of Dr. Frank's. The angle question brings up an even more important general matter completely forgotten by Dr. Frank, one which is almost the center of my work on this, and that is that the obstacles are not independent. It is not possible to ascribe a waiting time to one obstacle that does not depend on whether the obstacle next to it has not already broken through. There is a zipper effect. If one obstacle goes through, the angle that the dislocation makes on the new obstacle has changed, and the waiting time depends on this. These geometrical factors do not enter into the equation that Dr. Frank derives, despite the fact that it looks general.

SEEGER: Before I give the floor to Dr. Frank, I should like to make a comment from the chair on the temperature dependence of the activation energies and entropies and the validity of the Arrhenius equation. I disagree completely with what you say, for the following reason: If you have constant temperature independent activation energy and temperature independent entropy, then these are two unrelated quantities and they may have any value you dream of. If you consider, now, temperature dependent values, then at a fixed reference temperature—like room temperature—the two absolute magnitudes are also unrelated, but the temperature dependencies are absolutely coupled, by the following equation:  $T \frac{dS}{dT} = \frac{dH}{dT}$ . In fact, assuming a temperature dependence or finding a temperature dependence for one of the quantities gives a temperature dependence of the other—not its absolute magnitude. So, there is no difficulty whatsoever. The kind of proliferation of possibilities which you indicated simply does not exist on thermodynamic grounds. If you have a curved Arrhenius plot, say  $\ln D$  against  $1/kT$  you determine the slope at one point, which is equal to minus  $H$  at that particular temperature,  $T$ . Then from the temperature dependence of the function  $H$  determined from the equation I mentioned, you get the temperature dependence of the entropy. I really cannot see the physical basis of your remarks.

KOCKS: The Stuttgart people and many other people always write on the ordinate  $\ln(\dot{a}/\dot{a}_0)$ . That's not an operational parameter. You are there assuming that  $\dot{a}_0$  is constant.

SEEGER: But only the absolute magnitude. If you assume that the other parameters are temperature independent . . .

KOCKS: Yes, *assume*.

SEEGER: In fact, you don't have to assume. If you measure the temperature dependence of  $S$ , you can separate it from the measured temperature independence of  $\dot{a}_0$ .

KOCKS: No, sir, that is not true.

SEEGER: Well, let's agree to disagree.

FRANK: First of all I want to thank Professor Seeger for having answered most of the questions which were addressed to me . . .

AUDIENCE: General laughter.

FRANK: But, what I wanted to say is connected to what you have called the zipper effect. You are completely right that the overcoming of the different obstacles of various heights are not independent from each other and that one has to account for this zipper effect, but, you see, in my expressions for the waiting times, I have a set of parameters called  $P$ , and I may use one of these parameters in order to describe this zipper effect. The problem which is left—and on this point I agree with you—is the calculation of the interaction potential between the moving dislocation and the dislocation obstacle when overcoming the obstacle by zippering. I admit that we did not account for this zippering effect in our application to neutron irradiated copper single crystals.

MITCHELL: Since this is a conference on fundamental aspects of dislocation theory, with the emphasis on the theory, I would like to ask Dr. Schoeck and Dr. Frank if the most appropriate thermodynamic potential for the discussion of dislocation phenomena should not be the measure which has the independent variables  $V$ ,  $T$  and  $\mu$ , because glide processes occur at constant volume and climb processes occur when one has a deviation in the chemical potential. Therefore one needs the chemical potential,  $\mu$ , as the independent thermodynamic variable and not  $N$ .

SCHOECK: You have to select your thermodynamic potential according to your problem. When during the deformation process you have formation of point defects, and this is a rate controlling factor, then of course you have to introduce the chemical potential of the vacancies or point defects into your rate equation. But this complicates the matter very much, and the expression for the rate equation often becomes very

complicated. The form of the rate equation then depends sensitively on the finer details of the formation of point defects by moving jogs and on such questions as to whether a dislocation is a good or bad sink for vacancies.

On the other hand, if you assume a simple glide process and if intersections or other localized obstacles are rate controlling, then you can neglect the formation of point defects. In this case the appropriate thermodynamic potential is the Gibbs free energy, which depends on the applied stress, the internal stress and the temperature.

HAASEN: What we would really like to do is construct a macroscopic strain rate theory from parameters we can measure microscopically. Now, there is no doubt that we can measure dislocation velocities and dislocation densities, but as Dr. Kocks has rightly said we cannot easily measure mobile dislocation densities. In certain cases, however, we might have a chance to get the mobile dislocation density. If it is true that dislocations get stuck in configurations like dipoles, or pile ups, or something, then there are physical properties which can differentiate between single dislocations and dipoles. This afternoon I will try to explain that maybe the electrical properties of dislocations in semi-conductors which have been a very useful material in constructing such a microscopic strain rate theory, might be a tool. Perhaps, then, we can separate dislocations in a locked configuration from free dislocations and thus the mobile dislocation density might be a measurable parameter.

LOTHE: I just want to put on record that I disagree that the attempt frequency should just be the lowest mode.

SEEGER: Alright. I think there are quite a few people who will agree with you. It's really a very complicated problem and one has to take into account the flexibility of dislocations in detail, etc.

HIRTH: I would like to write on the board. I would like to agree with what Dr. Kocks said about not being able to abstract the pre-exponential from the free energy. Suppose we have some mean jump frequency that is composed of a pre-exponential factor and an exponential containing the free energy  $\Delta G$  divided by  $kT$ —incidentally, this could apply as well to diffusion as to dislocation jumps—and suppose that  $\Delta G$  and  $\nu_o$  are functions, say, of stress and temperature. We could then write

$$\nu_o(\sigma, T) \exp(-\Delta G(\sigma, T)/kT) = \nu'_o \exp(-\Delta G'(\sigma, T)/kT),$$

where  $\nu'_o$  is not a function of stress or temperature and

$$\Delta G'(\sigma, T) = \Delta G(\sigma, T) + kT \ln \nu''_o(\sigma, T),$$

where  $\nu''_o$  is that part of  $\nu_o$  that is a function of  $\sigma$  and  $T$ . Then, unless one independently knows information about the stress and temperature dependence of the pre-exponential—either from theory or from

some other measurements—when one operates on this equation, there is no way of separating the two terms  $\Delta G$  and  $\nu_o$ . So, one cannot resolve the issue on the sole basis of mechanical property data.

SEEGER: I appreciate your point. I agree there is a difference whether you have processes where the relationship between the Arrhenius function  $\exp(-G/kT)$  is something which is fixed by the physical situation, as is the case when you calculate the concentration of point defects, and a case like you have discussed where there is a certain freedom. In diffusion processes, however, I think this difficulty does not arise since whatever you write for  $\nu_o$  is more or less fixed by the modes of vibration of the crystal, etc.; so it is really a matter of principle rather than actual importance. But I agree there is a difference.

GRANATO: I'd like to ask Professor Lothe why he feels that the attempt frequency should not be the lowest mode.

LOTHE: The lowest mode attempt frequency corresponds to an activation process which goes more or less in phase all over the segment. However, one could also think of activation processes where the applied stress does not do quite so much work, but on the other hand the line tension is more relaxed; and one can show that starting with these as equilibrium configurations, they have the same total activation energy to first order. This means that there are a number of activated configurations with the same energy to first order as the lowest mode configuration which is the one you seem to be counting when you use the dependence  $1/l$ .

SEEGER: I have come across this point when considering tunneling effects where the effective mass enter very heavily, and if it were such that it's only the lowest mode that's the important one, then you would move an enormous effective mass. You could do much better if you moved only a little bit of the dislocation; what you then lose in work, you gain by far in the exponential factor. This is also true, but not so markedly, in the case of ordinary thermal activation.

GRANATO: Those effects would be taken into account in the entropy term—that is, the effect of the other modes. The attempt frequency only means the lowest mode. All the rest are really entropy terms.<sup>6</sup>

LOTHE: It really comes down to a matter of definition of what you call the pre-exponential term.

SEEGER: What Professor Lothe would say, presumably, is that it is simply not enough to write  $\nu_o \exp(-\Delta G/kT)$  and take the  $\nu_o$  as proportional to  $1/l$ . So you would have to use a modified form for  $l$  or give the full treatment for the other modes—but you shouldn't forget the other modes.

<sup>6</sup> See footnote 3 page 1107.

FRANK: I think Dr. Schoeck has shown that you have to put the total entropy into the free enthalpy of activation which enters the Boltzmann factor. On the other hand, Professor Granato has demonstrated that you can put the entropy arising from these various activated states into the entropy factor. My feeling is that when we calculate, for example, the free enthalpy of activation by means of the theory of elasticity, we automatically take these terms into account. This is because in the formulation given by Schoeck nothing is said about the sort of entropy entering the  $\Delta G$  term. It is the total entropy.

SCHOECK: I would like to come back to Professor Hirth's statement that it is impossible to get the pre-exponential factor out of experiments. I agree only conditionally with his statement.

HIRTH: I stated it conditionally.

AUDIENCE: General laughter.

SCHOECK: The problem is really that before you try to analyze a thermally activated process, you should know what the process is so that you can construct the appropriate model with an appropriate rate equation. Once you have chosen a model, you can calculate the effective activation energy and the activation volume and compare their temperature, stress and strain dependence with what you determine experimentally.

The quantities you measure experimentally depend, of course, on whether your pre-exponential factor is constant or whether it changes during the experiment. If it changes, it introduces, however, in your experimental values some characteristic dependence on temperature and maybe other variables which are at variance with what you would expect from the model, and hence you may be able to subtract it out. I agree this approach is not without pitfalls, and in complicated systems might not work well. However, you may try different possibilities until you come up with a self-consistent picture.



# ON THE MECHANISM OF CROSS-SLIP OF DISLOCATIONS AT PARTICLES

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The effect of the misfit strain field upon the mechanism of cross-slip of dislocations at impenetrable particles in two-phase alloys is considered. The strain field is found to have a profound effect of the activation energy for cross-slip.

**Key words:** Activation energy; cross slip; mechanical properties; misfit strain; precipitation hardening.

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## I. Introduction

When a crystal containing dispersions of small particles is plastically deformed, the dislocations moving through the crystal generate rows of prismatic loops at the particles. These loops have the Burgers vector of the primary dislocations, and the rows lie along the Burgers vector direction. Such rows of loops have been observed at low strains for a number of different systems, for example in copper with silica or cobalt particles (Humphreys and Martin [1]), in copper with alumina particles and in copper-zinc alloys with alumina particles (Hirsch and Humphreys [2]), in aluminum with silicon particles (Martin and Stewart [3]), and in magnesium with particles of unknown origin (Hirsch and Lally [4]). The phenomenon is quite general, and the loops appear to be produced by a cross-slip mechanism (Hirsch [5]). The geometrical arrangements expected for impenetrable particles have been discussed by Hirsch and Humphreys [2]; however, the details of the cross-slip mechanism have not yet been discussed. Gleiter [6] has considered in some detail the problem of cross-slip and formation of prismatic loops at particles with misfit strains for the case in which the dislocations can pass through the particle during the sequence of steps leading to the eventual formation of prismatic loops. However, Gleiter based his arguments entirely on the local stresses present, without considering the activation energy controlling the various

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Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough, Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

cross-slip steps involved. The object of the present paper is to study the effect of misfit strain on the activation energy for cross-slip. It will be shown that the strain field due to the particle misfit has a profound effect on the activation energy, even when the local force on the total dislocation is small. The implication of this effect on the various cross-slip steps involved in the formation of prismatic loops is considered, for the case of impenetrable particles.

## II. The Effect of the Misfit Strain on Dislocation Width

In this section a general expression will be derived for the force on an arbitrary element of glide dislocation due to a spherical coherent inclusion; the special case of extended dislocations in the fcc lattice will then be considered.

The displacement field  $u_r$  of a spherical coherent inclusion of radius  $R$  and linear misfit  $\epsilon$ , embedded in an infinite isotropic elastic continuum (Mott and Nabarro [7]), is

$$u_r = \begin{cases} \epsilon R^3/r^2, & r \geq R \\ \epsilon r, & r < R \end{cases}$$

where  $r$  is the radial distance from the centre of the inclusion. This displacement field gives rise to a stress field  $\sigma_{ij}$  in the matrix given by

$$\sigma_{ij} = \frac{2G\epsilon R^3}{r^3} \left( \delta_{ij} - \frac{3x_i x_j}{r^2} \right), \quad r \geq R. \quad (1)$$

where  $G$  is the shear modulus of the matrix and  $\delta_{ij}$  is the Kronecker delta.

Consider an element of dislocation of unit length lying in the  $x_1 x_2$  plane at a point  $(x_1, x_2, x_3)$ , and having a Burgers vector  $\mathbf{b}$  also in the  $x_1 x_2$  plane. Using the FS/RH sign convention, the force per unit length in the slip plane exerted on the dislocation is

$$F = \sigma_{31} b_1 + \sigma_{32} b_2, \quad (2)$$

with direction as shown in figure 1(i).

Next consider the interaction of the inclusion with a unit element of a dislocation dissociated in the  $x_1 x_2$  plane into two partial dislocations separated by a distance  $d$ . There will be a difference in the forces on the two partials due to their different distances from the inclusion. However, it can be shown easily that this difference will be of order  $d/r$ , and for ribbon widths small compared with the radius of the inclusion, can be neglected; the forces will be calculated as if both partial elements were

situated at their mean distance from the inclusion, taken as  $(x_1, x_2, x_3)$ . We assume the partial elements to be parallel, of equal length, and to have Burgers vectors  $\mathbf{b}_p$  of equal magnitude. Choosing the  $x_2$  axis parallel to the Burgers vector of the total dislocation, we have for the forces per unit length,  $F_+$  and  $F_-$ , on the partials with Burgers vectors making angles  $+\theta, -\theta$ , respectively, with the  $x_2$  axis

$$F_+ = \frac{6Gb_p\epsilon R^3 x_3}{r^5} (x_2 \cos \theta + x_1 \sin \theta) \quad (3)$$

$$F_- = \frac{6Gb_p\epsilon R^3 x_3}{r^5} (x_2 \cos \theta - x_1 \sin \theta),$$

where the positive directions of  $F_+, F_-$  are shown in figure 1(ii). Note the change in sign of positive force, due to the negative stress field components in (1). There is a total force on the dissociated dislocation element:

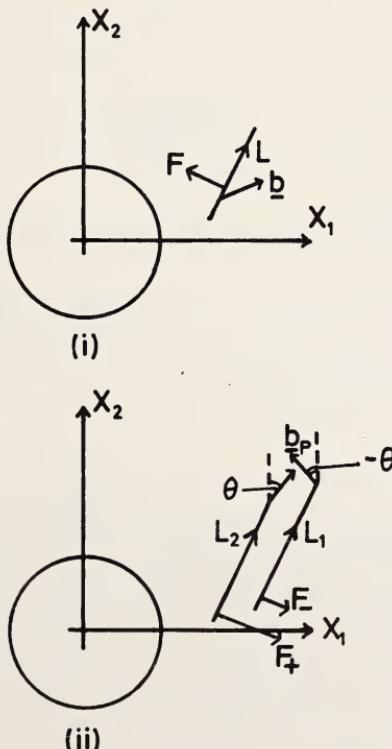


FIGURE 1. (i) Definition of the positive direction of force  $F$  on the dislocation  $L$ , assuming the FS/RH convention. (ii) The positive directions of the forces  $F_+$  and  $F_-$  on the partial dislocations  $L_1, L_2$ .

$$F = F_+ + F_- = \frac{12Gb_p\epsilon R^3 x_2 x_3 \cos \theta}{r^5}, \quad (4)$$

and a difference in the forces on the two partials:

$$\Delta F = F_+ - F_- = \frac{12Gb_p\epsilon R^3 x_1 x_3 \sin \theta}{r^5}, \quad (5)$$

where the positive directions of  $F$ ,  $\Delta F$  are those of  $F_+$  in figure 1(ii).

In general the dislocation will be in equilibrium around the inclusion under the influence of the interaction force  $F$ , given by (4), the externally applied stress, and the self-stress of the dislocation. The differential equation governing the equilibrium shape is given by Gleiter [6]. Assuming that the curvature of the partials is sufficiently small for them to be considered locally straight and parallel, their equilibrium separation will be determined by their mutual interaction, the force due to the intervening ribbon of stacking fault, and the force  $\Delta F$  given by (5). The effect of the particle force  $\Delta F$  may be seen most easily by combining it with the stacking fault energy  $\gamma$  to define an effective stacking fault energy  $\gamma^*$  given by

$$\gamma^* = \gamma \pm \frac{12Gb_p\epsilon R^3 x_1 x_3 \sin \theta}{r^5} \quad (6)$$

the choice of sign depending on whether the  $+\theta$  or  $-\theta$  partial is nearer to the inclusion.

The equilibrium separation  $d^*$  of the partials is given in terms of the separation  $d$  in the absence of the inclusion stress field by

$$d^* = d\gamma/\gamma^*. \quad (7)$$

The effective fault energy is evidently equal to the stacking fault energy if the two partial Burgers vectors are parallel to the total Burgers vector ( $\theta=0$ ), and thus the modification in  $\gamma$  is due to the difference in character between the partial dislocations and the total dislocation, e.g., for an extended screw dislocation, the change in  $\gamma$  is due to the edge components of the partial dislocations. It is also of interest to note that the change in  $\gamma$  changes sign with  $x_1 x_3$ . Thus for a dislocation lying on the slip plane  $x_3=\text{constant}$ , the effect of the inclusion will be to constrict the dislocation on one side of the inclusion, and to extend it further on the other side. It should also be noted that the constricting or extending effect can be large even though the total force on the dislocation is zero, i.e., at  $x_2=0$ .

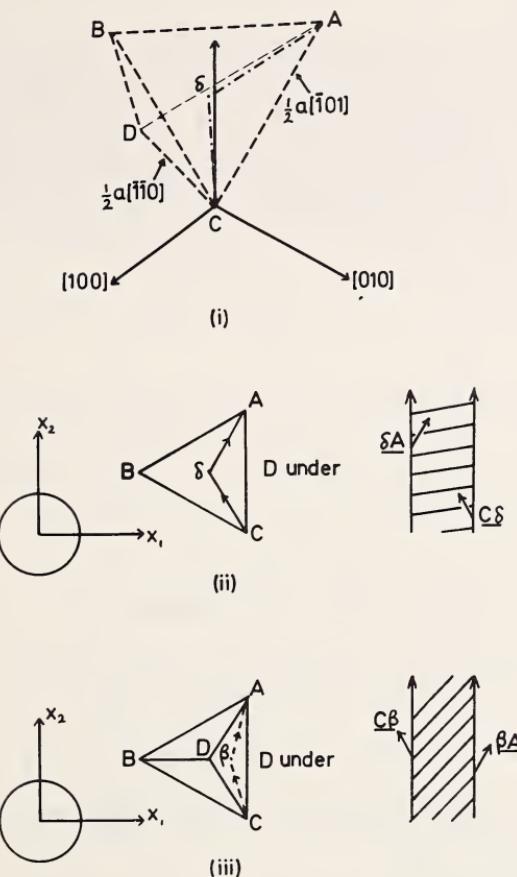
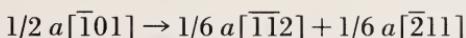


FIGURE 2. Thompson's tetrahedron, drawn relative to (i) cube axes. (ii) primary slip plane axes. (primary plane is ABC). (iii) primary slip plane axes, showing cross-slip plane (ADC); dislocation on cross-slip plane viewed from inside tetrahedron.

It is convenient at this point to restrict discussion to glide dislocations in the fcc lattice. Figure 2(i) shows a diagram of the Thompson tetrahedron relative to the crystal axes, and figure 2(ii) shows the orientation of the tetrahedron relative to the chosen inclusion axes  $[\bar{1}2\bar{1}]$ ,  $[\bar{1}01]$ ,  $[111]$  (such that the primary slip system is  $(111)[\bar{1}01]$ ). A primary  $1/2 a[\bar{1}01]$  dislocation can dissociate on the  $(111)$  plane according to the reaction



with the order of the partials as shown in figure 2(ii). Thus in (6) we take the positive sign.

In figures 3(i)–(iv) is shown qualitatively the effect of the difference in the forces on the two partials for positive and negative dislocations, and for positive and negative misfit  $\epsilon$ . For  $\epsilon > 0$ , both positive and negative dislocations are constricted for  $x_1 x_3 > 0$ , and are extended further for  $x_1 x_3 < 0$ ; the reverse applies for  $\epsilon < 0$ . In figures 3(v) and (vi) the effect is shown on a positive edge dislocation bowed out around the inclusion,

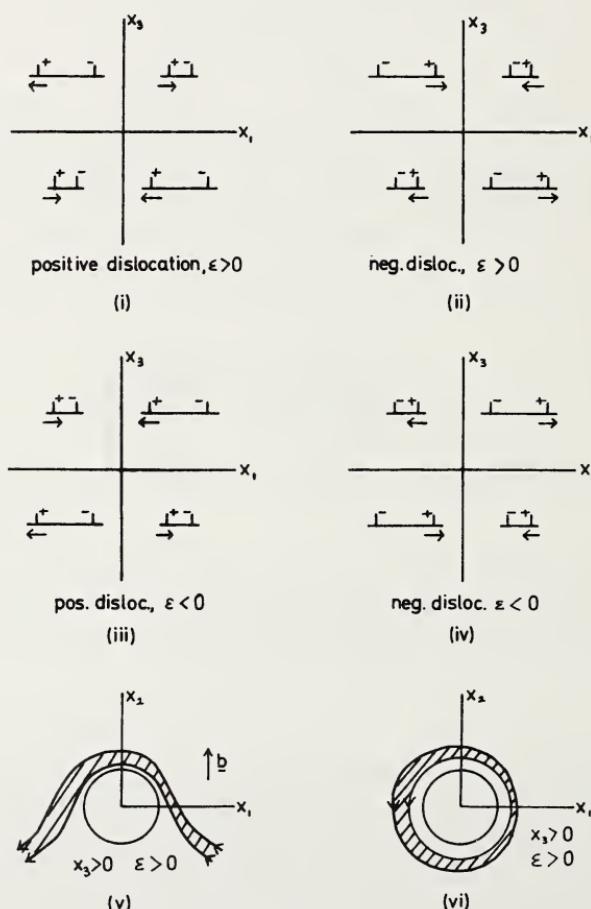
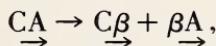
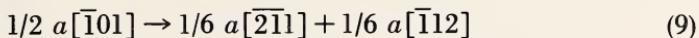


FIGURE 3. Schematic diagrams of the influence of the particle stress field: (i)–(iv) on the width of dissociated dislocations. (v) on the width of a positive edge dislocation bowed out around the particle. (vi) on the width of a positive Orowan loop around the particle.

and on an Orowan loop formed from such a dislocation, respectively, for the case  $x_3 > 0$  and  $\epsilon > 0$ . It should be noted in figures 3(v) and (vi) that the edge components, for which  $x_1 = 0$  in (6), have their width unchanged by the inclusion stress field. It is clear that once the arms of the bowed edge dislocation in figure 3(v) reach screw orientation, cross-slip of the constricted arm can occur more easily than in the absence of the inclusion stress field, while cross-slip of the extended arm will be more difficult.

The force constricting the partials can be considerable; at the surface of the inclusion, at  $x_1 = x_3 = R/\sqrt{2}$ ,  $r = R$ , then  $\Delta F = 3Gb_p\epsilon$ , and for  $\epsilon = 10^{-2}$ ,  $\Delta F \sim Gb_p/30$ , which is of the order of the theoretical shear strength.

Once cross-slip has occurred, the  $1/2 a[\bar{1}01]$  dislocation can redissociate in the  $(\bar{1}\bar{1}1)$  (see fig. 2(iii)) cross-slip plane according to



with the order of the partials as in fig. 2(iii). The effective fault energy  $\gamma_c^*$  on the cross-slip plane is given in terms of the primary coordinates  $x_1, x_2, x_3$  by

$$\gamma_c^* = \gamma \mp \frac{12Gb_p\epsilon R^3}{9r^5} (x_1 + 2\sqrt{2}x_3)(x_3 - 2\sqrt{2}x_1) \sin \theta, \quad (10)$$

with the negative sign being chosen for a positive dislocation.

Figures 4(i) and (ii) show a projection on the  $x_2 = \text{constant}$  plane. The regions of constriction and extension on the primary and cross-slip planes are shown for positive dislocations and for positive  $\epsilon$  (fig. 4(i), corresponding to an inclusion larger than the cavity in the matrix) and negative  $\epsilon$  (fig. 4(ii)). For negative dislocations the diagrams are similar, but the order of the partials is reversed.

The inclusion exerts also a total force, which can assist cross-slip, on the dislocations of figure 4. The sign of the force changes with the sign of  $x_2 x_3$ , and with the sign of the dislocation. The arrows in figures 4(i) and (ii) show the sense of the total force for  $x_2 > 0$ ; for  $x_2 < 0$ , and for negative dislocations and  $x_2 > 0$ , the force is reversed. Thus for  $\epsilon > 0$ ,  $x_2 > 0$ , a positive dislocation will be driven in a clockwise circuit around the particle; for  $x_2 < 0$  the circuit will be anticlockwise. There are, of course, other forces on the dislocation, due to the applied stress, and due to the image interaction with the inclusion. The sense of the applied stress on

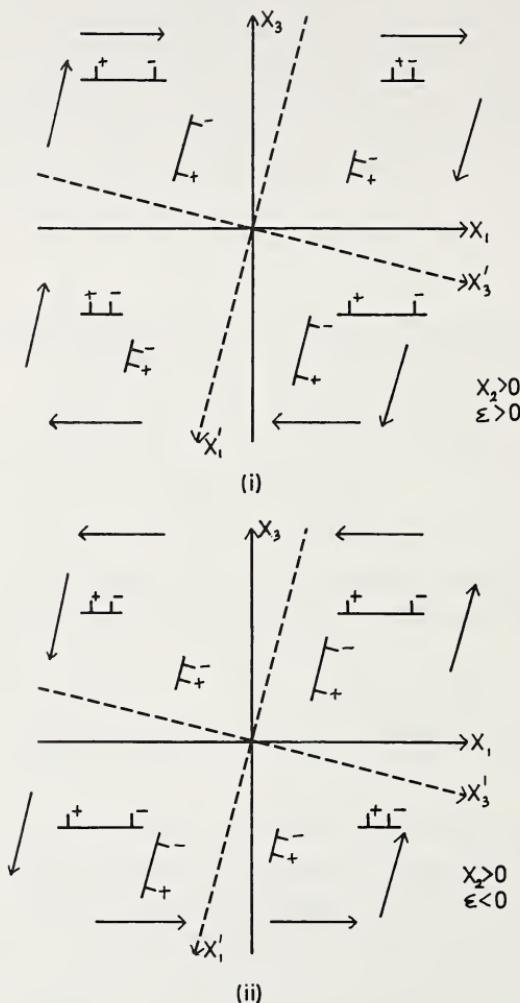


FIGURE 4. The regions of constriction and extension on the primary and cross-slip planes for positive dislocations and for positive  $\epsilon$ (i) and negative  $\epsilon$ (ii).

the cross-slip plane will depend upon the orientation of the stress with respect to the crystal axes; the image force will be complicated in form, but will in general repel all dislocations if the shear modulus of the particle is greater than that of the matrix, and vice versa.

Consider the cross-slip process for a bowed edge dislocation (fig. 3(v)) or an Orowan loop (fig. 3(vi)); the screw arm must cross-slip three times in order to bypass the inclusion. Some of these steps will be easy (labeled

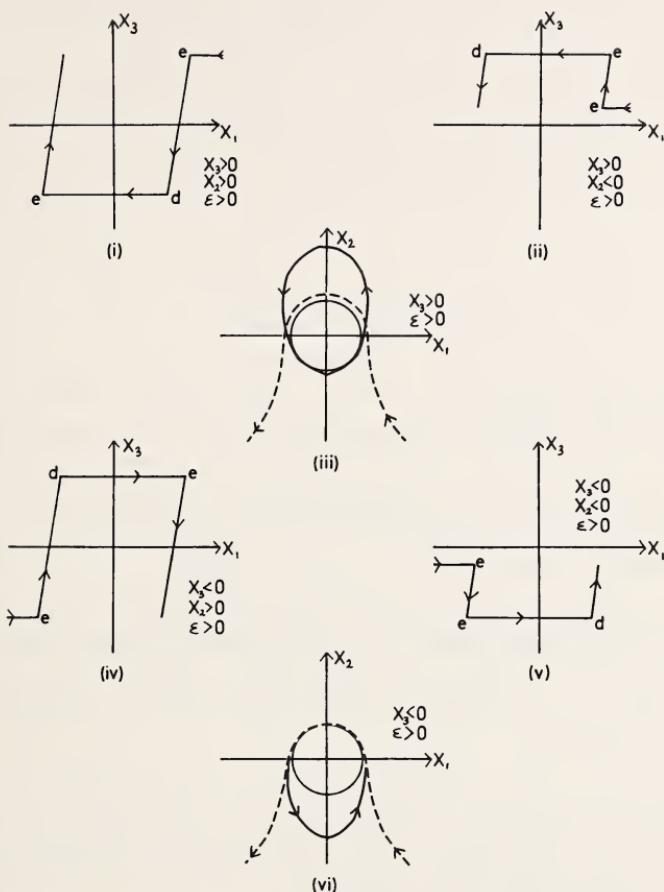


FIGURE 5. (i) and (ii) Possible cross-slip paths for a positive dislocation for  $x_3 > 0$ ,  $\epsilon > 0$ , and for  $x_2 > 0$ ,  $< 0$  respectively. (iv) and (v) Similar paths, for  $x_3 < 0$ . (iii) and (vi) Schematic diagram of the equilibrium shapes of a positive edge dislocation bowed out around the particle, and of a positive Orowan loop around the particle, for  $x_3 > 0$  and  $< 0$ , respectively.

“e” in fig. 5) because the dislocation is constricted by the inclusion stress field, others difficult (labeled “d” in fig. 5), because the cross-slipping dislocation is extended further.

Figures 5 (i) and (ii) show possible cross-slip paths for a positive dislocation at  $x_3 > 0$ , for  $\epsilon > 0$ , and for positive and negative  $x_2$ , respectively: figures 5 (iv) and (v) show similar paths for  $x_3 < 0$ . In each case two easy cross-slip steps and one difficult step are necessary. In the cases where the difficult step is the third (figs. 5 (ii) and (v)), cross-slip can be assisted somewhat by the attractive interaction of the cross-slipped dislocation

and the remaining arm of the loop. For this reason the circuits of figures 5 (ii) and (v) may be preferred, although as will be shown in section IV, this effect is relatively small for practical values of  $\epsilon$ .

It is also of interest to consider qualitatively the shape of the dislocation line in the neighbourhood of the inclusion, since cross-slip can occur only when the dislocation has local screw character. In the case of  $x_3 > 0$  (figs. 5 (i) and (ii)), a positive dislocation is repelled by the particle for  $x_2 > 0$ , and is attracted for  $x_2 < 0$ . For an Orowan loop, the expected equilibrium shape is shown in figure 5(iii). In the region of negative  $x_2$ , the loop will lie close to the particle, in equilibrium under the self-stress of the loop, the attractive particle interaction, and the repulsive image interaction: for positive  $x_2$  the loop will lie further from the particle, since the particle interaction is now repulsive. Thus it is likely that screw orientation will occur for  $x_2 > 0$ , so that cross-slip via the circuit of figure 5(i) is possible. In the case of a bowed dislocation, however (dashed line in figure 5(iii)), Gleiter [6] has shown that screw orientation is reached in the critical configuration at  $x_2 < 0$ . Thus cross-slip in this case is possible via the circuit of figure 5(ii).

For  $x_3 < 0$  (figs. 5 (iv) and (v)) the expected shapes are shown in figure 5(vi). Provided that the dislocation does not cut through the particle, both the Orowan loop and the bowed dislocation (dashed line) attain screw character for  $x_2 < 0$ , so that in both cases cross-slip via the circuit of figure 5(v) is possible.

The above discussion of the loop shape is highly simplified. For the small dislocation-particle distances involved, the precise shape of the inclusion and the anisotropy of the image stress will have a profound influence on the shape of the dislocation.

It should be noted that the magnitude of the driving stress can be considerable e.g., for  $x_2 = x_3 = R/\sqrt{2}$ , the driving stress on the primary plane is  $3\sqrt{3}Gb_p\epsilon$ , which for  $\epsilon = 0.01$  is again of the order of the theoretical shear strength.

### III. Conditions for Cross-Slip at Absolute Zero

In this section we consider the magnitude of the constricting effect of the inclusion stress field. It will be shown that the easy steps in the bypass mechanism can take place at absolute zero for suitable values of linear misfit  $\epsilon$  and stacking fault energy  $\gamma$ . We assume a dislocation in equilibrium around the inclusion, and consider a segment of screw orientation at the point  $(x_1, 0, x_3)$ . It is further assumed that constriction is complete when the two partials are separated by a distance less than or equal to the magnitude of the total Burgers vector.

For the sake of simplicity, and in order to assess the importance of the effect, we shall consider the maximum constricting stress for a given radius  $r$  from the particle centre; it follows from (5) that this occurs for  $x_1 = x_3 = r/\sqrt{2}$ . (It should be noted of course that for values of  $x_3 < R/\sqrt{2}$  this maximum cannot be attained, and for small values of  $x_3$  in particular the effective constricting stress will be considerably smaller.) Inserting these values in (6), together with  $\theta = 30^\circ$ ,  $b_p = b/\sqrt{3}$ , and  $d = Gb^2/16\pi\gamma$  (assuming Poisson's ratio to be 1/3), it is found, after some rearrangement, that complete constriction can occur for

$$1 \leq \left(\frac{r}{R}\right)^3 \leq \frac{\sqrt{3}\epsilon}{1/16\pi - \gamma/Gb}. \quad (11)$$

In figure 6 the maximum value of  $(r/R)$  satisfying (11) is shown as a function of the linear misfit  $\epsilon$  for various values of the dimensionless quantity  $\gamma/Gb$ .

These results suggest that at particles with large coherency strains, e.g., Co particles in Cu ( $\epsilon \sim 10^{-2}$ ), the screw dislocations (in the favourable positions) are completely constricted even at the absolute zero. On the other hand, the misfit strain expected from incoherent impenetrable oxide particles will be considerably less,  $\epsilon \sim$  a few times  $10^{-3}$ , estimated

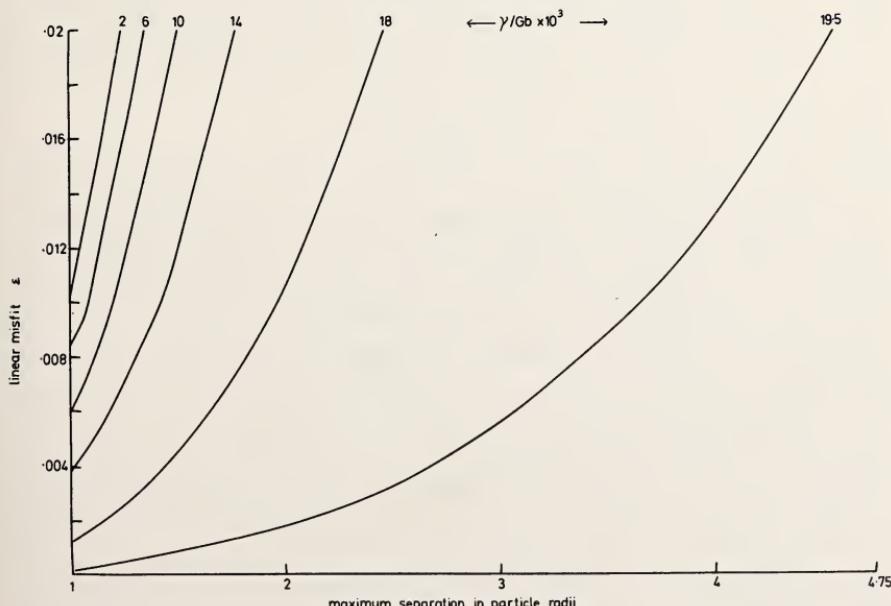


FIGURE 6. The maximum separation in units of particle radius,  $r/R$ , for which complete constriction can occur at the absolute zero, shown as a function of linear misfit  $\epsilon$  for various stacking fault energies.

from differences in the thermal contraction during cooling. For such alloys thermal activation would be needed at low temperatures if  $\gamma/Gb$  is too small. Thus for alloys with  $\gamma/Gb \sim 10^{-2}$  (e.g.,  $\gamma \sim 100$  ergs/cm<sup>2</sup> for Cu base alloys) thermal activation is required to complete the constriction; for Al base alloys ( $\gamma/Gb \sim 2 \times 10^{-2}$ ) the dislocations would be completely constricted at 0 K.

However the difficult cross-slip steps can never take place without the aid of thermal activation, since in this case the partials are extended rather than constricted by the inclusion stress field.

#### IV. Cross-Slip With the Aid of Thermal Activation

At finite temperatures the presence of thermal energy can assist the cross-slip process. Thermally activated cross-slip in the rapidly varying stress field around an inclusion will be a complex process, and the highly simplified models used below can do no more than give an estimate of the energy changes involved. We consider two simple models with the aid of the diagrams in figure 7. For cross-slip to occur, the dissociated screw dislocation of figure 7(i) must first be recombined over part of its length, forming constrictions at A and B (fig. 7(ii)). The energy necessary to effect this change can be divided roughly into two parts.

(a) The energy of the constrictions at A and B. Provided that the length AB is large compared with the dislocation width, this energy will be independent of the length AB, and may be written as  $2U_1$ , where  $U_1$  is the energy of a single constriction, assumed to include the effect of the work done by the applied and internal stresses.

(b) The energy required to recombine the dislocation over the length AB. Again, if AB is assumed large compared with the dislocation width, this energy will be linear in  $\ell$ , the length AB. If  $E_0$  and  $E_1$  are the energies per unit length of the constricted and dissociated configurations, respectively, with  $E_1$  assumed to include the effect of the work done by applied and internal stresses, then the recombination energy will be  $\ell(E_0 - E_1)$ .

If the length  $\ell$  becomes sufficiently large, the constricted part of the dislocation can redissociate on the cross-slip plane (Friedel [8], Escaig [9], (fig. 7(iii)), releasing energy  $\ell(E_0 - E_2) - 2U_2$  (the condition that this quantity be not less than zero defines the activation length), where the subscript "2" indicates reference to the cross-slip plane. The constrictions A and B are then attracted by a force  $E_2$ , and are drawn apart by a force  $E_1$ ; thus the configuration of figure 7(iii) will collapse into the fully cross-slipped state provided that  $E_1 > E_2$ , i.e., as shown below, provided that the separation of the partials is greater in the cross-slipped state than in the initial state.

Provided that these conditions are satisfied, cross-slip is possible by model (a), with activation length  $\ell_a^*$  and activation energy  $H_a^*$  given by

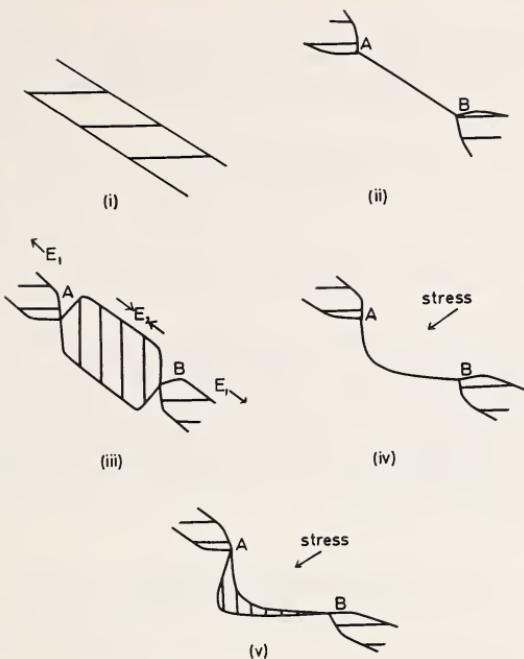


FIGURE 7. Schematic diagram of the activation processes. (i) The unperturbed extended dislocation. (ii) The dislocation constricted between A and B. (iii) Model (a): the dislocation is redissociated between A and B on the cross-slip plane without bowing out. (iv) Model (b): the dislocation is bowed out in the cross-slip plane without redissociation. (v) Model (c): the dislocation is both bowed out and redissociated in the cross-slip plane.

$$\begin{aligned}\ell_a^* &\simeq 2U_2/(E_0 - E_2) \\ H_a^* &\simeq 2U_1 + \ell_a^*(E_0 - E_1).\end{aligned}\quad (12)$$

When the total stress (i.e., the sum of the particle driving stress and the applied stress) on the dislocation is large, alternative mechanisms (figs. 7(iv), (v)) may be possible. The constricted (fig. 7(iv)) or redissociated (fig. 7(v)) segment of dislocation AB is glissile in the cross-slip plane, and can bow out under the influence of an applied stress. For a sufficiently high curvature (i.e. for a sufficiently high stress) the loop AB will become unstable, and cross-slip can occur. Consider first the case where the length AB in the critical state is too small to permit redissociation (fig. 7(v)). In this case (model (b)) the equations analogous to (12) are given by (Friedel [8], Escaig [10])

$$\begin{aligned}\ell_b^* &\simeq \frac{2}{\tau b} \sqrt{2E_0(E_0 - E_1)} \\ H_b^* &\simeq 2U_1 + \ell_b^*(E_0 - E_1),\end{aligned}\quad (13)$$

where  $\tau$  is the total stress on the dislocation.

Next consider the case in which the length AB is sufficiently large to permit redissociation in the cross-slip plane (fig. 7(v), model (c)). The activation length and energy are now given by (Duesbery and Hirsch [11])

$$\ell_c^* \approx \frac{2}{\tau b} \sqrt{2E_0(E_2 - E_1)}$$

$$H_c^* \approx 2U_1 + 2U_2 + \ell_c^*(E_2 - E_1). \quad (14)$$

Equations (14) are valid only for  $E_2 \geq E_1$ , since for  $E_2 < E_1$  the critical length and the activation energy will be given by (12).

The unknown quantities  $U$  and  $(E_1 - E)$  can be estimated from elasticity theory by established methods (Escaig [10]; Duesbery [12]), and only the results are given here. For dissociated screw dislocations in the fcc lattice we put

$$2U \approx 0.0536Gb^3 \sqrt{\ln \frac{d^*}{b}} \cdot \frac{d^*}{b} \left(1 - \frac{b}{d^*}\right)^2$$

$$(E_0 - E) \approx 0.0199Gb^2 \left( \ln \frac{d^*}{b} - 1 + \frac{b}{d^*} \right), \quad (15)$$

where  $d^*$  is the separation of the partials on the relevant slip plane in the presence of the imposed stress fields.

As mentioned above, in order for cross-slip to be possible by model (a), the inequality  $d_2^* > d_1^*$  must be satisfied; cross-slip may be more favourable by model (b), if  $\ell_b^* < \ell_a^*$ , but cross-slip by model (c) will be unfavourable. If  $d_2^* < d_1^*$ , however, cross-slip must occur by models (b) or (c), since in this case the cross-slipped state of model (a) is unstable. If  $\ell_b^* < 2U_2/(E_0 - E_2)$ , model (b) will be the more favourable; if  $\ell_b^* > 2U_2/(E_0 - E_2)$ , model (c) will be preferred.

A little manipulation of (6) and (10) shows that cross-slip from the primary plane to the cross-slip plane is possible by model (a) provided that

$$(\sqrt{2}x_3 - x_1)(x_3 + \sqrt{2}x_1) > 0. \quad (16)$$

Conversely, cross-slip from the cross-slip plane to the primary plane is possible by model (a) only if the left-hand side of (16) is negative.

It should be noted that the condition (16) for the primary-cross-slip plane step to be possible by model (a) immediately precludes the possibility of the reverse process by the same mechanism. Similarly, the stress-activated models (b) and (c) are not reversible, since activation requires the formation of an unstable loop of dislocation. Thus the rate of formation

of prismatic loops by these mechanisms will be controlled by that cross-slip step requiring the largest activation energy, and is not given by the product of the rates for all three necessary steps.

The activation energies for cross-slip have been calculated as a function of position for various stacking fault energies, linear misfit values, and for several applied stresses, using the equations given above. Figures 8 (i) and (ii) show the variation of activation energy around the inclusion for stacking fault energy  $\gamma = 0.008$  Gb (corresponding roughly to 80 ergs/cm<sup>2</sup>), for linear misfit  $\epsilon = 0.005$ , and for zero applied stress. Figure 8(i) shows the primary to cross-slip plane activation energy, while figure 8(ii) shows the cross-slip back to primary plane activation energy. In both cases values are shown for  $x_3 > 0$  only; figures for  $x_3 < 0$  can be obtained by rotation of the diagrams by 180° about the  $x_2$  axis. In the case of the stress-aided mechanisms, the value of  $x_2$  was chosen to maximise the driving stress at fixed  $x_1$ ,  $x_3$  (i.e., at  $x_2^2 = 1/4(x_1^2 + x_3^2)$ ); in the case of mechanism (a), the

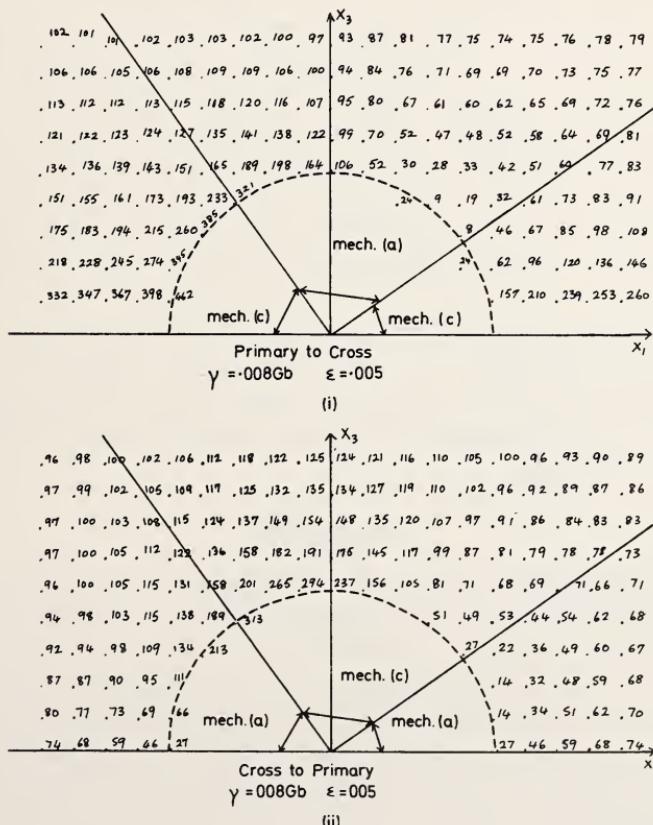


FIGURE 8. The variation of the activation energy, in units of 0.001 Gb<sup>3</sup>, with position around the particle for stacking fault energy  $\gamma = 0.008$  Gb, linear misfit  $\epsilon = 0.005$ , (i) for primary to cross-slip plane steps, and (ii) for cross to primary slip plane steps.

value shown is the lesser of the two calculated at  $x_2 = 0$  and  $x_2^2 = 1/4(x_1^2 + x_3^2)$ . The favourable regions of mechanisms (a) and (c) are clearly shown; it is found that mechanism (b) begins to operate only for total stresses in excess of  $\sim 0.02$  G.

Figure 8 shows that for  $\gamma = 0.008$  Gb,  $\epsilon = 0.005$ , the controlling "difficult" cross-slip step requires an activation energy  $\sim 1/8$  Gb<sup>3</sup>. In this case the activation energy is likely to be overestimated, since the cross-slipping dislocation is extended by the particle stress. Cross-slip may be easier at a larger value of  $|x_2|$ , such that the driving stress is still large, while the extending stress is smaller.<sup>1</sup>

In order to investigate the cross-slip process in more detail, one particular cross-slip sequence (corresponding to fig. 5(ii)) was chosen, with coordinates  $(0.80R, \pm 0.44R, 0.40R)$ ;  $(R, \pm 0.70R, R)$ ,  $(-R, \pm 0.70R, R)$  for the first, second and third steps, respectively. Figures 9 (i)–(iii) show the activation energies for these steps as a function of stacking fault energy for zero applied stress and for linear misfits  $\epsilon = 0.005, 0.010$ . Calculations have also been made for nonzero applied stresses, but the difference in activation energy is small. For example, in figure 9(iii), an applied stress of 0.01 G on the cross-slip plane reduces the activation energies shown by less than 10 percent. Since applied stresses greater than  $\sim 0.001$  G are unlikely to occur in dispersion-hardened fcc. materials, it seems likely that the applied stress will have little influence on the cross-slip process. The reason for the relatively small effect due to the applied stress is that the internal stress from the particle is considerably greater.

It should be noted that the coordinates selected for the cross-slip sequence of figure 9 are not those for which maximum constriction occurs. Thus there is no anomaly in the finite values of activation energy in figure 9 at stacking fault energies for which figure 6 would predict complete constriction.

## V. Discussion

The experimental observations give (a) some information about the cross-slip paths (c.f. fig. 5), and (b) about the activation energies involved.

(a) Humphreys (private communication) has examined the loop structures in a Cu–20 percent Zn alloy, sectioned normal to the slip plane with the slip direction contained in the plane of the foil. The loops are always less than half the particle diameter high, and the top edge of the loop is approximately at the same height as the top of the particle. The

<sup>1</sup> For dislocations on planes close to the equator, the first "easy" step in the cross-slip sequence also has a high activation energy.

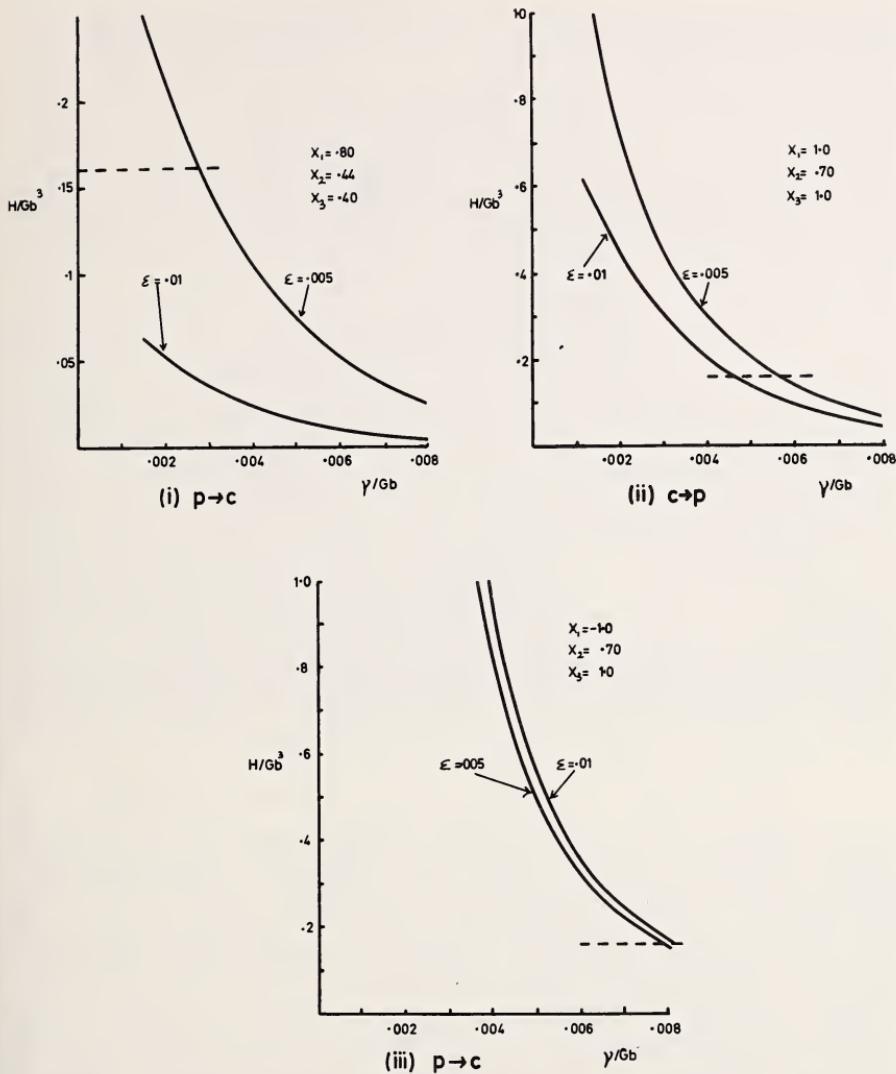


FIGURE 9. (i), (ii), and (iii) show the activation energies for the first, second, and third cross-slip steps, respectively, as a function of stacking fault energy, for linear misfits  $\epsilon = 0.005$  and  $\epsilon = 0.010$ .

loop shapes are therefore in accordance with paths 5(ii) and 5(v). The size of the loops is also in accord with this mechanism.

(b) It is pointed out by Hirsch and Humphreys [2] that it is difficult to decide from the experimental evidence whether prismatic loops are formed as a result of a dislocation bypass mechanism, or by indirect means e.g., cross-slip of Orowan loops. It is therefore of interest to consider whether the formation of prismatic loops could account quantitatively for the observed strain rate. The number of Orowan loops produced per

particle per second is given in terms of the plastic strain rate  $\dot{\epsilon}$  by (Hirsch and Humphreys [2], eq 22)

$$\frac{dN}{dt} = \frac{2R}{b} \dot{\epsilon}. \quad (17)$$

If the strain rate is to be supportable by prismatic loop formation (i.e., if prismatic loops are formed in preference to Orowan loops) then the rate of cross-slip must not be less than the rate of Orowan loop formation in (17), i.e.,

$$\frac{2R}{b} \dot{\epsilon} \leq \frac{2R}{\ell^*} \cdot \frac{\nu_D b}{\ell^*} \exp(-H/kT), \quad (18)$$

where  $\ell^*$  is the activation length,  $2R/\ell^*$  an estimate of the number of available activation sites,  $\nu_D$  is the Debye frequency, and  $\nu_D b/\ell^*$  the vibration frequency of a dislocation with wavelength  $\ell^*$ ;  $k$  is Boltzmann's constant and  $T$  the absolute temperature.

Assuming  $\nu_D = 10^{13} \text{ s}^{-1}$ ,  $\ell^* \sim 30b$ , (18) reduces to

$$\dot{\epsilon} \leq 10^{10} \exp(-H/kT). \quad (19)$$

For deformation at room temperature ( $T = 300 \text{ K}$ ), with a typical strain rate of  $10^{-4} \text{ s}^{-1}$ , equation (19) places an upper limit on the activation energy of  $0.81 \text{ eV}$ , or about  $0.16 \text{ Gb}^3$ . For activation energies greater than this, Orowan loops will be formed before prismatic loops.

From figure 9, with  $\dot{\epsilon} = 0.005$ , it can be seen that this limiting value corresponds to  $\gamma/Gb \gtrsim 0.0028, 0.0056, 0.0079$ , respectively, for the first, second and third cross-slip steps, respectively. It is clear from figure 9(iii) that the rate-determining difficult step is more sensitive to stacking fault energy than to the misfit, and thus we would expect a transition between prismatic loop formation and Orowan loop formation as the stacking fault energy is decreased.

There is evidence that such a transition occurs (Humphreys, [13]; Hirsch and Humphreys, [2]; Orowan loops are observed in an alloy of Cu-30 percent Zn containing alumina particles (fig. 10), but the critical stacking fault energy is  $\lesssim 20 \text{ ergs/cm}^2$ , in contrast to the value  $\sim 80 \text{ ergs/cm}^2$  suggested by the above theory.

There are however a number of factors which make detailed comparison with experiment difficult. Firstly, the parameter  $\dot{\epsilon}$  for the particles under observation is not known. Secondly, Orowan loops could first be formed during the deformation and then subsequently cross-slip, aided possibly by further Orowan loops formed later and adding to the internal stress, which is not taken into account in the calculation. The structure observed for the alloys of lowest stacking fault energy consists of Orowan plus prismatic loops suggesting that this mechanism operates in this



FIGURE 10. Orowan loops around alumina particles in a Cu-30 percent Zn alloy.

case. Thirdly, a considerable time interval ( $\sim 10^5$  s) elapses between carrying out the deformation and observing the structures by electron microscopy at room temperature. In principle therefore Orowan loops could cross-slip during this time interval at room temperature. However, after deformation at room temperature, and in the case of Cu containing silica or alumina particles also after deformation at 77 K, the structures observed suggest that most of the cross-slip processes occur during the deformation, although the possibility of perhaps one Orowan loop being left around the particle and subsequently cross-slipping cannot be ruled out. Another uncertainty arises from the non-spherical shape of the particles which introduces deviation from spherical symmetry in the stress field.

It is also possible that a different mechanism may be responsible, for low stacking fault energies. It is clear from (12) & (14) that for the operative mechanisms, the activation energy cannot be less than the sum of the constriction energies, which for wide dislocation energies can be very large. It is not likely that refinement of the calculations would reduce the

constriction energies by the factor of 10 necessary to explain experimental results. A possible alternative mechanism in such circumstances was suggested by Fleischer [14]. In this mechanism the  $1/6 a[\bar{2}11]$  partial on the primary plane can redissociate in the cross-slip plane, forming a nonplanar configuration, according to



if the cross-slip is through an obtuse angle, or



if the cross-slip occurs through an acute angle; in either case a sessile dislocation results at the intersection of primary and cross-slip planes. The dislocation is then pinned, so that the large driving stress of the inclusion can be used to constrict the remaining  $1/6 a[\bar{1}\bar{1}2]$  primary partial. At stacking fault energies  $\geq 60$  ergs/cm<sup>2</sup> the separations of the partials in the intermediate configurations are smaller than the total Burgers vector, so that cross-slip by this mechanism would be indistinguishable in this case from the mechanisms considered in detail in the previous sections. However, for lower stacking fault energies it is likely that the Fleischer mechanism would require an activation energy appreciably smaller than the mechanisms discussed above.

In conclusion it should be noted that the particle strain field has a profound effect on the activation energy for cross-slip, that so far the observations are in qualitative agreement with the theory, but that at present it appears that cross-slip at the particle is even easier than expected are the basis of the theory described in this paper.

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## **Discussion on Paper by M. S. Duesbery and P. B. Hirsch.**

**BULLOUGH:** Have you allowed for change in line shape, such as bowing out around the obstacles?

**DUESBERY:** No, we haven't.

**BULLOUGH:** This effective stacking fault energy is based on straight dislocations, then?

**DUESBERY:** Yes, it is based on the assumption that the partial elements are straight and parallel. The particles are very large, of the order of 2,000 Å in diameter, so that this might not be a bad assumption.



# THEORIES OF THERMALLY ACTIVATED PROCESSES AND THEIR APPLICATION TO DISLOCATION MOTIONS IN CRYSTALS

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Thermally activated processes involving dislocations are usually treated by applying the theory of absolute reaction rates and the string approximation of dislocations. In the first part of this paper the limits of validity of these treatments are discussed. A paper of T. Geszti is briefly reviewed in which it is shown that in processes involving *point defects* deviations from the rate theory must be expected if the energy exchange between defect and lattice waves is slow compared with the average time between jumps, e.g. if localized or quasi-local vibrations contribute essentially to the defect motion. It is pointed out that the localized modes of dislocations may also lead to deviations from the rate theory.

In the second part a treatment of the double kink relaxation (Bordoni relaxation) based on the Kramers-Brinkman diffusion theory of chemical reactions is given. After showing that in f.c.c. metals the influence of the Peierls potential is so small that on dislocation loops only one kink pair must be considered explicitly whereas the remaining parts of the loops may be described by the string approximations, diffusion equations for the loop motion are derived. Under certain conditions these equations are equivalent to a system of reaction rate equations. Exact solutions of this system are not yet available. However, the behaviour of dislocation loops in the amplitude independent region of internal friction measurements may be extrapolated combining results of two limiting cases: a double well model and a simplified multi-well model.

The relaxation strength and the preexponential factor of the relaxation time calculated have the same orders of magnitude as in measurements of the Bordoni peak. The loop length dependence of the damping peak is in good agreement with neutron-irradiation measurements. The characteristic half-width of the Bordoni peak may partly be explained using loop length and stress distributions.

**Key words:** Bordoni-peaks; dislocation motion; kink relaxation; mechanical properties; thermal activation.

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## I. Introduction

The plastic behaviour of crystals is to a considerable extent determined by thermally activated processes involving dislocations. These processes are mostly treated by applying the theory of absolute reaction rates and the string approximation of dislocation. The purpose of this paper is to discuss the limits of validity of these treatments with a view of more recent developments both in the theory of thermally activated processes and in dislocation dynamics.

As an example for the application of the Kramers-Brinkman diffusion theory of chemical reactions to dislocation problems a treatment of double kink relaxation (Bordoni relaxation) will be briefly reviewed.

## II. Theories of Thermally Activated Processes

The theory of thermally activated processes was originally elaborated for chemical reactions. The well-known "transition state theory" has been developed for defects in crystals by Vineyard [1]. In this theory the transition of a crystal in an atomic jump process from a stable equilibrium state  $i$  in  $N$ -dimensional configuration space to another one  $j$  over a single saddle-point  $S$  is considered. The jumping rate  $\Gamma_{ij}$  from potential well  $i$  to  $j$  is calculated as the one-sided current going out from well  $i$ , directed perpendicular to the hypersurface  $S_{ij}$  in the configurational space dividing well  $i$  from  $j$ . Equilibrium distribution functions are assumed in the potential well and at the saddle-point. Employing the theory of small oscillations in the high temperature approximation leads to the well-known expression for the jumping rate:

$$\Gamma_{ij} = \nu_{\text{eff}} \cdot e^{-\Delta\phi/kT}, \quad \nu_{\text{eff}} = \left( \prod_{l=1}^N \nu_l \right) / \left( \prod_{l=1}^{N-1} \nu'_l \right). \quad (1)$$

$\Delta\phi$  is the potential energy difference between the saddle-point and the ground state  $i$ .  $\nu_l$  are the eigen frequencies in the ground state,  $\nu'_l$  the eigen frequencies in the activated state.

Equation (1) is frequently applied to thermal activated motion of dislocations, assuming plausible values for the jump frequency  $\nu_{\text{eff}}$ .

Granato et al. [2] have actually calculated the effective jump frequency  $\nu_{\text{eff}}$  in (1) for different obstacles. The eigen-frequencies of both states were determined in the framework of the vibrating string model.

The applicability of the transition state theory is limited since Brownian motion in the saddle-point region and deviations from equilibrium dis-

tribution functions may occur. This contradicts the assumptions of the transition state theory. In the case of point defects the situation has been clarified by Geszti [3] in a thorough investigation.

Geszti points out that loss of energy and loss of momentum are two entirely different aspects of defect motion. He finds that in hopping processes (characterized by an activation energy  $\Delta\phi \gg kT$ ) the basic dissipation process is that of momentum. This process occurs during the jump of the defect over the barrier by turning from directed motion on the barrier into irregular oscillation around the reached equilibrium state. The loss of momentum takes place within a time  $t_p$  much shorter than the meantime between two jumps over the barrier, i.e.,

$$t_p \ll \frac{1}{\Gamma_{ij}}. \quad (2)$$

$t_p$  is of the order of a few lattice vibration periods, i.e.,  $t_p \approx \omega_D^{-1}$  ( $\omega_D$  = Debye frequency).

For the loss of energy two limiting cases can be distinguished:

(a) the case of fast thermalization, where extreme (jumping) energy values are created by random phase-coincidence of the normal modes and are destroyed within a time  $\tau \approx (\omega_D)^{-1}$  as short as  $t_p$ . This mechanism has been investigated by Rice [4]. It is in this case that the predictions of rate theory are fully realized.

(b) a case of low thermalization, where localized or quasi-local vibrations give contributions to the motion of the defect comparable with that of all the non-localized modes. The intrawell thermalization of the defect is dominated by a quantity slowly varying with respect to  $t_p$  (say, the energy of the local or quasi-local vibration). In this case deviations from the rate theory must be expected. A treatment of this case has been given by Prigogine and Bak [5].

In order to check the applicability of the transition state theory to dislocations one has to investigate the mechanisms of energy exchange between dislocation and lattice.

The situation is rather transparent in the case of the double kink relaxation process since kinks have only one degree of freedom and their mass and viscosity are rather well-defined quantities if one excludes the double kink creation proper. As pointed out by Seeger and Schiller [6], the rate theory may in this case be replaced by Kramers' [7] respectively Brinkman's [8] diffusion theory.

In the case of depinning from point obstacles more recent results of dislocation dynamics should be considered. Different authors have found localized normal modes for infinitely long screw and edge dislocations

[9–11]. Besides resonance modes for screw dislocations exist. It may be possible that these modes, modified by the finite loop length, give rise to deviations from the transition state theory.

### III. Application of Kramers' Diffusion Theory to the Double Kink Relaxation Process

#### III.1. Properties of dislocation loops in the Peierls potential

##### A. EQUILIBRIUM CONFIGURATION

We consider a pinned dislocation loop in the Peierls potential and describe it by the distance between the pinning points  $L$  ("loop length"), the angle  $\varphi$  to a close-packed direction and by the applied (constant) stress  $\sigma_i$ . For loops that have a tangent to a close-packed direction several equilibrium configurations exist. It is only these loops that are capable of taking part in the double kink relaxation process. This process has been proposed for the interpretation of the Bordoni peak by Seeger [12]. The static equilibrium of a dislocation loop is best discussed by means of an energy diagram used by Alefeld [17] showing the loop energy versus the area  $F$  swept over by the bowing dislocation. Figure 1b gives the special case of vanishing internal stresses and absence of geometric kinks ( $\sigma_i=0$ ,  $\varphi=0$ ). The energy increases in portions of  $2W_k$ . Calculations for a dislocation in copper show (see fig. 1a) that the mutual attraction between the kinks of a created pair plays a negligible role beyond a distance of  $1.5 w$  ( $w$ =kink width). Therefore a long plateau in the diagram exists. Kinks at the ends of the loop are pushed aside when a new pair is created leading to an increase of the energy at the end of the plateau. By applying a stress the energy diagram is tilted to one side.

The first two energy troughs become equally deep when the condition

$$a\mathbf{b}L\sigma = 2W_k \quad (2)$$

is fulfilled ( $a$ =distance between Peierls valleys,  $\mathbf{b}$ =Burgers vector). For stronger stresses  $\sigma$  always two or more troughs on nearly the same energy level exist. Figure 2 illustrates this situation. On the dislocation loop three regions may be distinguished then. In region I the kinks coalesce, in region II they are well distinct and in region III the dislocation runs along a close-packed direction. The parabolic rise of the lowest trough energies is caused by an increase of the elastic line energy. For the treatment of the double kink relaxation this increase, the length  $L_{III}$  and the area  $\Delta F$  between the two energetically most favourable configurations must be determined.

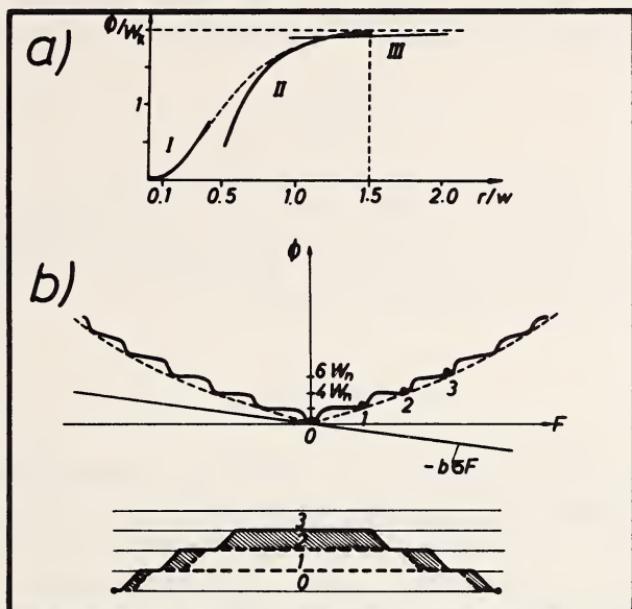


FIGURE 1. Energy diagram for a dislocation in the Peierls potential.

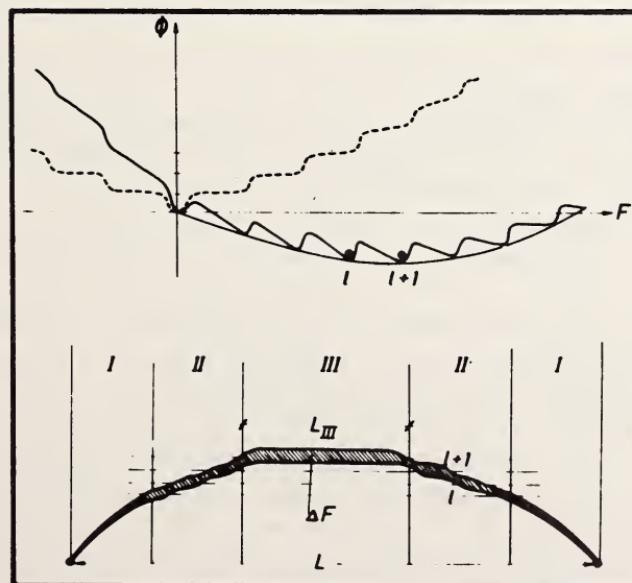


FIGURE 2. Tilted energy diagram for a dislocation under stress.

In fcc metals the kinks coalesce already at low kink densities since the Peierls energy is low compared with the elastic line energy. The kink width  $w$  of a single kink is given by the expression ( $G$  = shear modulus)

$$\frac{w}{a} \approx \frac{Gb^2a}{2W_k} \approx 35. \quad (3)$$

Thus very few kinks are fully distinct on a loop and one may neglect region II. In region I the string approximation may be applied. Variation of the elastic energy to the number of double kinks and simultaneous consideration of the equilibrium condition

$$\sigma b = \frac{S(\psi)}{R} \quad (4)$$

( $S(\psi)$  = line energy dependent on dislocation character,  $R$  = radius of curvature) yields values for  $\Delta F$  and  $L_{III}$ . We quote only interpolation formulae which are valid for all amounts of bowing out:

$$L_{III} = \frac{2W_k}{v\sigma} \cdot L; \Delta F = \frac{aL}{2} \cdot \left[ 1 + \left( \frac{2W_k}{v\sigma} \right)^2 \right]; v = a\mathbf{b} \cdot \mathbf{L}. \quad (5)$$

## B. NON-EQUILIBRIUM CONFIGURATIONS

In internal friction measurements transitions between equilibrium configurations are induced. In these, the loops must run through different non-equilibrium configurations. Figure 3 shows several such configurations. In (a) an unrealistic configuration in the pure kink picture is given. A description of this loop would require a variable number of kink coordinates. In the kink chain on the left side a double kink has been created. This pair cannot contribute to the relaxation strength because it must vanish in separating. Creation of kinks in this region brings about only fluctuations of the dislocation around its equilibrium configuration. The remaining deviations from the equilibrium position in (a) require high energies and therefore are rather improbable. We assume that transitions between equilibrium positions take place by the lowest deviation possible: the action of only one kink pair. This is justified by the fact that the thermal energy  $kT$  is small compared with the elastic line energy ( $Gb^2a$ ) in the vicinity of the Bordoni peak and therefore only small fluctuations in position occur for not too high loop lengths ( $L < 10^4a$ ). The process of bowing out looks then as follows: in one direction a kink pair is created and separated by stress to the loop ends before the next pair is created. In the reverse direction the kinks in the pair created last separate from the loop ends

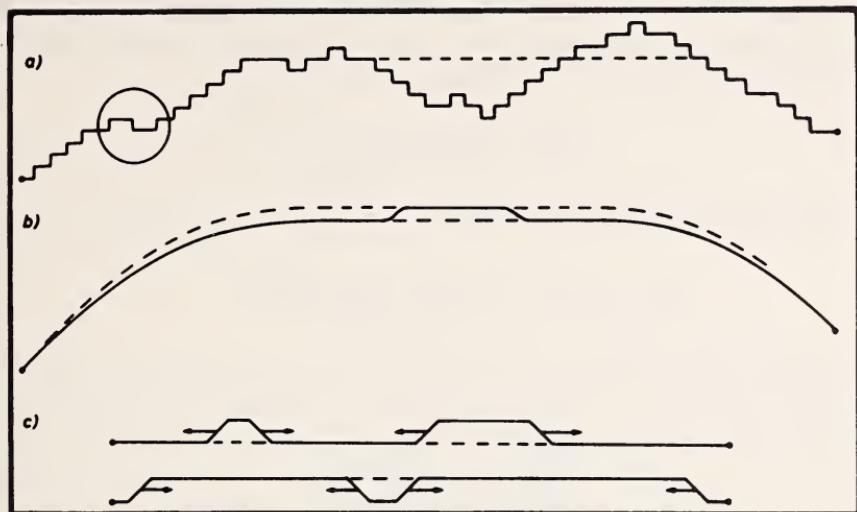


FIGURE 3. Non-equilibrium configurations of a dislocation.

and diffuse towards each other until the pair collapses. Only after this the next pair separates from the loop ends. Figure 3 shows an energetically less favourable transition (activation energy  $4W_k$ ) by means of two simultaneously moving double kinks.

### III.2. Diffusion model of double-kink relaxation

The motion of kinks along a dislocation line may be treated as one-dimensional diffusion of particles. Consider a dislocation containing only one kink pair. If  $x_1$  and  $x_2$  are the kink coordinates and  $m_k$  the kink mass, the following equations of motion may be set up:

$$\frac{dp_1}{dt} \equiv m_k \ddot{x}_1 = K + X_1(t); \quad \frac{dp_2}{dt} \equiv m_k \ddot{x}_2 = -K + X_2(t). \quad (6)$$

The force  $K$  is defined by the relation  $K = \partial\phi(r)/\partial r$  and consists of the attraction between the two kinks and a contribution due to stresses acting on the dislocation.  $X_i(t)$  is a statistical force due to the interaction of the  $i$ th kink with lattice vibrations and gives rise to a Brownian motion of the kinks. Starting from the above equations of motion (6) one may derive an equation for the distribution function  $g(x_1, x_2, p_1, p_2, t)$  in phase space following Kramers [7].

The statistical force  $X_i(t)$  is characterized by a relaxation time  $\tau_k = m_k/\eta_k$  ( $\eta_k$  = kink viscosity) which is a measure for the decrease of directed motion. Since  $\tau_k$  is short compared with oscillation periods applied in internal friction measurements in the interesting temperature

range ( $\tau_k = 10^{-10} - 10^{-11}$  s) Kramer's diffusion equation may be replaced by an equation in coordinate space which is known as Smoluchowski's equation. Introducing the coordinates

$$r = x_2 - x_1, \quad q = x_1 + x_2$$

and the density in coordinate space

$$\rho(q, r, t) = \int_{-\infty}^{+\infty} g(q, r, p, p_r) dp dp_r$$

this equation takes the form of an equation of continuity in the  $q, r$ -plane:

$$-\frac{\partial \rho}{\partial t} = \operatorname{div} \mathbf{j} = \frac{\partial j_q}{\partial q} + \frac{\partial j_r}{\partial r}. \quad (7)$$

The components of the current density  $\mathbf{j}$  are given by the following expressions:

$$\begin{aligned} j_q &= -\frac{2kT}{\eta_k} \cdot \frac{\partial \rho}{\partial q} \\ j_r &= -\frac{2kT}{\eta_k} \frac{\partial \rho}{\partial r} + \frac{2}{\eta_k} \cdot K(r) \cdot \rho. \end{aligned} \quad (8)$$

The first terms represent ordinary diffusion currents, the second term in  $j_r$  describes the convection of kinks in the field of force  $K(r)$ . Since the kinks move within the distance  $L$  between pinning-points and kink creation is probable only in one direction, eq (8) has to be solved in a region in the  $q, r$ -plane limited by the straight lines  $r = L - q$  and  $r = 0$ . The component of the current normal to the boundary must vanish. Another form of the diffusion equation is obtained by integrating over the coordinate  $q$ . Defining a density function

$$\bar{\rho}(r, t) \equiv \int_{q=-L+r}^{L-r} \rho(q, r, t) dq$$

and an integral flux in  $r$ -direction

$$J(r, t) \equiv \int_{q=-L+r}^{L-r} j_r(q, r, t) dq,$$

one gets an extended equation of continuity from eq (7):

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial J}{\partial r} = 2(j_r |_{q=L-r} + j_r |_{q=-L+r}). \quad (9)$$

For the current  $J$  the following expression holds:

$$J(r, t) = -\frac{2kT}{\eta_k} \cdot \frac{\partial \bar{\rho}}{\partial r} + \frac{2}{\eta_k} K(r) \bar{\rho}(r, t) - \frac{2kT}{\eta_k} (\rho(q, r) |_{q=L-r} + \rho(q, r) |_{q=-L+r}). \quad (10)$$

The concept of diffusing particles breaks down at  $r=0$ , since then the kink properties ( $m_k, \eta_k, r$ ) become ill-defined. A simple model may be employed here.

If a loop is bowed out by the creation of several double kinks some idealization is necessary since the motion of both the kink pair and the loop ends must be taken into account. We assume that the kink pair entirely separates before the loop ends begin to glide. Suitable coordinates instead of  $x_1$  and  $x_2$  are the areas under the loop ends reckoned from the centre of the loop. The calculation runs on similar lines as in the case of one kink pair. The diffusion region takes a different shape as shown in figure 4.

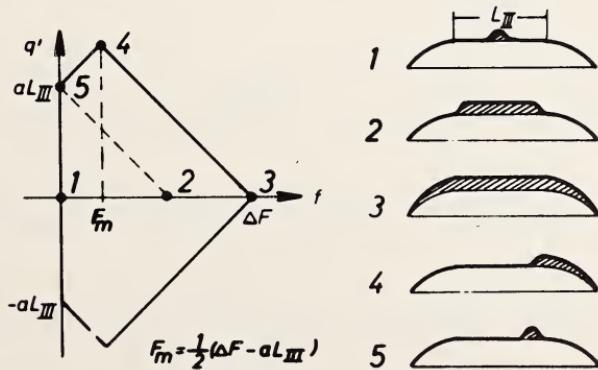


FIGURE 4. Region of diffusion for bowed-out dislocation.

For illustration the loop configurations for five points in the  $q', f$ -plane have been sketched. Configuration 1, 2, and 3 are symmetric ones, the others are unsymmetric. The coordinate  $q'$  is a measure for the shift of the loop to one side.

### III. 3. A multiple well model of double kink relaxation

Equation (9) and the corresponding equation for loops with several double kinks describe the anelastic behaviour of dislocation loops. A stress-strain-relation is obtained in principle by solving these equations for a given stress  $\sigma(t)$  as function of time and using the solutions  $\bar{\rho}(r, t)$  to calculate a mean anelastic strain by averaging over  $r$ .

An exact solution of Smoluchowski's equation is available if the following three conditions are fulfilled:

- (1)  $a b L \sigma_i > 2W_k$
- (2)  $\sigma_a/\sigma_i \ll 1$
- (3)  $2W_k \gg kT$ .

In the vicinity of the Bordoni peak we have  $2W_k \approx 9kT$ . Condition (1) ensures that several wells of comparable depth exist, condition (2) has the effect that the well character of the potential is only slightly altered by the applied stress  $\sigma_a$ . Condition (3) is necessary for the application of an approximate method due to Brinkman [8].

#### A. DERIVATION OF RATE EQUATIONS

Starting-point of Brinkman's method is the current  $J$  of eq (10), which may be written in the form

$$J(r, t) = -\frac{2kT}{\eta_k} \cdot e^{-\phi/kT} \cdot \frac{\partial}{\partial r} (\bar{\rho} \cdot e^{\phi/kT}) - \frac{2kT}{\eta_k} (\rho(q, r)|_{q=L-r} + \rho(q, r)|_{q=-L+r}).$$

Multiplying by  $\exp [\phi/kT]$  and integrating over the potential ridge yields ( $\xi_0 = kT/ab\sigma$ )

$$\int_0^{L-\xi_0} J \cdot e^{\phi/kT} dr = -\frac{2kT}{\eta_k} \bar{\rho}(r) \cdot e^{\phi/kT} \Big|_{r=0}^{L-\xi_0} - \frac{2kT}{\eta_k} \int_0^{L-\xi_0} (\dots) e^{\phi/kT} dr.$$

The main contribution to the integral on the left-hand side is given by the region near to the top of the barrier ( $S_{12}$ ). Since on the top the current  $J$  is nearly independent of  $r$  (owing to low density values and the validity of eq (9)),  $J$  may be taken out of the integral

$$\int_0^{L-\xi_0} J \cdot e^{\phi/kT} dr \approx J \int_{S_{12}} e^{\phi/kT} dr. \quad (11)$$

Assuming Boltzmann distributions for  $\rho(q, r)$  in the potential wells the current  $J$  may be calculated. By introduction of the occupation numbers

$$n_1 = \int_{r=0}^{1.5w} \bar{\rho}(r) dr \quad \text{and} \quad n_2 = \int_{r=1.5w}^L \bar{\rho}(r) dr$$

eq (11) takes the form of a rate equation:

$$J = -\dot{n}_1 = \Gamma_{12} n_1 - \Gamma_{21} n_2. \quad (12a)$$

For loops with several double kinks one gets a system of rate equations:

$$\begin{aligned} -\dot{n}_1 &= J_{l, l+1} - J_{l-1, l} \\ J_{l, l+1} &= \Gamma_{l, l+1} n_1 - \Gamma_{l+1, l} n_{l+1}. \end{aligned} \quad (12b)$$

The jumping rates are defined by the following expressions

$$\begin{aligned} \Gamma_{12} &= \frac{2kT}{\eta_k} \left/ \left( \int_1 \left( 1 - \frac{r}{L} \right) \cdot e^{-\frac{\phi}{kT}} dr \int_{S_{12}} e^{\frac{\phi}{kT}} dr \right) \right., \quad \xi_0 = \frac{kT}{ab\sigma} \\ \Gamma_{21} &= \frac{2kT}{\eta_k} \cdot \frac{L}{\xi_0} \left/ \left( \xi_0 \cdot e^{-\frac{\phi(L)}{kT}} \cdot \int_{S_{12}} e^{\frac{\phi}{kT}} dr \right) \right. \end{aligned}$$

$$\Gamma_{l, l+1} = \frac{2kT}{\eta_k} \left/ \left( \int_l \left( 1 + \frac{f}{aL_{III}} \right) \cdot e^{-\frac{\phi(f)}{kT}} df \int_{S_{l, l+1}} e^{\frac{\phi(f)}{kT}} df \right) \right.$$

$$\Gamma_{l+1, l} = \frac{2kT}{\eta_k} \cdot \frac{L_{III}}{\xi_0} \left/ \left( \xi_0 \cdot e^{-\frac{\phi(f)}{kT}} \cdot \int_{S_{l, l+1}} e^{\frac{\phi(f)}{kT}} df \right) \right.$$

Explicit forms are

$$\Gamma_{12} = \Gamma_0 \cdot e^\gamma \cdot e^{-\frac{2W_k}{kT}}, \quad \Gamma_{21} = \Gamma_0 \cdot \lambda \frac{v\sigma}{kT} \cdot e^{-\frac{v\sigma}{kT}},$$

$$\Gamma_0 = \frac{2\alpha^2}{\pi\eta_k} \frac{e^{\frac{v_0\sigma}{kT}}}{\left( \frac{\alpha}{2\beta} + \frac{1}{\lambda} \right)}$$

$$\alpha^2 = 2, 31 \cdot 2W_k/w^2, \beta^2 = 0, 33 \cdot 2W_k/w^2, \lambda = \frac{\pi ab\sigma}{\alpha\sqrt{\pi kT}}, \frac{v}{v_0} = \frac{abL}{1.5 abw}$$

$$\Gamma_{l, l+1} = \Gamma'_0 \frac{e^\gamma \cdot e^{-\frac{2W_k}{kT}}}{\left(1 + \frac{kT\lambda'}{\pi abL_{III}\sigma'}\right)},$$

$$\Gamma_{l+1, l} = \Gamma'_0 \lambda' \frac{abL_{III}\sigma'}{kT} e^{-\frac{b\Delta F\sigma'}{kT}},$$

$$\Gamma'_0 = \frac{2\alpha^2}{\pi\eta_k} \cdot \frac{e^{\frac{v_0\sigma'}{kT}}}{\left(\frac{\alpha}{2\beta} + \frac{1}{\lambda'}\right)},$$

$$\sigma' = \sigma - \sigma_{ww}, \lambda' = \frac{\pi ab\sigma'}{\alpha\sqrt{\pi kT}}.$$

The jumping rates  $\Gamma_{ij}$  are functions of the curvatures  $\alpha$  and  $\beta$  of the potential curve (see fig. 1). The factor  $e^\gamma$  ( $\gamma \approx 3/4 \pi$ ) describes the variation of the oscillation entropy of the dislocation by double kink creation.  $\sigma_{ww}$  is a parameter (having the dimension of a stress) which describes the interaction of the kinks of the same sign at the loop ends.

The system of eqs (12) may be written in matrix form

$$\mathbf{A} \cdot \mathbf{n} + \dot{\mathbf{n}} = 0, \quad (13)$$

where  $\mathbf{n}$  is the  $m$ -dimensional vector of occupation numbers ( $\mathbf{n} = \{n_1, n_2, \dots, n_m\}$ ) and the square matrix  $\mathbf{A}$  contains the jumping rates  $\Gamma_{ij}$ .

## B. SOLUTION OF THE RATE EQUATIONS FOR LOW EXTERNAL STRESSES

We restrict ourselves to the linear anelastic response of the loops to an external stress  $\sigma_a$ . Requiring that

$$\frac{v\sigma_a}{kT} \ll 1$$

we may expand the matrix  $\mathbf{A}(\sigma)$  at  $\sigma = \sigma_i$  ( $\sigma = \sigma_i + \sigma_a$ ), retaining only the linear term in  $\sigma_a$ :

$$\mathbf{A} = \mathbf{A}_0 + \Delta \mathbf{A}, \quad (\Delta \mathbf{A} \sim v \sigma_a).$$

The *ansatz*

$$\mathbf{n} = \mathbf{n}_0 + \Delta \mathbf{n}$$

leads to the following inhomogeneous linear system of differential equations (a second order term is neglected)

$$\mathbf{A}_0 \cdot \Delta \mathbf{n} + \Delta \dot{\mathbf{n}} = -\Delta \mathbf{A} \cdot \mathbf{n}_0, \quad (14)$$

where  $\mathbf{n}_0$  solves the equations

$$\mathbf{A}_0 \mathbf{n}_0 + \dot{\mathbf{n}}_0 = 0. \quad (15)$$

Solutions of eq (15) are of the form

$$\mathbf{n}_{0k} = \boldsymbol{\eta}_k \cdot \exp[-t/\tau_k], \quad k = 0, 1, 2, \dots, m-1.$$

$\tau_k$  are eigenvalues of the corresponding eigen-equation

$$(\mathbf{A}_0 - \frac{1}{\tau} \mathbf{J}) \cdot \boldsymbol{\eta} = 0. \quad (16)$$

The vectors  $\boldsymbol{\eta}_k$  form a complete set of eigen-functions, with which the solution of eq (14) may be constructed. For a periodic stress  $\sigma_a = \sigma_{a0} \cdot \exp[i\omega t]$  one obtains

$$\Delta \mathbf{n} = - \sum_{k=1}^{m-1} \frac{\boldsymbol{\eta}_k^* \cdot \Delta \mathbf{A} \cdot \mathbf{n}_0}{1/\tau_k + i\omega} \boldsymbol{\eta}_k, \quad \sum_{l=1}^m \Delta n_l = 0. \quad (17)$$

At long times after switching on the external stress  $\mathbf{n}_0$  is given by a solution of the static equation  $\mathbf{A}_0 \cdot \mathbf{n}_0 = 0$ .

Eigenfunctions for the exact matrix  $\mathbf{A}_0$  in which the parabolic increase of the loop energy (see fig. 2) is taken into account are not available yet. Figure 5 illustrates under which simplifying conditions the problem could be solved. The main contribution to the relaxation strength comes from the wells with the highest occupation numbers (in the centre of model A). This situation may be roughly approximated by taking all jumping rates equal ( $\Gamma_{ij} = \Gamma$ ) and determining a suitable number  $m$  of potential wells (model B). This number is estimated in model D by distinguishing only

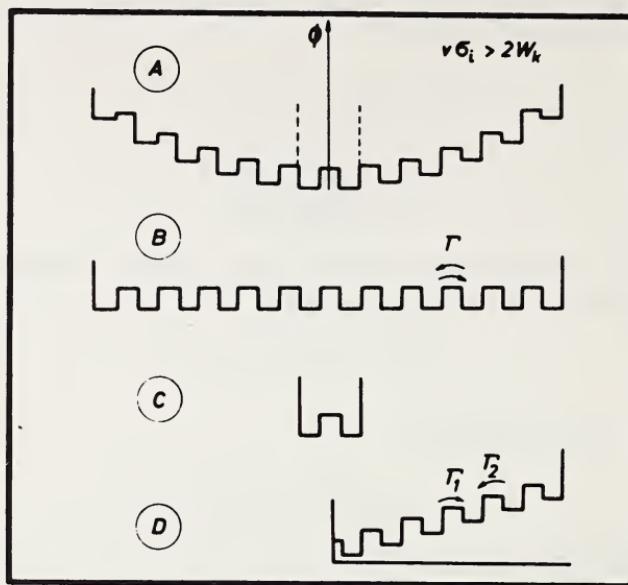


FIGURE 5. Different multi-well models (schematic).

two jumping rates ( $\Gamma_1$  and  $\Gamma_2$ ). Equation (16) could be solved for models B, C, and D in closed form (B is a special case of D). The double well model C gives nearly the same information as model B if only the solution with the lowest eigenvalue  $\tau_k$  is taken into account.

The resolved anelastic strain may be calculated from solutions  $\Delta n(t)$  by the following relation:

$$\Delta \epsilon_{\text{anel}} = b \sum_{l=1}^m \bar{F}_l \cdot 1 \cdot \Delta n_l, \quad (18)$$

where  $\bar{F}_1 \approx \bar{F} = \Delta F - 2kT/b\sigma_i$  for neighbouring wells. The logarithmic decrement  $\delta$  is given by the expression

$$\delta = -\pi \frac{\text{Im}(\epsilon_{\text{anel}})}{\epsilon_{\text{el}}}, \quad \epsilon_{\text{el}} = \sigma_a/M_{\text{el}}. \quad (19)$$

In the case of model  $\overline{B}$  ( $\Gamma_{ij} = \Gamma$ ) one obtains for the relaxation times  $\tau_k$  and the decrement  $\delta$ :

$$\tau_k = 1 / \left[ 2 \left( 1 - \cos \frac{\pi k}{m} \right) \right] \approx \frac{m^2}{\pi^2 k^2} \cdot \frac{1}{\Gamma} \quad \text{for} \quad \frac{\pi k}{m} \ll 1; \quad (20)$$

$$\tau(m=2) = 1/2\Gamma \quad \text{and}$$

$$\delta \sim \sum_{k'} g_{mk'} \frac{\omega \tau_{k'}}{1 + \omega^2 \tau_{k'}^2}; \quad (k' \text{ odd integer number}). \quad (21)$$

Thus the decrement is proportional to a sum of Lorentzian peaks. For the weighting factor  $g_{mk'}$  approximately the following expression holds:

$$g_{mk'} = \frac{8m^2}{\pi^4 k'^3} \quad \text{for} \quad \frac{\pi k'}{m} \ll 1; \quad g_{21} = \frac{1}{4}. \quad (22)$$

The main contribution to the relaxation strength is given by the lowest mode ( $k' = 1$ ). For example,  $g_{m3} = 1/27 g_{m1}$ . We therefore neglect all modes but the lowest.

An estimate of the number of considered wells  $m$  leads to the following relation:

$$m^2 \sim \frac{kT}{Gb^2 a} \cdot \frac{L}{a}.$$

For a maximal length  $L_{\max} = 10^4 a$ , a temperature  $T_{\max} = 150$  K and  $Gb^2 a = 4.26$  eV an upper limit of the number wells is obtained:  $m_{\max} = 22$ .

### III.4. Numerical results for the double-well model

#### A. RELAXATION TIME

In figure 6 the relaxation time  $\tau(m=2)$  is plotted in a logarithmic scale as a function of  $1/T$  for different loop lengths. The preexponential of  $\tau$

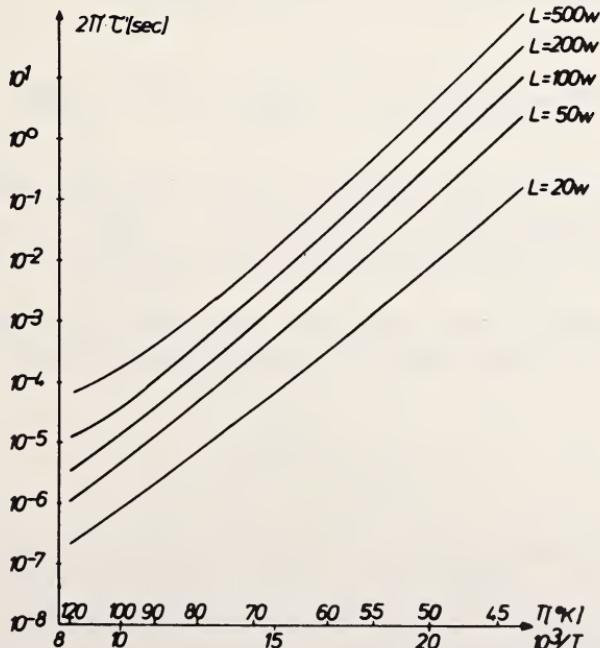


FIGURE 6. Relaxation time as a function of temperature in the double-well case (parameter is the loop length  $L$ ).

turns out to be of the same order of magnitude as those measured although no adaptable parameter is involved. This must be considered a success of our diffusion model. The relaxation time is approximately proportional to the loop length. Therefore the Bordoni peak shifts to slightly lower temperatures by shortening of the loops (on account of the maximum condition  $\omega\tau(T_{\max}) = 1$ ).

### B. RELAXATION STRENGTH

The relaxation strength of the double kink relaxation may be estimated by assuming plausible values for the dislocation density, the fraction of loops capable of relaxation and a mean loop length. The double-well model yields values for the relaxation strength that are lower than experimental values by a factor of about 40. This difference is reduced in a multi-well model when the reasonable assumption is made that about ten wells participate ( $m = 10$ ).

### C. HALF WIDTH OF THE DAMPING PEAK

Since the relaxation time depends on loop length and stress a broadening of the damping peak is to be expected when distribution functions for these variables are assumed.

The following distribution function was employed:

$$n(L_1\sigma_i)dLd\sigma_i = \frac{C}{\Lambda} \cdot e^{-\frac{L}{\Lambda}} \frac{2}{\sqrt{2\pi\Delta\sigma}} e^{-\frac{\sigma_i^2}{2(\Delta\sigma)^2}} \cdot dLd\sigma_i. \quad (23)$$

Here  $n(L, \sigma_i)dLd\sigma_i$  is the number of loops with lengths between  $L$  and  $L + dL$  and under a stress in the interval  $\sigma_i, \sigma_i + d\sigma_i$ .  $C$  is a constant of normalization,  $\Lambda$  is the mean loop length,  $\Delta\sigma$  is the spread of the internal stresses.

It is reasonable to allow only for those loops that cannot act as dislocation sources, i.e., whose length is lower than the critical Frank-Read-length  $L_{\text{cr}}$ :

$$L < L_{\text{cr}} \equiv 2S/b\sigma_i.$$

Figure 7 gives experimental and calculated values of the half-width as a function of  $1/T_m$  (i.e., a frequency scale!). The filled circles represent Bordoni peak measurements collected by Niblett [13]. The other data represent peaks calculated with the distribution function eq (23)

$$(\Lambda \approx 0.5 \mu\text{m}, \Delta\sigma/G \approx 10^{-4}).$$

Figure 7 shows that the calculated values exceed that of a simple relaxation process (line parallel to the  $1/T_m$  axis) but that the broadening is not sufficient to explain the full width of measured Bordoni peaks. Further reasons for broadening may be involved.

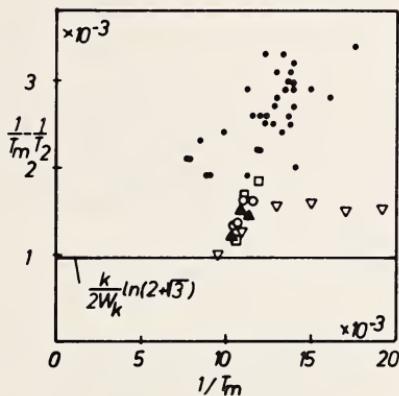


FIGURE 7. Half-width  $1/T_m - 1/T_2$  of measured (●) and calculated (other symbols) Bordoni peaks plotted against  $1/T_m$  ( $T_m$  = peak temperature,  $T_2$  = temperature ( $> T_m$ ) at which the damping is half the maximum value).

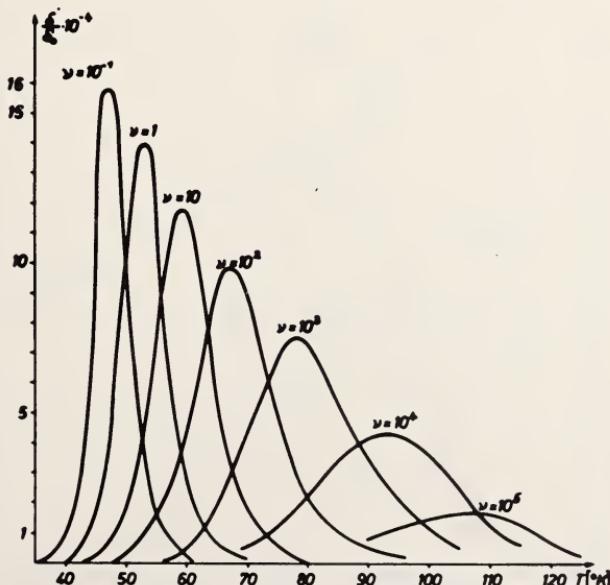


FIGURE 8. Calculated damping peaks for various frequencies (double-well model).

#### D. FREQUENCY DEPENDENCE OF THE RELAXATION STRENGTH

Figure 8 shows the behaviour of a calculated peak due to a variation of the frequency. The peak height is seen to decrease with frequency, as has been observed in copper [14] but not in silver, gold, palladium, and platinum [15].

#### E. LOOP LENGTH DEPENDENCE

Figure 9 gives results obtained with the double-well model. The spread  $\Delta\sigma$  of internal stresses and the frequency were taken constant and only the mean loop length  $\lambda$  was altered. An outstanding property of the peaks is a simultaneous decrease of the height and a shift to lower temperatures with decreasing loop length.

The peaks were calculated for comparison with a neutron-irradiation experiment on copper carried out by Thompson [16]. Figure 10 shows Thompson's results. The upper curve is measured after a 12 percent plastic strain, the second after an anneal of 24 hr at 150 °C and the others after different doses of irradiation. The mean loop length was determined

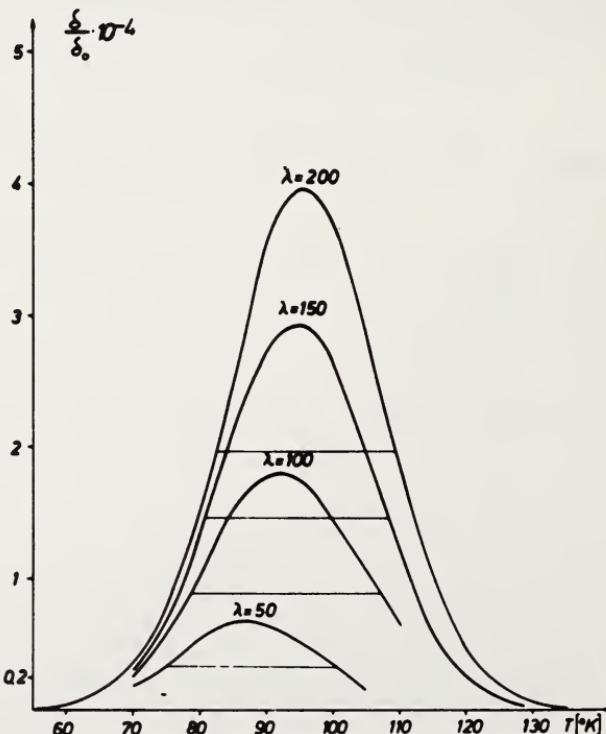


FIGURE 9. Calculated damping peaks for various mean loop lengths:  $\lambda \equiv \Lambda/w$ ;  $\Delta\sigma = 10^{-4}G$ ,  $2W_k = 0.115$  eV,  $\nu = 1.6 \cdot 10^4$  Hz (double-well model).

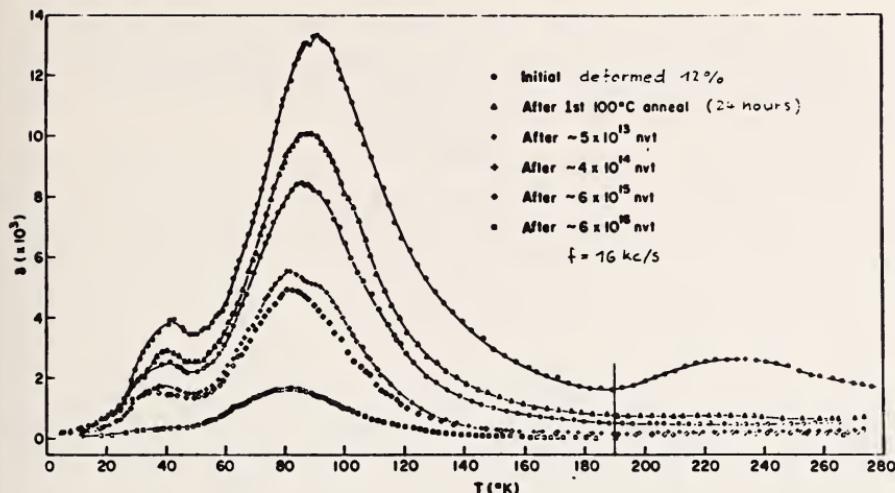


FIGURE 10. Variation of the Bordoni peak with increasing neutron-irradiation dose measured by Thompson [16].

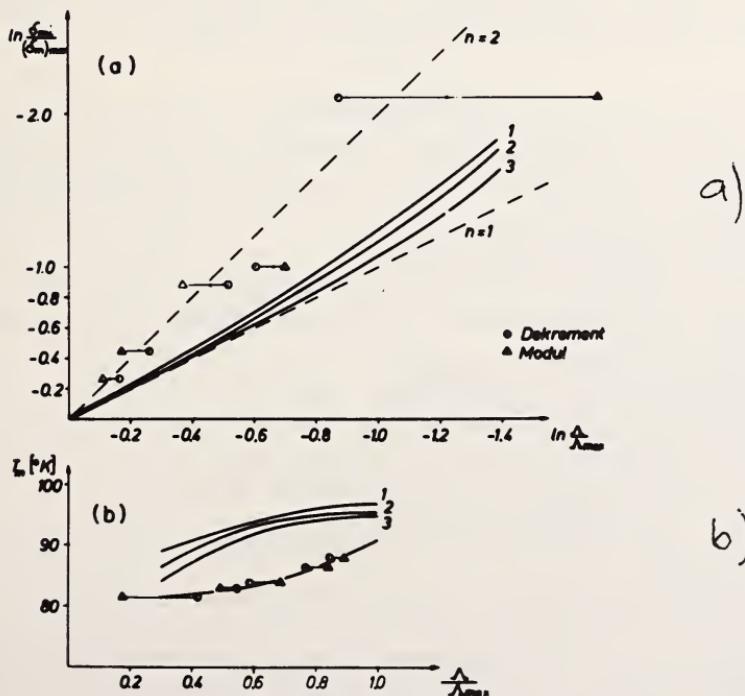


FIGURE 11. Comparison of loop-length dependence.

for each peak from modulus and decrement measurements at temperatures ( $T \approx 190$  K) far above the Bordoni peak by means of the Granato-Lücke-model. This permits a quantitative comparison between model and experiment of the loop length dependence.

In figure 11a the relative decrease of the height of the Bordoni peak with increasing dose is plotted against the relative variation of the mean loop length. For small doses the peak height decreases approximately proportional to  $\Lambda^2$ , for larger doses proportional to  $\Lambda^n$  where the exponent  $n$  lies between one and two. A clear decision is not possible because of the differences occurring between modulus and decrement values for the loop length. The solid line represents results for the double-well model ( $\Lambda_{\max} = 200 w$ ). The exponent  $n$  is near to one for  $\Lambda = 200 w$  and increases with decreasing loop length. In the multi-well model full agreement may be expected since the weighting factor  $g_{m1}$  is nearly proportional to  $\Lambda$ .

In figure 11b the peak temperature  $T_m$  is plotted as a function of relative loop length. The calculated shift of  $T_m$  agrees rather well with Thompson's results.

Summarizing one may say that the derived diffusion model is able to describe the loop length dependence of the Bordoni peak rather quantitatively. The characteristic half-width of the peak is only partly explained, however. The influence of other causes as for example the splitting of dislocations can therefore not be excluded.

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# SLIGHTLY DISSOCIATED DISLOCATIONS

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A modified Peierls-Nabarro model is used to calculate the relation between the separation of partials and stacking fault energy for an idealized dislocation dissociated into two equal pure screw partials. The resulting expression agrees with the inverse dependence obtained by equating the elastic repulsion of the partials to the attraction of the stacking fault, but unlike that result does not break down at zero separation. Also an argument is given that the width of such a dissociated dislocation should be considered as a complex quantity, with the imaginary part corresponding to the separation of the partials.

Key words: Dislocation stacking faults; Peierls-Nabarro mode.

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An inverse dependence on stacking fault energy of the separation of partials in a dissociated dislocation, while reasonable for large separations, is highly questionable when the separation is less than a few lattice spacings as in a dissociation model for low temperature flow stress of bcc metals [1]. The present note discusses some of the problems of slightly dissociated dislocations in terms of a Peierls-Nabarro model in the Foreman [2] modification applied to a screw dislocation dissociated into screw partials on one plane. While such a model is inadequate to describe the complex multiplanar dissociation presumed for a bcc screw dislocation, it does give the interesting result that the partials recombine at a definite stacking fault energy. In an earlier communication [3] it was shown for the Peierls barrier problem, assuming the dislocation configuration is known as an analytical displacement function  $U(x)$ , that partial separation is defined better as the separation of the poles of  $dU/dx$  nearest the partials in the complex coordinate plane than as the separation of the maxima of  $dU/dx$  on the real coordinate axis, due to the mutual distortion of the partials for slight dissociation. It will now be argued that the pole definition is also preferable for the multiplanar dissociation problem.

Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough, Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

Assume an analytical displacement function

$$U(x) = -\frac{b}{4\pi} \tan^{-1} \left( \frac{x+\sigma}{\omega} \right) - \frac{b}{4\pi} \tan^{-1} \left( \frac{x-\sigma}{\omega} \right), \quad (1)$$

appropriate for a Peierls-Nabarro model of a dissociated dislocation, which will be constructed later. Here  $b$  is the magnitude of the Burgers vector and  $\omega$  is the width of each partial. Width is also defined better in terms of the poles than in terms of the configuration, due to the mutual distortion of the partials for slight dissociation. For now, observe that the dislocation is already dissociated by  $2\sigma = 2\omega/\sqrt{3}$  according to the pole definition before there is any dissociation according to the maxima definition. This may explain the paradox of an apparently undissociated sessile b.c.c. screw dislocation in the computer model of Gehlen, Rosenfield and Hahn [4]. If indeed the explanation lies in their use of an inappropriate definition for dissociation, then a sessile to glissile transformation should occur in their computer model upon increasing the stacking fault energy on the possible dissociation planes.

A self-consistent Peierls-Nabarro model for a dissociated screw dislocation can be obtained from (1) by reversing the usual approach. Consider now the displacement function  $U(x)$  as known and the misfit shear stress function

$$f[U(x)] = \frac{\mu}{\pi} \int_{-\infty}^{+\infty} \frac{dU(x')/dx'}{x-x'} dx', \quad (2)$$

as unknown, where  $\mu$  is the shear modulus and the principal value of the integral is understood [5]. While the direct approach required solution of a nonlinear integral equation, the reverse approach requires mere integration to obtain

$$f[U(x)] = -\frac{\mu b}{4\pi} \left\{ \frac{x+\sigma}{\omega^2 + (x+\sigma)^2} + \frac{x-\sigma}{\omega^2 + (x-\sigma)^2} \right\}. \quad (3)$$

Since  $U(x)$  has an inverse on  $-b/4 < U < b/4$ , the function  $f(U)$  can be obtained from (3) by substitution. However, it will be more convenient to keep  $x$  as the independent variable for the final two steps of the present argument.

The first step is to satisfy Hooke's law in shear

$$df = -\mu \frac{d(2U)}{a}, \quad (4)$$

for the small strain at  $2U = \pm b/2$ , where  $a$  is the vertical spacing between the elastic media above and below the slip plane, and where  $2U$  is the relative displacement of the media. For large  $x$  the chain rule, with (1) and (3), gives

$$\omega = \frac{a}{2}. \quad (5)$$

The second step is to obtain the stacking fault energy  $\gamma$  of the model from the misfit energy density  $v(x)$ . This is obtained by integrating the misfit shear stress function  $f$  over the relative displacement  $2U$

$$v(x) = -2 \int_{-\infty}^x f[U(x)] \frac{dU(x)}{dx} dx, \quad (6)$$

which gives

$$v(x) = \frac{\mu b^2}{16\pi^2} \left\{ \frac{\omega}{\omega^2 + (x + \sigma)^2} + \frac{\omega}{\omega^2 + (x - \sigma)^2} + \frac{\tan^{-1} [(x + \sigma)/\omega] - \tan^{-1} [(x - \sigma)/\omega]}{\sigma} \right\}. \quad (7)$$

The first two terms can be identified with the misfit energy density due to the two partials and the remainder with the misfit energy density due to the stacking fault. The remainder at  $x = 0$  is taken as the stacking fault energy of the model

$$\gamma = \frac{\mu b^2}{8\pi^2} \frac{\tan^{-1} (\sigma/\omega)}{\sigma}. \quad (8)$$

For  $\sigma \gg \omega$  this agrees with the result obtained by equating the elastic repulsion of two parallel screw dislocations of Burgers vectors  $b/2$  to the attraction of the stacking fault, but unlike that result (8) does not break down at  $\sigma = 0$ . Rather there is a definite recombination stacking fault energy

$$\gamma_0 = \frac{\mu b^2}{4\pi^2 a}, \quad (9)$$

which for an f.c.c. lattice is  $0.031 \mu b$ . This recombination stacking fault energy is about midway between the  $0.056 \mu b$  obtained by Seeger [6], and the  $0.013 \mu b$  obtained by Duncan and Kuhlman-Wilsdorf [7].

It was asserted above that width and separation are better defined in terms of the location  $i\omega \pm \sigma$  of the poles nearest the real axis of the function  $dU/dx$  rather than in terms of the configuration  $U(x)$ . This can be illustrated in a two-harmonic Frenkel-Kontorova model described [3] earlier, in which the configuration is

$$U(x) = 2 \tan^{-1} [\sinh (\alpha x/2)/\alpha], \quad (10)$$

and the lattice mesh is  $h$ . For this model the Peierls barrier was found to be proportional to

$$\exp (-\pi l/\alpha) \{ \cos \theta + (\alpha/l) [\sin \theta / \sinh (\alpha \theta / l)] \}, \quad (11)$$

where  $l \equiv 2\pi/h$  and  $\theta \equiv (2l \cosh^{-1} \alpha)/\alpha$ . Actually it is not the poles in  $dU/dx$  which determine the barrier but the similarly located poles in the misfit energy density. The Peierls barrier is proportional to the lattice periodic component of the Fourier integral of the misfit energy density in the slip plane [8]. It is the evaluation of the factor  $\exp (2\pi i x/h)$  of the Fourier integrand at the poles of the misfit energy density function that gives the result (11). To define the dislocation width  $w$  in lattice units  $h$  so it is proportional to the common distance  $\omega = \pi/\alpha$  of the poles from the real axis makes more sense than to define width  $l$  in lattice units so it is inversely proportional to the slope of the dislocation at its center since this latter definition becomes unreasonable on splitting. If  $w$  and  $l$  are to agree for  $\alpha=1$  when there is no splitting, then  $w$  and  $l$  are related by  $w=l/\alpha$ . If additionally the separation  $s$  of the partials is taken to be the separation of the poles in lattice units, then in terms of  $w$  and  $s$  expression (11) becomes

$$\exp (-\pi w) \{ \cos (\pi s) + (1/w) [\sin (\pi s) / \sinh (\pi s/w)] \}. \quad (12)$$

The cosine term in (12) can be obtained by a simple argument that assumes each partial moves in a quasi-Peierls potential [3]. When this term dominates the other term in the brackets, the Peierls barrier can be viewed formally as proportional to the real part of an exponential  $\exp (-\pi [w + is])$  of a complex dislocation width, which incorporates partial separation as its imaginary part. The real and imaginary parts of dislocation width have often been confused in the assumption that any increase in dislocation width lowers the Peierls barrier.

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## Discussion on Papers by H. Engelke and R. Hobart.

SEEEGER: Could we divide the discussion first between the general aspects of thermally activated processes—such as questions of thermalization, validity of rate theories, diffusion theories, etc.—which were discussed in the beginning, and then the more specialized questions connected with the applications to Bordoni relaxation?

THOMSON: A few years ago we worked on much of the same material concerning the Peierls energy kink nucleation problem, and I am just wondering about something which came up at the time. Much has been said about how the system goes through the saddle point configuration and whether this is or is not in equilibrium. I gather that the assumption is usually stated that the time one stays in this activated state is small compared to the various times for collision processes going on during that activated state. I have been puzzled by this, because it seems to me that if one has an ensemble then this is taken care of automatically. If the entire system is in equilibrium presumably there are a number of dislocations and a number of activated processes in the lifetime of the experiment, and the requirement is stated in terms of the equilibrium of the entire ensemble. Then one does not have to talk about the time between various types of collisions during any given activated state. I wonder if I could ask the authors what their opinion of this is.

SEEEGER: May I give my personal opinion, because I have been discussing these questions with my collaborators. The point that Professor Thomson raised is right when he speaks about the application of statistical mechanics as a whole. I think it is quite true that these processes are included. If you would give an exact treatment based on statistical mechanics this problem would not arise. However, I think in the transition state theory you made a specific assumption saying that as soon as a representative point reaches a saddle point with an outward velocity, it will never come back. There you made a specific assumption and this assumption need not be right, but it has nothing to do with the validity of the statistical arguments. If you try to avoid this by saying that even if a particle is over the hill there is still a finite chance of coming back because of fluctuation—the particle is carrying out a sort of Brownian motion rather than what you ordinarily think of as a jump process—then you get into the range of validity of the Kramers-Brinkman theory which Mr. Engelke was alluding to. It turns out, fortunately, that if the conditions are such that you are uncertain whether one theory or the other is applicable then both give the same result. So, it's comforting to know

that both theories are not only right in their own domains where they are clearly applicable, but also in between. The transition theory gives the right result in those cases where there is a slight possibility of the jump being interrupted, but in the extreme cases where you have a barrier—as may happen in kink problems—which is thirty or forty atomic distances wide and fairly low, so that the particle really creeps up slowly and reverses its direction of motion many times, then, I think, the transition state theory would give you the wrong answer, because you are making an assumption which is patently not fulfilled.

BESHERS: I was going to remark that there are very simple proofs available for Professor Thomson's point. Fred Reif's new books on statistical mechanics<sup>1</sup> make your point quite clear in very elementary derivations. The applicability is a consequence of the equilibrium of the whole system.

THOMSON: Part of the reason for bringing my point up is that apparently it is not uniformly accepted that one can take the point of view I outlined.

SEEGER: But do you agree with the general point I made?

THOMSON: Yes.

ARSENAULT: When you had a plot of decrement versus temperature, you had various widths of peaks as a function of loop length. Were you considering that the loop was bowed out to equilibrium position due to some static stress?

Also, I wanted to raise a related question. When I looked at this problem sometime ago, one thing that confused me was that if you take a piece of copper and deformed it to produce the bias stress, you have a large range of loop lengths and a larger range of bias stresses. That led me to believe that it would be very difficult to get anything that resembled a peak out of the data as you would have just a huge background.

ENGELKE: I don't know what you mean exactly, but what I have assumed is a random distribution of loop lengths and, in addition, a normal distribution of internal stresses. Using this distribution you get bowed-out loops if the spread of the stresses is sufficiently large. Stresses play an essential role in the kink-relaxation process since an appreciable relaxation strength is produced only if the stresses are high enough ( $abL\sigma_i > 2W_k$ ).

ARSENAULT: Let me simplify the question. When the loop goes out to a bias stress, do you always get the two equilibrium positions almost the same irrespective of loop lengths?

<sup>1</sup> Reif, F., Fundamentals of Statistics and Thermal Physics (McGraw-Hill Book Co., New York, 1965), pp. 202-203, and Reif, F., Statistical Physics—Berkeley Physics Course, 5, (McGraw-Hill Book Co., New York, 1967).

ENGELKE: Yes.

SEEGER: You could also look at it this way: The activation energy is always close to that for formation of two kinks. That is the basic process. What we are talking about are two modifications: One involves a factor affecting the relaxation strength associated with the process. The other is that it is not quite true that the activation energy is two times the kink energy because stresses can help and there is a loop length effect, etc. This is what Mr. Engelke has been discussing, so he has really been discussing a modification of the basic idea that the Bordoni energy is simply the energy to form a kink pair.

BRAILSFORD: I have a question for Mr. Engelke related to Dr. D. O. Thompson's experiments. As you know, it has always been his thesis that the Bordoni peak consists of several independent components, corresponding to different types of dislocations for example. I was under the impression that he had shown that if you looked at the modulus defect change produced by irradiation, the positions of the independent components did not move with temperature. The overall shifting of the peak temperature, according to his interpretation, arises because of changes in the relative strengths of the various components. This is the main point of his paper. It appears to be in conflict with your interpretation of his attenuation data.

ENGELKE: The random loop distribution produces smooth damping curves, but can only roughly approximate the loop distribution existing in a real crystal. If you look at the Bordoni peaks measured by Dr. Thompson you will see various dents. In my opinion these are caused by different loop distributions. With a random distribution you can only roughly approximate the existing loop distribution in a crystal.

SEEGER: Perhaps I may try to summarize what the present situation seems to be? I think the interpretation of Dr. Thompson that all you see is just going up and down of components cannot be generally true. There seem to be genuine effects where the loop length comes in, and they seem to be accounted for by the double kink model if you take everything properly into account. Of all these what I call secondary effects, which are not simply described by my original proposal, there is only one that is left not completely accounted for. That is the peak width, and, in fact, the width that comes out of the kind of theory that Mr. Engelke considered is considerably broader than the single relaxation width, but it's still too small by a factor of two compared with the measured width. So, there is room for other modifications like the fact that dislocations are extended in copper, say, or for using quite different distributions of dislocations, such as one for screws and one for edges. I

think it should be left to specific experiments to clear up these final refinements.

BRAILSFORD: Would you not agree, however, that it is important that we look not just at the internal friction, but simultaneously at the modulus defect?

SEEEGER: Yes.

BESHERS: I just wanted to say that every picture we have, theoretical and experimental, of work hardening—including the original Taylor theory—gives you a non-random distribution of dislocations. That is, we talk about pile-ups or cell walls and about dislocations which are not in the pile-ups and not in the cell walls. I have not tried to analyze it myself, but the resulting distribution must be something that is at least bimodal—if one can give a one parameter analysis—if not more. So, until you find an experiment which gives you a random distribution of dislocations instead of pile-ups and the resulting cell walls, you just won't be able to disentangle these two.

SEEEGER: This may well be the answer. But it's a challenge to the experimentalist to create conditions where the Bordoni peak is half as wide as the normal one. Anyway, I still consider the question of peak width as open.

[Written contribution] In aluminum, Bordoni peaks of approximately the width corresponding to a single relaxation time with Arrhenius temperature dependence have been observed by Ameen.<sup>2</sup>

ARSENAULT: This was really my question earlier. It is my feeling it is hard to conceive of a model or of a dislocation arrangement where you would get a narrow peak. It seems to me that in any cold worked block, you would get an infinitely wide peak.

SEEEGER: I cannot agree with you about the infinite peak width. We are really dealing with small corrections to two basic peaks. You see, only those dislocations contribute which run fairly parallel to one of the close packed directions. So, the most random aspects of the dislocation distribution do not contribute. This was one objection against Dr. Thompson's interpretation. He needed at least six peaks, or something like that, so you would have to invoke not only dislocations running parallel to [110] directions in fcc crystals, but also along [211] directions, and reasons were not given why the [211] energies were so close to the [110] energies as to make the peaks overlap. Anyway, I don't think this state-

<sup>2</sup> Ameen, D. L., Materials Science Center, Report No. 50 (Cornell University, Ithaca, New York, 1962), pp. 26-27; Mayadas, A. F., Materials Science Center Report No. 429 (Cornell University, Ithaca, New York, 1966), p. 37.

ment of an infinitely wide peak is a fair one; I don't think you would expect this.

BULLOUGH: With reference to Dr. Hobart's paper, perhaps I could just refer him to Alan Foreman's Ph. D. thesis which was published in 1954.<sup>3</sup> He does both of the problems that you discuss in your paper.

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<sup>3</sup> Foreman, A. J. E., Ph. D. Thesis (Imperial College, London, 1954).



# THE BROADENING OF RESONANCE LINES BY DISLOCATIONS

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Dislocations and other defects in solids broaden sharp resonance lines in solids, such as spin resonance and optical zero phonon lines. The broadening is a result of the random strain fields produced, and the shape of the resonance line is a measure of the distribution of internal strains. Measurement of line shapes can give information which is different from that given by the more usual mechanical and transport studies of dislocations. We calculate the shapes of the resonance lines in terms of the properties of the individual defects which cause broadening, their density and their statistical distribution. The theory is applied to straight dislocations, infinitesimal loops, dislocation dipoles and to point defects.

**Key words:** Line broadening; optical zero phonon line; spin resonance; statistical methods for dislocations.

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Dislocations and other defects in solids often broaden sharp resonance lines, such as spin resonance lines and optical zero phonon lines. The broadening is a result of the random strain fields produced, and may give information additional to that from mechanical and transport studies. We discuss the calculation of the shapes of these resonance lines in terms of the properties of the defects which cause the strain fields: the statistical properties of their distribution, the perturbation fields of the individual defects, and their concentration. In particular we compare the effects of straight dislocations, dislocation loops and point defects.

The method we use is the so-called "Statistical Method," and its essential assumptions are these:

(I) The transition energy of any one of the centres giving rise to the resonance line shifts linearly with the local strain:

$$E = E_0 + E' \epsilon \quad (1)$$

where  $\epsilon$  is a suitable linear combination of the components of the local

strain tensor.  $E_0$  is the unperturbed energy and  $E'$  is a coupling coefficient.

(II) The contributions of the various defects (dislocations, loops, etc.) to the local strain  $\epsilon$  are simply additive

$$\epsilon(z_1, z_2, \dots, z_N) = \sum_{i=1, N} \epsilon(z_i). \quad (2)$$

Here  $z_i \equiv (r_i, \eta_i)$  where  $r_i$  is the position of the defect with respect to the centre studied and  $\eta_i$  denotes any relevant internal variables of the defect (e.g., the axis and Burgers vector for a straight dislocation). Equation (2) is the assumption of linear elasticity and (1) that of first-order perturbation theory. We can, of course, bypass the definition of the local strain,  $\epsilon$ , by combining (I) and (II) into the assumption that the shift in transition energy of any centre is simply the sum of contributions from each defect.

(III) The probability of a particular defect configuration,  $\{z_1, \dots, z_N\}$ , in which the positions and internal variables of the  $N$  defects all have definite values, is  $P(z_1, \dots, z_N) dz_1 \dots dz_N$ . We assume the individual defect distributions are independent of one another, so  $P$  can be factorised:

$$P(z_1, \dots, z_N) = p(z_1) \dots p(z_N) \quad (3)$$

This cannot be exact because it allows two defects to occupy the same site; (3) should, however, hold well at low defect concentrations. The statistical distribution function,  $p(z)$ , is closely related to the pair distribution function of the defects causing broadening with respect to the centres giving rise to the resonance line.

The general method was described in [1]; here we quote the results for the distribution of  $\epsilon$  and outline the proof in an appendix. Within the assumptions (I)–(III) these results are exact.

$$I(\epsilon) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \cdot e^{ix\epsilon} e^{-\rho J(x)} \quad (4a)$$

where  $\rho = N / \int dz p(z)$  is the density of defects, and

$$J(x) = \int dz p(z) [1 - \exp(-ix\epsilon(z))]. \quad (4b)$$

These equations give the distribution of microscopic strain,  $\epsilon$ , and hence (by (1)) the line shape, in terms of the strain fields of the individual defects,  $\epsilon(z)$ , the density of defects,  $\rho$ , and the statistical distribution of defects, specified by  $p(z)$ .

In addition to the basic assumptions, outlined above, for the purposes of this note we have assumed (a) that the host lattice can be treated as an isotropic elastic continuum (although we may restrict the Burgers

vectors to specific directions), in that the long-range elasticity theory forms of  $\epsilon(z)$  may be used, and (b) that the distribution of defects is statistically homogeneous. Our calculations will be made for MgO, so in all cases the Burgers vectors will be in one of the [110] directions; we usually assume all such directions occur with equal probabilities.

TABLE. *Line shapes and widths for different sources of broadening*

Defect	Line shape	Width $\Delta$
Straight dislocations.....	Nearly Gauss	$b\alpha_1 \sqrt{L}$
Infinitesimal loops.....	Lorentz	$b\alpha_2 A$
Dislocation dipoles.....	Lorentz	$b\alpha_3 Ll$
Point defects.....	Lorentz	$\alpha_4 \rho D$

Results are summarised in the table for straight dislocations, for infinitesimal loops with their planes normal to the Burgers vector, for dislocation dipoles with separation  $l$ , and for point defects of strength  $D$ .  $L$  is the length of dislocation per unit volume,  $\rho$  the number of point defects per unit volume and  $A$  the area of loops per unit volume. The distributions of strain are described by reference to the standard shapes:

$$\text{Lorentz: } I(\epsilon) \sim [\Delta^2 + (\epsilon - \epsilon_0)^2]^{-1}$$

$$\text{Gauss: } I(\epsilon) \sim \exp - \left[ 4 \ln 2 \left( \frac{\epsilon - \epsilon_0}{\Delta} \right)^2 \right].$$

$\Delta$  is the full width at half intensity of the distribution, and  $\epsilon_0$  the mean strain;  $\epsilon_0$  usually proves proportional to some macroscopic parameter, e.g., the change in lattice parameter for the point defect case.

The constants  $\alpha$  have been evaluated for two cases particularly useful in spin resonance:

$$\epsilon_{100} = 2\epsilon_{zz} - \epsilon_{xx} - \epsilon_{yy}$$

$$\epsilon_{111} = \epsilon_{xy} + \epsilon_{yz} + \epsilon_{zx}.$$

Straight dislocations:

$$b\alpha_1^{(100)} = 0.99 \cdot 10^{-7}/\text{cm}$$

$$b\alpha_1^{(111)} = 0.425 \cdot 10^{-7}/\text{cm}.$$

Infinitesimal loops:

$$b\alpha_2^{(100)} = 3.6 \cdot 10^{-8}/\text{cm}^2$$

$$b\alpha_2^{(111)} = 2.0 \cdot 10^{-8}/\text{cm}^2.$$

Point defects:

$$\alpha_4^{(100)} = 10.13$$

$$\alpha_4^{(111)} = 5.07.$$

With these figures the broadening should be significant ( $\Delta > 10^{-4}$ ) provided  $L \gtrsim 10^5$  or  $10^6 \text{ cm/cm}^3$ ,  $A \gtrsim 10^3$  or  $10^4 \text{ cm}^2/\text{cm}^3$  and  $\rho \gtrsim 50 \text{ ppm}$ . Dislocation dipoles are, in practise, always negligible. Note that, contrary to the usual supposition for random strains, simple Gaussian distributions never occur.

The predictions for straight dislocations in MgO have been compared in detail with spin-resonance experiments [1, 4]. The magnitude of the strain broadening, and the variation of the line shape and line width with magnetic field orientation are all in good agreement with experiment. However, the line-shape itself does not agree—theory gives a nearly Gaussian shape, whereas in MgO Lorentz shapes are observed. This discrepancy is probably a result of our oversimplification of the actual dislocation distribution in MgO. The nearly Gaussian shape for broadening by dislocations has been seen in NaCl [5], where the predictions for strain broadening by point defects were also verified in detail. No detailed check of the predictions for broadening by dislocation loops has been made, although zero-phonon lines in neutron-irradiated MgO appear to be broadened by this mechanism [6].

In summary we can predict the effects of dislocation and other lattice imperfections on resonance lines. The predictions, in terms of the individual defect perturbation fields, defect densities and defect distributions, are verified by experiment.

### Appendix

The probability that the perturbation  $\epsilon$  lines between  $\epsilon$  and  $\epsilon + d\epsilon$  is  $I(\epsilon)d\epsilon$ , and may be calculated from equations (1), (2), and (3) without further physical approximations.

Formally we can write

$$I(\epsilon) = \frac{1}{v^N} \int \cdots \int dz_1 p(z_1) \cdots dz_N p(z_N) \delta\{\epsilon - \epsilon(z_1, z_2, \dots, z_N)\}.$$

The delta function singles out the configurations where  $\epsilon(z_1, \dots, z_N)$  has the specific value  $\epsilon$ ;  $I(\epsilon)$  is simply the fraction of the possible configurations which have this value of  $\epsilon(z_1, \dots, z_N)$ . The statistical distribution function,  $p(z)$ , is normalised by

$$v = \int dz p(z).$$

Using the spectral representation of the delta function:

$$\delta(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{ixy}$$

we can write

$$I(\epsilon) = \frac{1}{2\pi} \cdot \frac{1}{v^N} \int_{-\infty}^{\infty} dx e^{ix\epsilon} \int dz_1 p(z_1) \dots \int dz_N p(z_N) \exp [-ix\epsilon(z_1, \dots, z_N)].$$

The innermost exponential factorises as a result of (2):

$$\exp [-ix\epsilon(z_1, \dots, z_N)] = \prod_{i=1}^N \exp [-ix\epsilon(z_i)]$$

so that

$$I(\epsilon) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{ix\epsilon} \left\{ \frac{1}{v} \int dx p(z) \exp [-ix\epsilon(z)] \right\}^N.$$

Using the definitions of  $\rho$  and  $J$  given in (4b)

$$I(\epsilon) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{ix\epsilon} \left\{ 1 - \frac{\rho^{J(x)}}{N} \right\}^N$$

which gives (4a) in the limit of large  $N$ .

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## Discussion on Paper by A. M. Stoneham.

BENNETT: Recently, Weisman and I<sup>1</sup> extended a nuclear magnetic resonance technique which turns out to be somewhat better than the calibrated lineshape method for studying these distributions of strains from dislocations. This is a technique (first introduced by Solomon in 1958)<sup>2</sup> of using pulsed NMR and measuring what is known as the quadrupolar echo. We have shown that this is a very powerful technique for measuring the actual distribution of the satellite lines rather than the reduction in intensity which is obtained when the satellite lines are too far out to be measurable as simply a broadening of the central line. So it would extend the applicability to the study of somewhat higher strains than the case you have talked about.

STONEHAM: Most of the experiments which have been done have generally been in spin resonance and optical techniques, and then they correspond to cases where there are strains in order of, shall we say, one part in 10,000. Now, the case you are mentioning deals with the situation where there are defects, generally speaking, closer to the centers than these which give rise to the resonance line in the spin resonance or optical cases. Then, the discrete structure of the lattice becomes important and gives rise to the satellite lines you mention.

ASHCROFT: Are these experiments carried out when the crystal is under a state of stress?

STONEHAM: No external stress.

ASHCROFT: Can you tell me how you normalize these widths?

STONEHAM: What one needs to know is the coupling coefficient to strain of the centers you are looking at, in other words, how much the line shifts per unit strain. This is usually obtained by a separate experiment in which there is a static external stress of the type you mentioned. In other words there is an assumption here that response to the local strain is the same as the response to a uniform stress. That becomes valid at the low concentration limit which is essential in some of the assumptions I made.

BULLOUGH: I wondered if you could comment on the possibility of using these kinds of methods to expose the non-linear strain field of dislocations.

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<sup>1</sup> Weisman, D., and Bennett, L. H., Phys. Rev. **181**, 1341 (1969).

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STONEHAM: I don't know how one would do it simply. What one can do is to look at the extreme wings of a resonance line. In that case in the low concentration limit the wings are dominated by the contribution of configurations in which there is, for instance, one dislocation near to whichever center you are looking at. In that case one should certainly be able to detect deviations from the simple  $r^{-1}$  dependence of the dislocation strain field provided you know something about the distribution of the dislocations and point defects, for instance if you assume that they are just randomly distributed. Unfortunately, both the strain field and the distribution are rather intimately coupled, and it may be difficult to separate the two effects.

SEEGER: There is also the point that since your Burgers vector is independent of the radius unless you are really in the core, the strain, if properly defined, will always be  $1/r$  unless you get right in the dislocation core. It's the stress that shows the non-linear deviations and your results are really sensitive to the strain and not the stress. So the region where your technique could be expected to show any non-linear effects is extremely small. It is the dislocation core proper, and not the region where in other experiments second-order effects could be expected to show up.

MARADUDIN: I would like to address my question to Dr. Stoneham, although it is prompted also by the question that Professor Ashcroft asked. In normalizing the widths, presumably one measures the shift in the center of the line due to an externally imposed strain. But, in fact, the strain actually acting at the defect site is different from the externally imposed strain. After all, the force constants about the defect and so forth are changed, so that in the resonance experiments the strain that is actually operative is the local strain. Is there any estimate of the differences or errors arising from this source?

STONEHAM: There are two points. The first point is that in the case of broadening by strains there is no need to make any corrections of the nature you have just mentioned, simply because all one is saying is that the coupling coefficient one measures is the shift in the resonance line per unit external strain—if one forgets about the changes in lattice constants. When one calculates what the strain broadening is, one also uses effectively, the formulae for the external strain due to other defects. In other words one is saying that the corrections due to the changes in local force constants are the same for the strains due to defects as they are for the case of the external stress. This is not necessarily a valid assumption, although it becomes increasingly valid at low concentrations when the more homogeneous strains are the most important ones. In other cases, though, particularly if you are interested in broadening by internal

electric fields, then it is essential to take into account some sort of local field correction. This is often very difficult to calculate, particularly in nuclear magnetic resonance cases.



# DISLOCATION PAIR INTERACTION IN A FINITE BODY

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The elastic interaction between dislocations in a finite body shows important features not found in an infinite body. For example, two like dislocations parallel to the axis of a cylinder repel each other only when they are close, but attract each other when their distance is comparable to the cylinder radius. Contours of the pair interaction energy are given for both screw and edge dislocations in a circular cylinder.

These new features appear not only when free surface conditions are demanded on the entire body, but even when approximate stress fields are used that demand some surface tractions, so long as no torques are transmitted through the body.

The relevant torques (bending moments) associated with an edge dislocation in a circular cylinder, which vanish when the mantle is traction free, may be made to vanish in general by a simple modification of the stress field of the edge dislocation.

Key words: Dislocation surface; interactions; dislocations; elastic interactions; finite elasticity.

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## I. FREE SURFACE CONDITIONS VERSUS INTERNAL STRESS CONDITIONS

Ideally, one might like to know the stress field  $\sigma_{ij}$  of a straight dislocation extending throughout a finite body under free surface conditions, i.e., so that the tractions<sup>1</sup>

$$T_i \equiv \sigma_{ij}n_j = 0 \quad (1)$$

on every surface element (unit normal  $n_j$ ). In practice, this goal is hard to achieve and of limited interest. Instead, stress fields of both screw and edge dislocations have been obtained for long cylinders and for thin plates,

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<sup>1</sup> Summation convention. All subscripts go from 1 to 3 unless stated otherwise.

fulfilling free surface conditions on the large surfaces, but not on the end surfaces of the cylinder or on the rim surface of the plate [1, 2]. Yet certain *averages* of the tractions over these small parts of the surface were made to vanish so that, by Saint Venant's principle [3], their effect would not penetrate far into the body. These less restrictive boundary conditions may be called "internal stress conditions."

For example, the torque developed by the simple stress field of a screw dislocation across any cross section of a cylinder has commonly been canceled by the superposition of another stress field without regard to the fact that both stress fields together do not lead to vanishing surface tractions on the ends of the cylinder.

Similarly, one may relax the free surface conditions everywhere, so long as certain averages of the tractions are zero and the "wavelength" of their variation is small compared to the specimen dimensions. We have found that more general boundary conditions like this, which are easier to satisfy than eq (1), often produce essential features of dislocation stress fields in a finite body. Let us therefore summarize these "internal stress" conditions, first regarding the "wavelength," then the vanishing of "certain averages."

For a finite body containing many dislocations, it is often stated that the surface effects penetrate to a depth comparable to the average dislocation spacing. It is true that the surface tractions, which would be demanded by an approximate stress field, would vary with a "wavelength" of the average dislocation spacing. Such an approximate stress field would therefore describe the state of affairs in the bulk of the body, provided the average of those surface tractions is also zero. This condition may be obviously satisfied in special cases, such as in a balanced distribution of positive and negative, but otherwise identical, dislocations. In general, however, any approximate stress field that limits surface effects to a thin layer has to satisfy additional conditions.

Consider separating off a part of the body by a plane cut  $C'$ , whose unit normal is  $n_j$ , and let the remaining part of the surface be called  $S'$ . The absence of body forces implies that the area integrals

$$\int_{C'} \sigma_{ij} n_j dS + \int_{S'} T_i dS = 0. \quad (2)$$

On the other hand, "internal stress conditions" demand

$$\int_{C'} \sigma_{ij} n_j dS = 0 \quad (3)$$

separately. In other words, the average of the surface tractions over  $S'$  must also vanish.

Similarly, the absence of body moments implies

$$\int_{C'} \epsilon_{ikl} x_k \sigma_{lj} n_j dS + \int_{S'} \epsilon_{ikl} x_k T_l dS = 0 \quad (4)$$

where  $x_k$  is the position vector from the origin and  $\epsilon_{ikl}$  is the permutation tensor. The first term in eq (4) represents the moments arising from torques (i.e., twisting and bending moments) being transmitted through the cut.

We may characterize these torques by defining a tensor  $M$ , the *torque tensor*, where the component  $M_{ij}$  is due to torques taken about the  $i$  axis which are transmitted through planes normal to the  $j$  axis. (In general  $M$  will not be symmetrical.) The first term in eq (4) then becomes  $n_j M_{ij}$ . "Internal stress conditions" demand that these torques also vanish:

$$M_{ij} \equiv \int_{C'} \epsilon_{ikl} x_k \sigma_{lj} dS = 0. \quad (5)$$

Therefore, the second term in eq (4), which is another average of the surface tractions over  $S'$ , must also vanish.

Equations (3) and (5) are trivially satisfied under free surface conditions (eq 1), but they are generally not satisfied if the stress field of a dislocation in an infinite body is used in the finite body. There are obviously intermediate solutions which satisfy conditions (3) and (5) but not (1).

## II. Elastic Interaction Between Dislocations

Consider a cylindrical body of cross-sectional area  $A$  containing a pair of dislocations parallel to its axis, one at a fixed position and the other intersecting the cross section at an arbitrary position  $x_n$ . Let  $I$  be the energy of interaction between the dislocations, i.e., the energy difference between the body containing the pair of dislocations and two identical bodies each containing one of them at corresponding positions. The average interaction energy

$$\bar{I} \equiv \frac{1}{A} \int I dS \quad (6)$$

where the integration is taken over all positions  $x_n$  on the cross section. If eq (6) is integrated by parts along the coordinates  $k$  in the plane, noting that  $I$  is zero for all positions  $x_n$  on the boundary, we obtain

$$\bar{I} = -\frac{1}{2A} \int x_k I_{,k} dS. \quad (7)$$

Let the dislocation at  $x_n$  have the Burgers vector  $b_j$ . The gradient of the interaction energy is then [4]

$$I_{,k} = -\epsilon_{kli}\sigma_{lj}b_jn_i \quad (8)$$

where  $\sigma_{lj}$  is the stress field of the fixed dislocation and  $n_i$  is a unit vector along the cylinder axis. Substituting into eq (7) and using eq (5) we find

$$\bar{I} = \frac{n_i b_j}{2A} \int_A \epsilon_{kli} x_k \sigma_{lj} dS = \frac{n_i b_j M_{ij}}{2A} = 0 \quad (9)$$

for an internally stressed body.

Since  $\bar{I}$  vanishes, the energy of interaction for the pair cannot have a unique sign and so two like (unlike) dislocations will not always repel (attract) each other. This result is in marked contrast to "infinite body interaction" where for example one always has two like screw dislocations repelling and their energy of interaction always positive.

$\bar{I}$  will be zero (eq 9) when the component  $M_{ij}$  due to torques transmitted through planes normal to the Burgers vector, taken about an axis along the dislocation line, is zero. This internal stress condition will be called the torque condition. Anticipating the results of the next section wherein we take the stress field for a dislocation in an infinite body and make corrections to it, eventually building up to a "complete solution" (free surfaces), the essential features of dislocation interaction appear when the torque condition alone is satisfied.

### III. Dislocation Interaction in Circular Cylinders

In order to illustrate the features of elastic interaction under various boundary conditions, we shall consider the interaction between a pair of dislocations lying parallel to the axis of a long circular cylinder of radius  $R$ . Let the  $z$  axis coincide with the cylinder axis and let the  $x$  and  $y$  axes be in the cylinder cross section. The analysis of the interaction is most transparent for the case of screw dislocations and we treat this first. Our approach will consist in taking the stress field for the dislocation in an infinite medium, make a correction so as to satisfy the torque condition, and finally make corrections to obtain a complete solution. A comparison of the interaction energy contours calculated from the various "corrected" stress fields enables one to see how the interaction is influenced as the free surface conditions are approached.

#### III. 1. Screw dislocations

$\bar{I}$  will be zero when the  $M_{zz}$  component of the torque tensor is zero, or in other words when no twisting torque is transmitted through the cross

section. (The twisting effect associated with a screw dislocation in a cylinder is well known [1, 2].) The torque condition can be satisfied by adding (we assume linear elasticity and small strains) to the infinite body stress  $\sigma_{\theta z}$  a stress  $\sigma'_{\theta z}$  which is proportional to the distance from the cylinder axis, the proportionality constant being determined by  $M_{zz}=0$ . A complete solution is obtained by then adding a stress  $\sigma''_{\theta z}$  which cancels the traction over the mantle (cylindrical surface) of the cylinder. This latter stress corresponds to the stress field of an image dislocation. The complete stress field is in equilibrium; therefore by Saint Venant's principle [3] we can ignore any effects due to the free surface condition on the ends of the cylinder.

Figures 1a, 1b, and 1c show contours of the interaction energy calculated from the complete, torque corrected, and infinite body stress fields, respectively.<sup>2</sup> The interaction under infinite body stress is quite distinct from the true interaction, but when the torque condition is satisfied all the essential features of the interaction appear. One can see that in a finite body the interaction energy does indeed change sign, and it is apparent from either figure 1a or 1b that the interaction force must also be zero for certain configurations. An extensive set of contours for the interaction energy and the radial component of the interaction force between a pair of screw dislocations in a cylinder was given in a previous paper using the complete solution for the stress field [5].

### III. 2. Edge dislocations

The relevant components of the torque tensor for edge dislocations with Burgers vectors along the  $x$  or  $y$  axes are  $M_{zx}$  and  $M_{zy}$ , respectively. These components are due to the bending torques, taken about the  $z$  axis, which are transmitted through planes normal to the  $x$  and  $y$  axes, respectively. When the tractions on the mantle vanish,  $M_{zx}$  and  $M_{zy}$  clearly must vanish. This is in contrast to the case of screws where the free surface and torque conditions were independent (section III. 1). Since the torques due to an edge dislocation have usually been ignored in the past, we shall treat them in detail at this point.

The following two identities are required; these can be verified with Gauss's theorem in the plane<sup>3</sup>

<sup>2</sup> Interaction energies were determined by the usual method [1] of integrating the appropriate stress components of the fixed dislocation over a "cut." When the mantle is not a free surface, this method must be considered an approximation since we ignore the work done by surface tractions. For consistency all cuts were parallel to the  $y$  axis.

<sup>3</sup> The bracketed index means no summation.

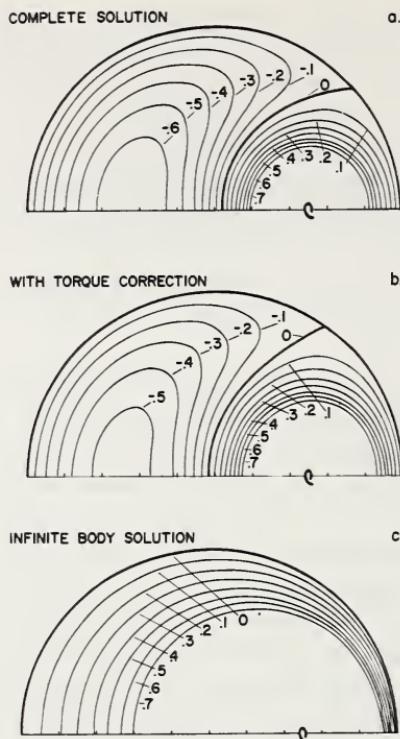


FIGURE 1. Interaction energy between one fixed dislocation (shown) and an identical dislocation at varying positions. The contour values are given in units of  $\frac{Gb^2}{4\pi}$ . (a) Complete solution. (b) With torque correction. (c) Infinite body solution.

$$\int_A x_{(i)} \sigma_{ij} dS = \frac{1}{2} \oint_C x_i^2 T_j ds \quad (10)$$

$$\int_A (x_i \sigma_{jn} + x_n \sigma_{ij}) dS = \oint_C x_i x_n T_j ds \quad (11)$$

where the closed curve  $C$  bounds a region  $A$  in the plane, and  $n_k (T_j = \sigma_{jk} n_k)$  is the unit normal to a given element of  $C$ . When the cylinder is *circular*, one can show

$$\begin{aligned} M_{zx} &= M_{xz}/\nu \\ M_{zy} &= M_{yz}/\nu \end{aligned} \quad (12)$$

where  $\nu$  is Poisson's ratio and we have assumed plane strain conditions. Thus for the special case of edges in circular cylinders, the torque condition can be stated in terms of the vanishing of the bending torques  $M_{xz}$

and  $M_{yz}$  which are transmitted through the cylinder cross section. It is clear that these kinds of torques must arise from the  $\sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy})$  component of the stress.

The only mention of the torques associated with edge dislocations appears to be a theorem attributed to Eshelby by Nabarro [2]: The vanishing of the tractions over the mantle of a cylindrical body (arbitrary cross-sectional shape) containing a dislocation parallel to its axis implies the vanishing of  $M_{xz}$  and  $M_{yz}$ . The proof given [2] invokes an incorrect formulation of the free surface condition on the mantle, and we shall give a correct proof since the result is of interest here.<sup>4</sup> Let the  $z$  axis coincide with the cylinder axis and let  $A$  be the cylinder cross section. We obtain from eqs (5), (10), and (11)

$$M_{xz} = - \int_A y \sigma_{zz} dS = \frac{\nu}{2} \oint_C (x^2 - y^2) T_y ds - \oint_C xy T_x ds \quad (14)$$

$$M_{yz} = \int_A x \sigma_{zz} dS = \frac{\nu}{2} \oint_C (x^2 - y^2) T_x ds - \oint_C xy T_y ds, \quad (15)$$

thus  $M_{xz} = M_{yz} = 0$  when  $T_i$  vanishes on the mantle.

Consider a dislocation with the Burgers vector parallel to the  $x$  axis, intersecting the cross section at a point on the  $x$  axis. We can make the torque correction in the following way.  $M_{yz}$  is zero by symmetry and we add a stress function

$$\chi = \frac{\alpha G b}{4\pi(1-\nu)R^2} y[(x-d)^2 + y^2] \quad (16)$$

to the infinite body stress function, where  $d$  is the displacement of the dislocation from the cylinder axis. This gives a  $\sigma_{zz}$  component of stress proportional to  $y$  and we determine the proportionality constant  $\alpha$  from  $M_{xz} = 0$ . A similar correction can be made if the Burgers vector is parallel to the  $y$  axis. The value of  $\alpha$  for the Burgers vector along the  $x$  axis is

$$\alpha = 1 - \frac{(d/R)^2}{2}, \quad (17)$$

and for the Burgers vector along the  $y$  axis it is

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<sup>4</sup> The present authors questioned the free surface conditions given in [2] on the basis of specific stress functions. The conditions given in [2] are in fact correct (J. Eshelby, private communication) if one allows for additional linear terms in the stress function. This does not affect the stresses.

$$\alpha = \frac{3[2 - 3(d/R)^2]}{2[3 + (d/R)^4]} \quad (18)$$

Bullough [6] has given the stress functions for complete solutions, these result in corrective terms which are more complicated functions of  $x$  and  $y$  than eq (16). We can again neglect the free surface condition at the ends of the cylinder (cf. screw dislocations).

Figures 2a and 2b show the interaction energy contours obtained with torque-corrected and infinite body stress fields, respectively. For this special case, with the fixed dislocation along the cylinder axis, the torque correction also removes the traction from the mantle, but in general this will not happen. We have thus labeled the torque corrected contours a complete solution, and of course *all* the features of finite body interaction are manifested under the torque corrected stress field. If the fixed dislocation is moved off the cylinder axis, the situation becomes analogous to that for screw dislocations. Adding the torque correction brings out the essential features of the interaction.

As a matter of interest we show in figures 3 and 4 several interaction energy contours obtained with complete solutions where the fixed dislocation is moved off the cylinder axis. One can see that the energy of interaction changes sign and also that there is a zero *radial* interaction force, i.e., not just with respect to the glide component. When two like dis-

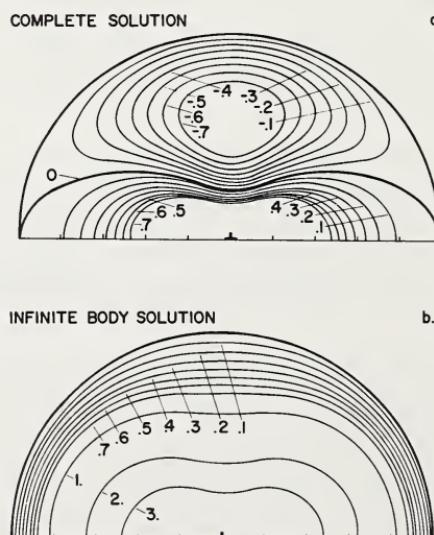
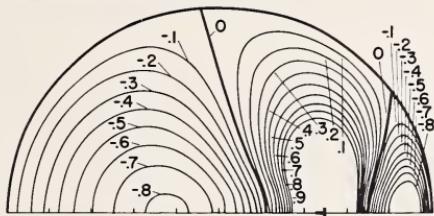


FIGURE 2. Interaction energy between one fixed dislocation (shown) and an identical dislocation at varying positions. The contour values are given in units of  $\frac{Gb^2}{4\pi(1-\nu)}$ .  
 (a) Complete solution. (b) Infinite body solution.

COMPLETE SOLUTION



COMPLETE SOLUTION

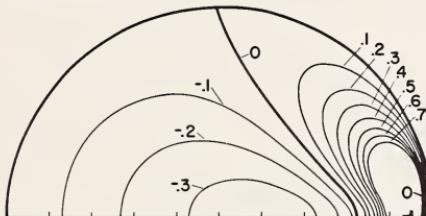
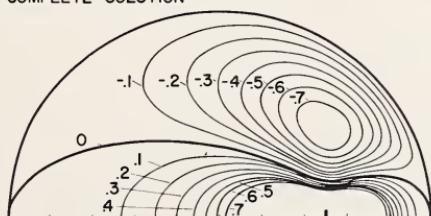


FIGURE 3. Interaction energy between one fixed dislocation (shown) and an identical dislocation at varying positions. The contour values are given in units of  $\frac{Gb}{4\pi(1-\nu)}$ .

COMPLETE SOLUTION



COMPLETE SOLUTION

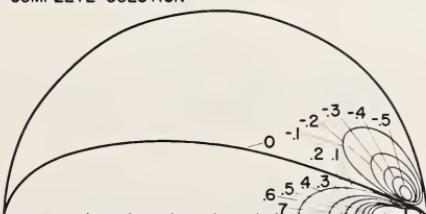


FIGURE 4. Interaction energy between one fixed dislocation (shown) and an identical dislocation at varying positions. The contour values are given in units of  $\frac{Gb^2}{4\pi(1-\nu)}$ .

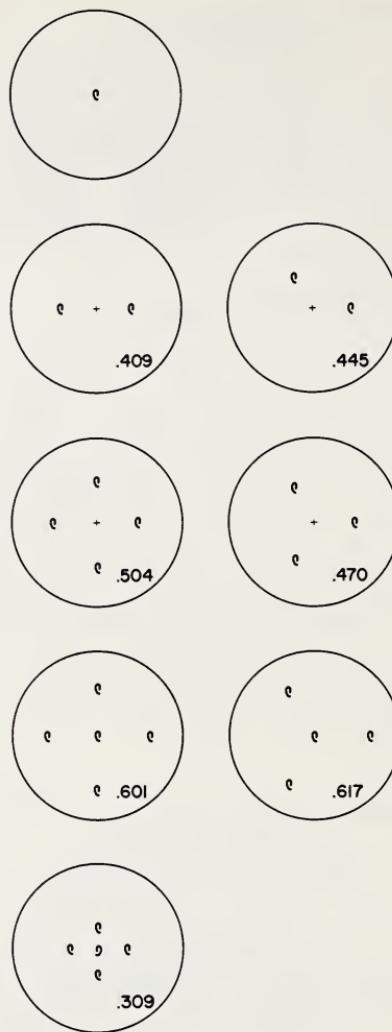


FIGURE 5. Some metastable screw dislocation configurations. (The distance from the axis is given in units of the cylinder radius.)

locations with Burgers vectors parallel to the  $x$  axis both lie on the  $x$  axis, the interaction force is always repulsive and the energy of interaction always positive.

#### IV. Metastable Configurations

We have seen that the interaction force between two dislocations will change sign. This suggests the existence of metastable configurations containing several dislocations. It has been shown that a single screw

dislocation is in metastable equilibrium when it lies along the axis of a circular cylinder [1].

The total energy of various arrangements was calculated using complete solutions for the stress fields, and we have found the metastable configurations of screw dislocations which are shown in figure 5. Because of their extreme symmetry, one would not really expect these to be physically significant except possibly in the cases of the dipoles. In no instance did we find similar metastable configurations made up of edge dislocations, even though figures 3 and 4 suggest they might exist.

### **V. Acknowledgement**

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# THE MEAN SQUARE STRESSES $\langle \sigma^2 \rangle$ FOR A COMPLETELY RANDOM AND A RESTRICTEDLY RANDOM DISTRIBUTION OF DISLOCATIONS IN A CYLINDRICAL BODY

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The paper gives a full proof of the author's earlier statement according to which the elastic interaction energy of completely randomly distributed dislocations vanishes. As a consequence the outer cut-off radius in the logarithmic factor of the elastic energy coincides with the external cylinder radius rather than with the mean dislocation spacing. The proof takes into account the elastomechanical boundary conditions which were neglected in the earlier paper. Further it is shown that for a restrictedly random distribution the outer cut-off radius is equivalent to the radius of the areas small compared with the cylinder cross-section, each of which contains the same number of dislocations randomly distributed over the corresponding area. In the special case that each area contains only one dislocation with arbitrary inside the area the outer cut-off radius degenerates to the mean dislocation spacing.

Key words: Dislocations; elasticity; statistical methods.

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The expression "random distribution" has been widely used in the literature for describing the dislocation patterns in deformed crystals. However, in an earlier paper the present author [1] has shown under some restrictive assumptions regarding the elastic boundary conditions that such a distribution yields to an unrealistic high value for the elastic energy or the mean square stresses.

The present paper deals with the calculation of the mean square stresses  $\langle \sigma^2 \rangle$  for two types of distributions of dislocations, which extend parallel to the axis of a cylindrical body with traction-free surfaces.

(i) The intersection points of the dislocations are completely randomly distributed over the cylinder cross section, all dislocations having the same Burgers vector  $\mathbf{b}$  in direction and sign.

(ii) The cross section is subdivided into equally sized areas, all containing the same number of dislocation intersection points. Within each

such area the intersection points are randomly distributed as in (i) ("restrictedly random distribution").

Using the linear theory of elasticity,  $\langle \sigma^2 \rangle$  may be splitted into two terms,

$$\langle \sigma^2 \rangle = \langle \sigma^2 \rangle_s + \langle \sigma^2 \rangle_i$$

where  $\langle \sigma^2 \rangle_s$  equals the sum of the mean square stresses due to the individual dislocations and  $\langle \sigma^2 \rangle_i$  denotes the interaction terms. (The subscripts  $s$  and  $i$  refer to "self-energy" and "interaction energy.") The two terms may be expressed as follows:

$$\langle \sigma^2 \rangle_s = \int_F \left[ \frac{1}{V} \int_v \sigma^2(\dot{r}, r) \cdot d^3r \right] \cdot \bar{P}^{(1)}(\dot{r}) \cdot d^2\dot{r}. \quad (1a)$$

$$\langle \sigma^2 \rangle_i = \int_F \int_F \left[ \frac{1}{V} \int_v \sigma(\dot{r}, r) \cdot \sigma(\dot{r}'', r) \cdot d^3r \right] \cdot \bar{P}^{(2)}(\dot{r}', \dot{r}'') \cdot d^2\dot{r}' \cdot d^2\dot{r}''. \quad (1b)$$

$\sigma(\dot{r}, r)$  stands for the stress component under consideration at the position  $r$  inside the traction-free body.  $\sigma(\dot{r}, r)$  is originated by a dislocation line with its intersection point at  $\dot{r}$  in the cross section  $F \cdot V =$  volume of the body,  $\bar{P}^{(1)}(\dot{r}) \cdot d^2\dot{r}$  means the probability for finding any dislocation inside the area  $d^2\dot{r}$  at the position  $\dot{r}$ .  $\bar{P}^{(2)}(\dot{r}', \dot{r}'') \cdot d^2\dot{r}' \cdot d^2\dot{r}''$  denotes the probability for one dislocation in the area  $d^2\dot{r}'$  at  $\dot{r}'$  and another dislocation in  $d^2\dot{r}''$  at  $\dot{r}''$ .  $\bar{P}^{(1)}$  and  $\bar{P}^{(2)}$  are distribution functions averaged over an infinitely large number of individual distributions, obtained under the same statistical conditions. For the problem under consideration this averaging is necessary, since for an individual distribution  $\langle \sigma^2 \rangle$  may deviate strongly from the average value in either direction.

Now we make use of the dislocation theorem, according to which a traction-free body containing a locally constant dislocation density remains stress-free [2, 3]. For the distribution model (i) it comes out that  $\bar{P}^{(1)} = \text{constant}$  and  $\bar{P}^{(2)} = \text{constant}$ . Then it is easy to arrive from eq (1) to

$$\langle \sigma^2 \rangle_i = 0, \quad (2a)$$

$$\langle \sigma^2 \rangle = \langle \sigma^2 \rangle_s = \rho \cdot b^2 \cdot C \cdot \log \tilde{R}_0/r_0. \quad (2b)$$

$\rho$  = dislocation density,  $C$  is a constant depending on the stress component concerned,  $\tilde{R}_0 = \alpha_0 \cdot R_0$ ,  $R_0$  = cylinder radius defined as  $R_0 = \left(\frac{F}{\pi}\right)^{1/2}$ ,  $\alpha_0$  = a constant in the order of 0.5,  $r_0$  = inner cut-off radius.

After evaluating  $\bar{P}^{(1)}$  and  $\bar{P}^{(2)}$  for the distribution (ii) one finds for  $R_0 \gg R_p \gg \rho^{-1/2}$ ,  $R_p$  = radius of the sub-areas,

$$\langle \sigma^2 \rangle = \rho \cdot b^2 \cdot C \cdot \log \tilde{R}_p / r_0, \quad (3)$$

$$\tilde{R}_p = \alpha_p \cdot R_p, \quad \alpha_p \approx \alpha_0.$$

Equation (2) confirms exactly the author's [1] earlier statement, according to which the effective outer cut-off radius in  $\langle \sigma^2 \rangle$  coincides for a completely random distribution approximately with the cylinder radius. The distribution model (ii) may be extrapolated to one dislocation per sub-area, corresponding to  $R_p = (\pi\rho)^{-1/2}$ . For this extreme case, which may be better denoted as a "quasi-homogeneous" distribution, eq (3) results in an effective outer cut-off radius in the order of the mean dislocation spacing. Such a value for the outer cut-off radius was assumed to hold also for completely random distributions [4, 5], which is in contrast to eq (2).

It is easy to verify that eq (2) remains valid also for dislocations of mixed signs as long as no correlation exists between the "plus" and "minus" dislocations. The same is to show for eq (3), if all sub-areas contain the same fractions of "plus" and "minus" dislocations. The full-length paper has been submitted to *Acta Met.* [6].

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# THEORETICAL ASPECTS OF KINEMATICAL X-RAY DIFFRACTION PROFILES FROM CRYSTALS CONTAINING DISLOCATION DISTRIBUTIONS

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The paper deals with a theoretical study of the Fourier transform of the X ray diffraction line profiles from crystals containing dislocation distributions. The theory is based mainly on a calculation of spatial averages of powers of the strains  $\epsilon_n$ , where  $\epsilon_n$  means the differential strain perpendicular to the reflecting planes averaged over a certain length  $n$  ( $n$  = variable of the Fourier transform). The second power average  $\langle \epsilon_n^2 \rangle$  is calculated in a closed form for a restrictedly random dislocation distribution. However, the result is approximately valid also for other distributions. The contributions of the averages of higher powers of  $\epsilon_n$  are taken into account in an approximate manner. The expression derived for the Fourier transform depends on the two parameters  $\rho$  and  $R_e$ , where  $\rho$  is the dislocation density.  $R_e$  is equivalent to the effective outer cut-off radius which appears for instance in the logarithmic factor of the elastically stored energy. The result which is applicable for  $R_e \gtrsim \rho^{-1/2}$  is discussed in comparison with the theory of Krivoglaz and Ryaboshapka, in which a completely random dislocation distribution is assumed, and with the theory of diffraction from distorted crystals mainly developed by Warren and Averbach.

**Key words:** Diffraction profiles; dislocation diffraction; kinematic x-ray diffraction; statistical methods for dislocations.

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## I. Introduction

X-ray diffraction profiles  $I(\theta)$  ( $\theta$  = angle of diffraction) from deformed crystals display a broadening compared with the theoretical line width of perfect crystals. This line broadening has been studied for many years in various experimental and theoretical investigations [1-5]. If the influence of stacking faults can be neglected, the broadening can be attributed mainly to the strain fields of the (deformation-induced) dislocations (strain broadening).

Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough, Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

In the past, broadened x-ray line profiles from deformed crystals were often analysed by means of a Fourier analysis method of the type mainly developed by Eastabrook and Wilson [1] and by Warren and Averbach [2, 4]. In this method, the broadening is analysed in terms of the "mean particle size" (mean size of the coherently scattering crystal regions) and the "mean square strains"  $\langle \epsilon^2 \rangle$  (see section II). There are, however, some fundamental difficulties preventing a straightforward interpretation of these results in terms of dislocation density and dislocation distribution.

Therefore, in developing a theory of kinematical diffraction from deformed crystals, it became expedient to incorporate, from the beginning, the existence of the dislocations as the sources of internal lattice strains. In several theoretical papers special, more or less oversimplified, crystal models were treated. (Therefore the conclusions of these papers are not directly applicable to experimental results.) For instance, some papers concerned themselves with the diffraction from a cylindrical crystal containing a single perfect dislocation [6-9], a single imperfect dislocation terminating a stacking fault [10], or a small number of perfect dislocations [11]. The asymptotic tails of the line profiles were studied in [12].

So far, the theory of Krivoglaz and Ryaboshapka [13] (in the following, K & R) is the most highly developed one. This theory uses a method especially developed for problems of scattering from crystals containing point defects and is based on the assumption that the cylindrical crystal contains a large number of straight parallel dislocations which are randomly distributed over the entire crystal cross-section. This theory predicts that the diffraction line profile is represented by a Gaussian function with a half-width which is proportional to the square root of the dislocation density and which depends logarithmically on the radius  $R_0$  of the model crystal. Applying the results of the K & R theory to experimentally determined diffraction profiles, the meaning of this parameter  $R_0$  (which comes out to be closely connected with the outer cutoff radius, see below) remains completely unclear. This difficulty results from the random distribution of the dislocations as assumed in the K & R theory. In fact, it has been shown by Wilkens [14, 15, 16] that such a distribution is not a suitable model distribution for the problem under consideration.

It is well known that properties of dislocated crystals which are based on spatial averages of second-power products of stress or strain tensor components depend on an outer cutoff radius  $R_e$ . As an example we mention the volume density  $E$  of the elastically stored energy, generally written in the form

$$E = \frac{G}{4\pi} b^2 \cdot \rho \cdot \log R_e/r_0 \quad (1.1)$$

where  $G$  shear modulus,  $b$  modulus of the Burgers vectors,  $\rho$  dislocation density,  $r_0$  inner cutoff radius.  $R_e$  is a characteristic parameter which for deformed macroscopic crystals depends on the internal structure of the dislocation distribution (caused by the deformation) rather than on the crystal dimensions.

Wilkens and Bargouth [17] have applied the K&R theory to experimentally determined diffraction profiles from deformed copper single crystals. Tentatively they identified the above-mentioned radius  $R_0$  with a characteristic spacing of the dislocation distribution and thus arrived at values for the dislocation density which were in a fairly good agreement with values determined by transmission electron microscopy.

Stimulated by this agreement we investigate in the present paper the kinematical x-ray diffraction profiles, expressed by their Fourier transforms, for non-random, i.e., physically more realistic dislocation distributions. This first paper is restricted to a rather simplified model: the cylindrical crystal contains one set of parallel dislocations of one slip system. The distribution of the dislocations over the crystal cross section is not tightly specified. However, as a special distribution which allows some detailed calculations we treat the case of a restrictedly random distribution which contains the effective outer cutoff radius  $R_e$  as a free adjustable parameter [14–16]. A subsequent paper [18] will deal with the extension of the theory to crystals with several sets of dislocations and with a discussion of methods for a separate determination of the two parameters,  $\rho$  and  $R_e$ , from the diffraction profiles.

Although electron transmission microscopy has proved to be a powerful tool for the determination of the dislocation density and distribution in various crystals [19, 20], the determination of  $\rho$  and  $R_e$  from x-ray diffraction profiles may be of interest especially for such substances which are difficult to investigate by electron microscopy, for instance because of a too high dislocation density ( $\rho > 10^{10} \text{ cm}^{-2}$ ) or due to difficulties in the preparation of the transmission specimens.

## II. The Basic Equations

Let us consider the diffraction profile  $I_g$  obtained from a set of lattice planes characterized by the reciprocal lattice vector  $\mathbf{g}$ . The function  $I_g$  is assumed to be given as a function of the coordinate  $S$  of the reciprocal lattice

$$S = \frac{2}{\lambda} (\sin \theta - \sin \theta_0) \cong \frac{2 \cos \theta_0}{\lambda} (\theta - \theta_0), \quad (2.1)$$

$\lambda$  = x-ray wavelength,  $\theta$  = diffraction angle,  $\theta_0$  = Bragg angle of the undistorted lattice.

$I_g(S)$  shall be normalized corresponding to

$$\int I_g(S) dS = 1 \quad (2.2)$$

and may be expressed by its Fourier transform  $A_g(n)$ ,

$$I_g(S) = \int A_g(n) \exp(2\pi i n S) dn, \quad (2.3)$$

$$A_g(n) = \int I_g(S) \exp(-2\pi i n S) dS. \quad (2.4)$$

Since we confine ourselves in the present paper to symmetric functions  $I_g(S)$  the Fourier transform  $A_g(n)$  will be symmetric and real, too. Therefore, it is sufficient to consider for the rest of the paper only positive values of  $n$ .

Neglecting the so-called particle size broadening,  $A_g(n)$  may be written in the form [1, 2, 4]

$$A_g(n) = \langle \exp(2\pi i g \cdot \epsilon_n) \rangle, \quad (2.5)$$

where

$$\epsilon_n = \frac{1}{n} \left[ u_g \left( \mathbf{r} + \frac{1}{2} n \cdot \mathbf{e}_o \right) - u_g \left( \mathbf{r} - \frac{1}{2} n \cdot \mathbf{e}_o \right) \right] \quad (2.6)$$

$$= \frac{1}{n} \int_{-n/2}^{+n/2} \epsilon_0(\mathbf{r} + s \cdot \mathbf{e}_o) ds. \quad (2.7)$$

$u_g$  stands for the component of the displacement vector  $\mathbf{u}$  parallel to  $\mathbf{g} \cdot \mathbf{e}_o$  = unit vector parallel to  $\mathbf{g}$ .

$$\epsilon_0 = \lim_{n \rightarrow 0} \epsilon_n \quad (2.8)$$

denotes the differential strain parallel to  $\mathbf{g}$  which may be calculated from the strain tensor  $\boldsymbol{\epsilon}$  by means of

$$\epsilon_0 = \mathbf{e}_o \cdot \boldsymbol{\epsilon} \cdot \mathbf{e}_o. \quad (2.9)$$

Further,

$$\langle \dots \rangle = \frac{1}{V} \int_v \dots d^3 \mathbf{r}, \quad V = \text{crystal volume}, \quad (2.10)$$

means in eq (2.5) the spatial average taken over all atom pairs with distance  $n \cdot \mathbf{e}_o$ .

Developing  $A_g(n)$  into a power series, we obtain [1, 2, 4]

$$A_g(n) = 1 - \frac{1}{2!} (2\pi g n)^2 \langle \epsilon_n^2 \rangle + \frac{1}{4!} (2\pi g n)^4 \langle \epsilon_n^4 \rangle + \dots + \quad (2.11)$$

This series can be transformed into an exponential form

$$A_g(n) = \exp (T_1 + T_2 + T_3 + \dots +) \quad (2.12)$$

with

$$T_1 = -\frac{1}{2!} (2\pi g n)^2 \langle \epsilon_n^2 \rangle \quad (2.13a)$$

$$T_2 = \frac{1}{4!} (2\pi g n)^4 [\langle \epsilon_n^4 \rangle - 3 \langle \epsilon_n^2 \rangle^2] \equiv T_2^* - \frac{1}{2} T_1^2; \quad (2.13b)$$

$$T_3 = -\frac{1}{6!} (2\pi g n)^6 [\langle \epsilon_n^6 \rangle - 15 \langle \epsilon_n^4 \rangle \langle \epsilon_n^2 \rangle + 30 \langle \epsilon_n^2 \rangle^3] \quad (2.13c)$$

$$\equiv T_3^* - T_2^* \cdot T_1 + \frac{1}{3} T_1^3.$$

In the method of Warren and Averbach [2, 4], it is assumed that the frequency distribution of the  $\epsilon_n$  within the crystal volume may be approximated by a Gaussian function. Under this assumption all terms  $T_k$  with  $k \geq 2$  vanish. Below, we will see that this is not the case due to the high strains near the dislocation cores.

### III. The Dislocation Distribution

In this paper we consider distributions of straight parallel dislocations all of them belonging to the same slip systems (i.e., all Burgers vectors are either parallel or antiparallel to a reference direction). The dislocations as well as the  $z$ -axis of a cartesian coordinate system are oriented parallel to the axis of a cylindrically shaped crystal which we assume to be elastically isotropic.  $F_0$  means the area of the cylinder cross section and  $N_0$  the number of distributed dislocations. Hence the dislocation density  $\rho$  is given by

$$\rho = \frac{N_0}{F_0}. \quad (3.1)$$

The position vectors within the cross section area of the dislocations will be denoted by  $\dot{\mathbf{r}}_i$ ,  $i=1 \dots N_0$ . We define  $\hat{\epsilon}_0(\dot{\mathbf{r}}, \mathbf{r})$  as the differential strain at the position  $\mathbf{r}$  produced by a dislocation at the position  $\dot{\mathbf{r}}$ .

Making use of the analytically simple solution of  $\hat{\epsilon}_0$  which is valid for straight dislocations in an infinite body (this assumption will be justified below), it follows

$$\hat{\epsilon}_0 = \text{function of } \mathbf{r} - \dot{\mathbf{r}}, \quad (3.2a)$$

$$\hat{\epsilon}_0 = \text{independent of the } z\text{-coordinate.} \quad (3.2b)$$

Under these conditions, eq (2.7) can be reformulated by substituting the integration over  $\mathbf{r}$  by an integration over  $\dot{\mathbf{r}}$ . Hence

$$\epsilon_n(\mathbf{r}) = \sum_{i=1}^{N_0} \hat{\epsilon}_n(\dot{\mathbf{r}}_i, \mathbf{r}) \quad (3.3)$$

with

$$\hat{\epsilon}_n(\dot{\mathbf{r}}_i, \mathbf{r}) = -\frac{1}{m} \int_{-\frac{m}{2}}^{+\frac{m}{2}} \cdot \hat{\epsilon}_0(\dot{\mathbf{r}}_i + \mathbf{e}'_0 \cdot s, \mathbf{r}) ds, \quad (3.4)$$

$m = n \cdot \sin \psi$ ,  $\mathbf{e}'_0$  = unit vector parallel to the projection of  $\mathbf{g}$  (or  $\mathbf{e}_0$ ) on the plane of the cylinder cross section ( $x-y$ -plane).  $m \cdot \mathbf{e}'_0$  = corresponding projection of  $n \cdot \mathbf{e}_0$ .

$\psi$  = angle between  $\mathbf{g}$  and the direction of the dislocation line ( $z$ -axis).

For the following it is expedient to use, instead of the variable  $n$ , the projected variable  $m$ . Since both variables can be interchanged easily we retain the notations  $A_g(n)$ ,  $\epsilon_n$ , and  $\hat{\epsilon}_n$ , even when these functions are expressed in terms of  $m$ .

With respect to the distribution of the dislocation positions we restrict ourselves to "quasi-periodical" distributions, where the length  $\Lambda$  of the quasi-period of the distributions is small compared with the diameter of the cylinder cross section. In this context quasi-periodical means that the local dislocation density has a much smaller variation when averaged over areas of minimum diameter  $\Lambda$  than would be expected for a completely random distribution of the intersection points  $\dot{\mathbf{r}}_i$  over the cross section. As a special, mathematically transparent case of such a quasi-periodical distribution we treat a "restrictedly random" distribution which was introduced by the present author in preceding papers [14, 15, 16].

A restrictedly random distribution is defined in the following way: The cylinder cross section is subdivided into sub-areas all of which are of

the same size  $F_p$ . Each sub-area contains the same number  $N_p^+$  and  $N_p^-$  dislocations with positive and negative Burgers vectors respectively. Consequently,

$$N_p = N_p^+ + N_p^-, \quad \rho = \frac{N_p}{F_p}. \quad (3.5)$$

Within each sub-area the  $N_p$  intersection points  $\mathbf{r}_i$  are completely randomly distributed. As shown in [15] such a distribution (for which the length  $\Lambda$  corresponds to  $\approx \sqrt{F_p}$ ) has the property that, for spatial averages of second power products of strain tensor components, the elasto-mechanical boundary conditions may be neglected if the condition

$$\sqrt{F_p} \ll \sqrt{F_0} \quad (3.6)$$

holds. (It appears reasonable that under the condition  $\Lambda \ll \sqrt{F_0}$  the same conclusion holds for other quasi-periodical distributions.) Hence, with eq (3.6) we may use for  $\epsilon_0$  the infinite body solutions, see above.

#### IV. Calculation of $\mathbf{T}_1$

In the same way as the elastically stored energy  $E$ , the mean square of the differential strain  $\epsilon_0$  may be expressed in the form

$$\langle \epsilon_0^2 \rangle = (b/2\pi)^2 \pi \cdot \rho \cdot C \cdot f_0; \quad f_0 = \log \frac{R_e}{r_0}. \quad (4.1)$$

The constant  $C$  depends on the type of the dislocation involved and on the orientation of  $\mathbf{g}$  with respect to the dislocation line and to  $\mathbf{b}$ .

$$C = \sin^2 \psi \cdot C', \quad C' = \cos^2 \psi, \text{ for screw dislocations}; \quad (4.2)$$

$$C = \sin^2 \psi \cdot C', \quad C' = \sin^2 \psi \cdot F(\gamma), \text{ for edge dislocations}, \quad (4.3a)$$

$$F(\gamma) = \frac{1}{8} (1 - \nu)^{-2} \cdot [1 - 4\nu + 8\nu^2 + 4(1 - 2\nu) \cos^2 \gamma]. \quad (4.3b)$$

$\nu$  = Poisson's ratio,  $\gamma$  = angle between  $\mathbf{b}$  and the projection of  $\mathbf{g}$  on the  $x$ - $y$ -plane,  $r_0$  = inner cutoff radius ( $r_0 \approx b$ ). As for the elastic energy, the effective outer cutoff radius  $R_e$  is determined by the dislocation distribution. In general  $R_e$  cannot simply be identified in terms of characteristic

spacings of the dislocation distribution. However, for a restrictedly random distribution it has been proved in [15] that  $R_e$  is closely related to the "radius"  $R_p$  of the sub-areas,

$$R_p = \sqrt{\frac{F_p}{\pi}}. \quad (4.4)$$

It came out that

$$f_0 = \log \frac{R_e}{r_0} = \log \frac{R_p}{r_0} - \alpha \quad (4.5)$$

with  $\alpha = \frac{1}{4}$  for screw dislocations. A similar value of  $\alpha$  is expected for other than screw dislocations.

According to eq (3.4)  $\epsilon_n$  is obtained from  $\epsilon_0$  by smearing the dislocation cores over the distance  $m = n \cdot \sin \psi$  in the  $x-y$ -plane. From a mathematical point of view this smearing procedure suppresses the divergence of the strain in the dislocation core. However, the inner cutoff radius  $r_0$  as introduced in eq (1.1) and (4.1) is physically determined as a proper limit of the applicability of the linear theory of elasticity. Consequently, with increasing  $m$  the inner cutoff radius  $r_0$  may not be neglected unless the strain divergence is more effectively suppressed by the  $m$ -smearing than by the  $r_0$  cutoff. This point was studied in more detail for a single screw dislocation in an earlier paper [8], in which we found that for a calculation of  $\langle \epsilon_n^2 \rangle$  the inner cutoff  $r_0$  may be neglected if  $m$  is larger than about  $10 r_0$ .

Under this condition it was found in [8] that for a single dislocation  $\langle \hat{\epsilon}_n^2 \rangle$  may be derived from  $\langle \hat{\epsilon}_0^2 \rangle$  by the following substitution

$$\log r_0 \text{ (in } \langle \hat{\epsilon}_0^2 \rangle \text{)} \rightarrow \log m - \beta \text{ (in } \langle \hat{\epsilon}_n^2 \rangle \text{)} \quad (4.6)$$

with  $\beta = 2$  for screw dislocations. Since the main displacement component of an edge dislocation resembles that of a screw dislocation, we may set tentatively  $\beta = 2$  for all types of dislocations.

Considering a crystal containing a large number  $N_0$  of dislocations distributed over the crystal cross section it appears reasonable that a similar substitution as eq (4.6) holds at least as long as  $m$  is small compared with the mean dislocation spacing  $\rho^{-1/2}$ . This assumption could be proved in detail for the special case of a restrictedly random distribution, for which  $\langle \epsilon_n^2 \rangle$  could be calculated in a closed form, see appendix 1. As a result one obtains

$$\langle \epsilon_n^2 \rangle = (b/2\pi)^2 \cdot \pi \cdot \rho \cdot C \cdot f(m/R_e). \quad (4.7)$$

The function  $f(m/R_e)$  is plotted in figure 1. The rather lengthy expression for  $f$  is given in the appendix. For small arguments we find the approximation

$$f(m/R_e) = \log \frac{R_e}{m} + 2, \quad (4.8)$$

which coincides with the substitution of  $\log r_0$  in eq (4.1) according to eq (4.6). As demonstrated in figure 1 the simple approximation eq (4.8) holds with a 10 percent accuracy up to  $m/R_e \approx 2$ . Later we shall find that the function  $f$  will be needed in general only for arguments which are small compared with this upper limit. Therefore we conclude that eqs (4.7) or (4.8) are suitable approximations also for other dislocation distributions as long as they do not deviate drastically from a restrictedly random distribution. Within this approximation we obtain for the first term  $T_1$  in the exponent of eq (2.12)

$$T_1 = \frac{\pi}{2!} (g \cdot b)^2 \cdot C' \cdot \rho \cdot m^2 \cdot f(m/R_e). \quad (4.9)$$

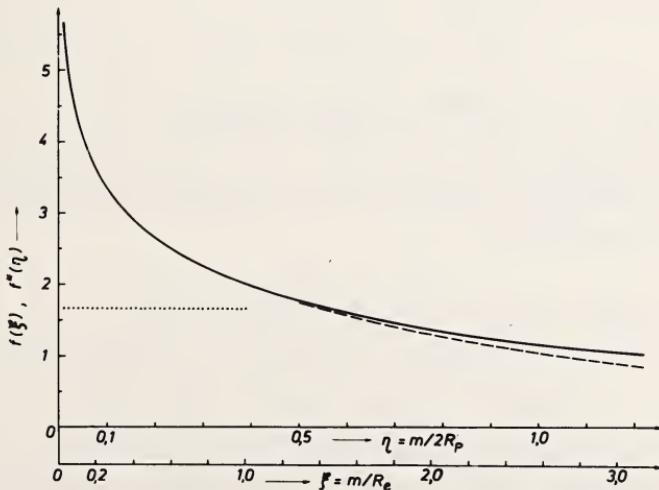


FIGURE 1 The functions  $f(\xi)$  and  $f^*(\eta)$  as given by eq (A.8). Full line =  $f(\xi)$  and  $f^*(\eta)$ ; dashed line = approximation according to eq (4.8); dotted horizontal line = constant  $p$  according to eq (7.6).

## V. The Higher Approximations $T_k$ , $k \geq 2$

In order to elucidate the structure of the terms  $T_k$  with  $k \geq 2$  we have studied  $T_2$  in more detail.  $T_2$  is proportional to  $\langle \epsilon_n^4 \rangle - 3\langle \epsilon_n^2 \rangle^2$ , which for

$n \rightarrow 0$  degenerates to  $\langle \epsilon_0^4 \rangle - 3\langle \epsilon_0^2 \rangle^2$ . Therefore an inspection of the latter expression gives a first clue. In the appendix 2  $\langle \epsilon_0^4 \rangle$  is calculated for a restrictedly random distribution of screw dislocations. We will report here only the conclusions which can be drawn from the results and which we believe to be qualitatively valid also for other types of distributions.

In order to have a simple description we subdivide  $\langle \epsilon_0^4 \rangle$  into three terms which are differentiated by a lower subscript. The same subdivision will be used also for  $\langle \epsilon_n^4 \rangle$  and  $T_2^*$  respectively.

(1) Irrespective of the dislocation distribution, the leading term of  $\langle \epsilon_0^4 \rangle$  is given by

$$\begin{aligned}\langle \epsilon_0^4 \rangle_{(1)} &= \sum_{i=1}^{N_0} \langle \hat{\epsilon}_0^4(\dot{\mathbf{r}}_i, \mathbf{r}) \rangle \\ &\cong N_0 \langle \hat{\epsilon}_0^4(0, r) \rangle \cong (b/2\pi)^4 \cdot \rho \cdot C^2 \cdot \frac{3\pi}{8} 1/r_0^2.\end{aligned}$$

(2) The second term  $\langle \epsilon_0^4 \rangle_{(2)}$  is mainly determined by the expression

$$3 \sum_{i \neq j} \langle \hat{\epsilon}_0^2(\dot{\mathbf{r}}_i, \mathbf{r}) \cdot \hat{\epsilon}_0^2(\dot{\mathbf{r}}_j, \mathbf{r}) \rangle. \quad (5.2)$$

All the individual integrands of the volume integration  $\langle \dots \rangle$  are positive. This means there is no mutual cancelling due to the different signs of the Burgers vectors  $\mathbf{b}_i, \mathbf{b}_j$  and, or due to the antisymmetry of the individual strain components  $\hat{\epsilon}_0$ . For a restrictedly random distribution the result is (appendix 2)

$$\begin{aligned}\langle \epsilon_0^4 \rangle_{(2)} &= 3(b/2\pi)^4 \cdot \pi^2 \cdot \rho^2 \cdot C^2 \left[ f_0^2 - f_0 + \frac{15}{16} \right] \\ &= 3\langle \epsilon_0^2 \rangle^2 - 3(b/2\pi)^4 \cdot \pi^2 \cdot \rho^2 \cdot C^2 \left[ f_0 - \frac{15}{16} \right]\end{aligned} \quad (5.3)$$

with  $f_0$  as defined in eqs (4.1) and (4.5). The first part of  $\langle \epsilon_0^4 \rangle_{(2)}$  exceeds the second one by the factor  $f_0$  (of the order of 5–10).

(3) In the appendix 2  $\langle \epsilon_0^4 \rangle_{(3)}$  is calculated as

$$\langle \epsilon_0^4 \rangle_{(3)} = \frac{1}{N_p} \left\{ \langle \epsilon_0^4 \rangle_{(2)} + \frac{3}{2} (b/2\pi)^4 \cdot \pi^2 \cdot \rho^2 \cdot C^2 \left[ f_0 - \left( 2 \log 2 + \frac{\pi^2}{6} - \frac{1}{12} \right) \right] \right\}. \quad (5.4)$$

In the next section we find that our approximation is applicable only for  $N_p \gg 1$ . Consequently we may neglect  $\langle \epsilon_0^4 \rangle_{(3)}$  in comparison to the preceding terms of  $\langle \epsilon_0^4 \rangle$ .

(4) Calculating  $\langle \epsilon_0^4 \rangle - 3\langle \epsilon_0^2 \rangle^2$  we see that both terms  $\langle \epsilon_0^2 \rangle^2$  cancel each other. We are thus left with

$$\langle \epsilon_0^4 \rangle - 3\langle \epsilon_0^2 \rangle^2 \approx \langle \epsilon_0^4 \rangle_{(1)} - 3(b/2\pi)^4 \cdot \pi^2 \cdot \rho^2 \cdot C^2 \left( f_0 - \frac{15}{16} \right) \quad (5.5)$$

where, due to  $r_0^{-2} \gg \rho$ , the first term on the right hand side outweighs the second one strongly.

(5) If we now turn from  $\epsilon_0$  to  $\epsilon_n$ , it is easy to show that neglecting  $r_0$   $\langle \epsilon_n^4 \rangle_{(1)}$  may be written in the form

$$\langle \epsilon_n^4 \rangle_{(1)} = (b/2\pi)^4 \cdot \rho \cdot D_2 \cdot 1/m^2 \quad (5.6)$$

The constant  $D_2$  will not be needed explicitly. The necessary integrations for the term  $\langle \epsilon_n^4 \rangle_{(2)}$  could not be performed. However, the factor  $f_0$ , which diverges logarithmically in  $r_0$ , appears in eqs (5.3) and (5.4) due to the same reasons as in  $\langle \epsilon_0^2 \rangle$  (area integration over the quadratic singularities in the dislocation cores). Therefore, it seems reasonable to assume that for sufficiently small  $m/R_e$  the  $f_0$ -factors in  $\langle \epsilon_n^4 \rangle_{(2)}$  may be replaced by the function  $f(m/R_e)$  of eqs (4.7) and (4.8). That means,

$$\langle \epsilon_n^4 \rangle_{(2)} + \langle \epsilon_n^4 \rangle_{(3)} - 3\langle \epsilon_n^2 \rangle^2$$

diverges only logarithmically with diminishing  $m$ , compared with

$$\langle \epsilon_n^4 \rangle_{(1)} \sim m^{-2}.$$

(6) Subdividing  $T_2^*$ , eq (2.13b), in the same manner as  $\langle \epsilon_0^4 \rangle$  we find that

$$T_{2(1)}^* = \frac{1}{4!} (g \cdot b)^4 \cdot \rho \cdot D'_2 \cdot m^2; D'_2 = D_2 \sin^{-4} \psi, \quad (5.7)$$

is of the same order in  $m$  as  $T_1$ ; and for small  $m$  the rest of  $T_2$  may be neglected compared with  $T_{2(1)}^*$ .

(7) With respect to the higher approximations  $T_k$ ,  $k \geq 3$ , similar conclusions could be drawn. For small  $m$  there exists a leading term  $T_{k(1)}^*$  analogously defined as  $T_{2(1)}^*$  which is rather independent of the dislocation distribution.

$$\begin{aligned}
 T_{k(1)}^* &= \frac{(-1)^k}{(2k)!} (2\pi g n)^{2k} \langle \epsilon_n^{2k} \rangle \\
 &\cong \frac{(-1)^k}{(2k)!} (g \cdot b)^{2k} \cdot \rho \cdot D'_k \cdot m^2.
 \end{aligned} \tag{5.8}$$

(8) Consequently, in restriction to small values of  $m$  the sum of the higher order terms  $\sum_{k=2}^{\infty} T_k$  may be approximated by the sum  $\sum_{k=2}^{\infty} T_{k(1)}^*$  of the leading terms. We write the sum in the form

$$\sum_{k=2}^{\infty} T_{k(1)}^* = \frac{\pi}{2} (g \cdot b)^2 \cdot \rho \cdot C' \cdot m^2 \cdot K_{\nu} \tag{5.9}$$

with  $\nu = |\mathbf{g} \cdot \dot{\mathbf{b}}| = g \cdot b \cdot |\cos \Psi|$  for screw dislocations. In the appendix 3 it is shown that the constant  $K_{\nu}$  can be calculated without explicit knowledge of the constants  $D'_k$ . In figure 2,  $K_{\nu}$  is plotted for  $\nu = 1$  to 6. The full line corresponds to an interpolation curve

$$K_{\nu} = K_1 + \log \nu, \tag{5.10}$$

which we will need later. Similar as for the calculations of  $\beta$ , eq (4.6), we assume that as a first approximation  $K_{\nu}$  is dependent of the type of the dislocations.

(9) One further conclusion regarding the higher order terms  $T_k$ ,  $k \geq 3$ , should be mentioned. Subtracting  $T_{3(1)}^*$  (which is included into  $K_3$ ) from  $T_3$  it is found by a qualitative discussion that the leading parts of  $T_3 - T_{3(1)}^*$  are of a similar structure to  $T_2^* \cdot T_1$  and  $T_1^3$  and consequently

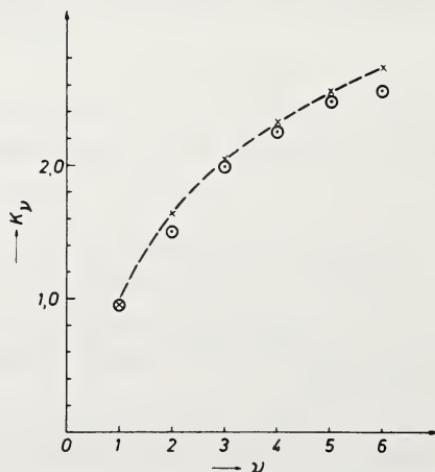


FIGURE 2  $\odot = K_{\nu}$  as derived in appendix 3.  $\times$  and dashed line =  $K_1 + \log \nu$ .

are compensated to a great extent by the term  $(-T_2^* \cdot T_1 + \frac{1}{3} T_1^3)$ , which is included in the complete expression of  $T_3$  (see eq (2.13c)). This mutual compensation (see also item (4) above) which we expect to apply also for  $k \geq 4$  justifies from a mathematical point of view the transition from the power series eq (2.11) to the exponential form of eq (2.12).

Making use of eqs (4.9) and (5.9),  $A_g(n)$  is given in the “quadratic approximation” by

$$A_g(n) = e^{-Q} \quad (5.11)$$

with

$$Q = \frac{\pi}{2} (g \cdot b)^2 \cdot C' \cdot \rho \cdot m^2 [f(m/R_e) - K_\nu]. \quad (5.12a)$$

We introduce a normalized coordinate

$$\xi = m/R_e \quad (5.13)$$

and a dimension-free parameter

$$N_e = \rho \cdot R_e^2 \cdot \pi \quad (5.14)$$

as a characteristic parameter of the dislocation distribution. Then the exponent  $Q$  may be written as

$$Q = \frac{1}{2} (g \cdot b)^2 C' \cdot N_e \cdot \xi^2 \cdot [f(\xi) - K_\nu]. \quad (5.12b)$$

## VI. Limits of the Applicability of Eq (5.12)

According to the above derivation eq (5.12) is expected to be most accurate for small  $\xi$ . We therefore define a critical value  $Q$  in such a way that for  $Q > Q_c$  the neglected terms in the exponent of  $A_g(n)$  exceed a critical fraction  $q$  of  $Q$ . In the present calculation  $Q_c$  can only be estimated, since even the next term which is proportional to  $(g \cdot b \cdot m)^4 \cdot \rho^2$  could not be calculated. However, a rough estimate may be obtained from the neglected terms of  $T_2$  the  $m$ -dependences of which are approximately known. We refer here only to the results of this estimate. For  $q = 0.15$  follows  $Q_c = 0.4, 0.8$  and  $1.1$  for  $N_e = 3, 10$  and  $100$  respectively. However, due to the alternating signs of the  $T_k$  it is expected that this estimate yields rather too small values of  $Q_c$ . Therefore considering the Fourier transformation of  $A_g(n)$ , i.e., the intensity profile  $I_g(S)$ , we assume that with  $N_e \geq 5$  the exponent  $Q$  in the form of eq (5.12) may be accurate

enough for a correct reconstruction of at least the flanks and tails of  $I_g(S)$ .

Apart from the neglection of the higher order terms of  $Q$ , eq (5.12) bears a real meaning, from a mathematical point of view, only as long as  $Q = Q(\xi)$  increases with increasing  $\xi$ . If we substitute  $f(\xi)$  for simplicity by the approximation of eq (4.8) it follows, for  $\nu = 1$  and  $C' = \cos^2 \psi$  (screw dislocations), that

$$\frac{dQ}{d\xi} = 0 \quad \text{for} \quad \xi = \xi_{\max} \cong 1.74 \quad Q(\xi_{\max}) \cong 0.76 \cdot N_e. \quad (6.1)$$

For  $\xi > \xi_{\max}$  the function  $A_g(n)$  diverges. In order to avoid this divergence eq (5.12) must be terminated for  $\xi > \xi_{\max}$ , for instance by putting  $A_g(n) = 0$  for  $\xi > \xi_{\max}$ . Such a termination ( $= \exp(-0.76 \cdot N_e)$ ) leads to characteristic oscillations in  $I_g(S)$  which, however, are irrelevant for  $N_e \geq 5$  (leading to  $\exp(-0.76 \cdot N_e) \lesssim 0.02$ ).

We see that both points of view, (1) neglection of the higher order terms, and (2) avoiding the divergence of  $A_g(n)$ , yield about the same lower limit of  $N_e$  for the applicability of eq (5.12).

Formally the termination of  $A_g(n)$  can be avoided with only minor perturbation of  $Q$  in that region which is relevant for the flanks and tails of  $I_g(S)$ . For this purpose we define another outer cutoff radius  $R'_e$  by

$$f(m/R_e) - K_\nu \cong f(m/R'_e), \quad (6.2)$$

where  $R'_e$  is adapted by means of eq (4.8)

$$R'_e = R_e \cdot e^{-K_\nu}. \quad (6.3)$$

With this substitution the exponent  $Q$  is transformed to  $Q'$ ,

$$Q' = \frac{1}{2} (g \cdot b)^2 \cdot C' \cdot N_e \xi^2 f(e^{K_\nu} \cdot \xi) \quad (6.4)$$

$$= \frac{\pi}{2} (g \cdot b)^2 \cdot C' \cdot \rho \cdot m^2 \cdot f(m/R'_e).$$

Since  $f(\xi)$  is proportional to  $\xi^{-1}$  for  $\xi \rightarrow \infty$  (see appendix 1),  $Q'$  is a monotonically increasing function and

$$A_g(n) = e^{-Q'} \quad (6.5)$$

a monotonically decreasing function of  $\xi$ . Therefore, even for  $N_e$  in the

order of 1, the Fourier transformation of  $A_g(n)$  in the approximation of eq (6.5) will result in "smooth" curves of  $I_g(S)$ , which are expected to be at least qualitatively correct as far as the flanks and tails of  $I_g(S)$  are concerned.

## VII. Application of the Warren-Averbach Analysis

As has been done before [8], we will treat the theoretically calculated Fourier transform  $A_g(n)$  of the diffraction profile  $I_g(S)$ , as if both functions,  $I_g(S)$  and  $A_g(n)$ , were determined experimentally. The reason is that we are interested to see how the "mean particle size" (assumed to be infinite in the present calculation) and the "mean square strains" as derived by the Warren-Averbach method [2-4] are related to the dislocation distribution.

Denoting  $A_g^e$  as the Fourier transform of the diffraction profile as derived from the experiment,  $A_g^e$  is split into two functions [2, 4]

$$A_g^e(n) = A_p^e(n) \cdot A_{g,s}^e(n), \quad (7.1)$$

where  $A_p^e$  is independent of the order of the reflexion involved and describes the particle size broadening of  $I_g(S)$ . The strain broadening is given by

$$A_{g,s}^e(n) = \exp(-2\pi^2 g^2 n^2 \langle \epsilon_n^2 \rangle^e), \quad (7.2)$$

where  $\langle \epsilon_n^2 \rangle^e$  should be equal to the above defined mean square strain  $\langle \epsilon_n^2 \rangle$  (see eqs (2.13a), (4.7)).

We assume that the diffraction profiles  $I_{g_0}^e$  and  $I_{2g_0}^e$  of the first two orders from the same set of lattice planes are known. Then  $A_p^e$  and  $A_{g,s}^e$  can be separated [2, 4]

$$\log A_p^e(n) = \frac{1}{3} [4 \log A_{g_0}^e - \log A_{2g_0}^e] \quad (7.3)$$

$$\langle \epsilon_n^2 \rangle^e = (6\pi^2 g_0^2 n^2)^{-1} [\log A_{g_0}^e - \log A_{2g_0}^e]. \quad (7.4)$$

We apply these equations to  $A_g(n)$  as calculated in eq (5.12). Setting  $\nu=1$  and  $\nu=2$  for  $g=g_0$  and  $g=2g_0$  respectively we obtain

$$A_p^e(n) = \exp\left(-\frac{2\pi}{3} (K_2 - K_1) \rho \cdot m^2\right) \text{ with } \frac{2\pi}{3} (K_2 - K_1) \cong 1.15, \quad (7.5)$$

$$\langle \epsilon^2 \rangle^e = (b/2\pi)^2 \cdot C \cdot \rho \cdot (f(m/R_e) - p), \quad p = \frac{(4K_2 - K_1)}{3} \cong 1.7. \quad (7.6)$$

For small  $m$  the particle size function  $A_p^e$  is curved towards the abscissa

$(d^2A_p^e/dm^2 < 0)$ . Such a behaviour of  $A_p^e$  has often been observed experimentally and has been discussed in the literature under the name "hook effect" [4, 8, 21, 22]. On the other hand, from a theoretical point of view a downward curvature of  $A_p^e$  is excluded, if the particle size broadening is assumed (as, e.g., in [2, 4]) to be caused by well-defined discrete boundaries like large angle boundaries, outer crystal surfaces, or extended stacking faults. Such a "discrete" boundary means: a given atom lies, for all pair distance vectors  $n \cdot \mathbf{e}_0$ , either inside or outside a given "particle" or "coherently scattering crystal region."

As discussed in earlier papers [8, 21], in macroscopic crystals containing distributed dislocations such a clear "either-or" distinction is not possible. As an example: Small angle boundaries may act as coherence boundaries for  $n \gg d$ , if  $d$  is the dislocation spacing in the small angle boundary. However, for  $n \ll d$  both adjacent crystal regions belong to the same "coherently" scattering particle [21].

Following a commonly used experimental procedure we extrapolate the steepest slope of  $A_p^e$  down to the abscissa. Using eq (7.5) the abscissa is intersected at  $m = 1.3 \cdot \rho^{-1/2}$ , which coincides rather well with the mean dislocation spacing. Although this latter result appears to be reasonable it should not be overestimated since the validity of eq (7.5) is perhaps restricted to rather small values of  $m$  which do not allow such an extrapolation.

Comparing the "experimentally" determined mean square strains  $\langle \epsilon_n^2 \rangle^e$  with the theoretically predicted form of eq (4.7) we see that the experimental logarithmic factor comes out too small by about 1.7. As a further consequence with increasing  $n$  the slope of  $\langle \epsilon_n^2 \rangle^e$  is considerably steeper than the "true" slope of  $\langle \epsilon_n^2 \rangle$ .

These anomalies of both "experimental" terms  $A_p^e$  and  $\langle \epsilon_n^2 \rangle^e$  are not included in the conventional interpretation of the results of the Warren-Averbach analysis. It is noticeable that they have been found already in the above mentioned earlier paper [8] which was concerned with a similar analysis of the calculated diffraction profiles from a crystal containing only one single screw dislocation. It is obvious from the present paper (which differs in its method considerably from [8]) that these anomalies are due to the constant  $K_v$ , i.e., due to the contribution of the higher order terms  $T_k$  with  $k \geq 2$  which is neglected in the Warren-Averbach analysis and which comes from the large strains in the vicinity of the dislocation lines.

### VIII. Comparison With the Theory of Krivoglaz and Ryaboshapka

Starting from a completely random dislocation distribution the K&R theory arrives at an expression for  $A_g(n)$  which agrees with eq (5.12) of the present paper, if the factor  $\log (R_0/m \cdot \nu)$  (K&R) is identified with

$(f(m/R_e) - K_\nu)$  (this paper). Using for  $f(m/R_e)$  and  $K_\nu$  the approximations of eqs (4.8) and (5.10) this leads to the equation

$$\log \frac{R_e}{m \cdot \nu} + \alpha - K_1 = \log \frac{R_0}{m \cdot \nu} \quad \text{or} \quad R_e = R_0 e^{(K_1 - \alpha)}. \quad (8.1)$$

Consequently our representation for  $A_g(n)$  agrees fairly well with that of K&R, if the effective outer cutoff radius  $R_e$  as used in the present paper is equated (apart from the factor  $\exp(K_1 - \alpha) \approx \exp(-1)$ ) to the crystal radius  $R_0$ . This is a reasonable result, since for a completely random dislocation distribution the effective outer cutoff radius coincides approximately with the crystal radius [14-16].

In the theory of K&R the completely random dislocation distribution is used as an essential and basic assumption. Therefore the consequent application of the K&R theory to diffraction profiles from macroscopic crystals leads to extremely large, and physically unrealistic, outer cutoff radii. However, in the more general treatment of the present paper we could show that the above mentioned basic assumption of K&R is not necessary for obtaining a comparatively simple expression for  $A_g(n)$ . This expression should be applicable to physically reasonable dislocation distributions with outer cutoff radii  $R_e$  down to values in the order of magnitude of the mean dislocation spacing  $\rho^{-1/2}$ .

If the instrumental broadening of the experimentally determined diffraction profile must be subtracted, as, i.e., in the Fourier method (see [4]), the comparison between experimental and theoretical line profiles is most easily performed in terms of the Fourier transform  $A_g(n)$ . However, under certain experimental conditions [17, 23, 24] the instrumental broadening can be neglected. Then it may be easier to compare the line profiles directly.

In the paper of K&R, the theoretical line profiles were calculated by an analytical Fourier transformation of  $A_g(n)$ . This procedure was carried out using some mathematical approximations which are most justifiable when  $N_0 = \rho \cdot R_0^2 \pi$  is very large. It was found that the line profile  $I_g(S)$  may be represented by a Gaussian function whose half width (or integral width) is proportional to  $\sqrt{\rho} \cdot \log \left\{ \frac{N_0}{2} \log \frac{N_0}{2} \right\}$ . As a consequence of this "Gaussian approximation," the two independent parameters of the dislocation distribution,  $\rho$  and  $R_0$  (corresponding to  $\rho$  and  $R_e$ , or  $\rho$  and  $N_e = \rho \cdot R_e^2 \pi$ , in the more general treatment of the present paper), cannot be determined separately.

A more detailed inspection of  $A_g(n)$  as given by eqs (5.12) or (6.4) of the present paper confirms the conclusion of K&R insofar as, for a given value of  $N_e$ , the width of the profile is proportional to  $\sqrt{\rho}$ . The Gaussian

function, however, is a good approximation for  $I_g(S)$  only for extremely large values of  $N_e$ . With decreasing  $N_e$  the tails of  $I_g(S)$  increase in height and extension. Thus by measuring the width as well as the shape of  $I_g(S)$  both parameters,  $\rho$  and  $N_e$ , can be determined independently from each other. We shall deal with this question in more detail in a subsequent paper [18].

### IX. Appendix 1. Calculation of $\langle \epsilon_n^2 \rangle$ for a Restrictedly Random Distribution of Screw Dislocations

The infinite body approximation of the displacement vector  $\mathbf{u}$  of a single screw dislocation lying in the  $z$ -axis of a cartesian coordinate system is given by

$$\mathbf{u} = \frac{b}{2\pi} [0, 0, \varphi], \quad (\text{A.1})$$

$\varphi$  = polar angle in the  $x$ - $y$ -plane

We set

$$\mathbf{e}_0 = [\sin \psi, 0, \cos \psi] \quad (\text{A.2})$$

which means, for screw dislocations, no restriction of generality. With eq (2.9) it follows

$$\hat{\epsilon}_0(0, \mathbf{r}) = \frac{b}{2\pi} \sin \psi \cdot \cos \psi \cdot \frac{\sin \varphi}{r'}, \quad r' = \sqrt{x^2 + y^2}, \quad (\text{A.3})$$

Following [15, 16] we may write  $\langle \epsilon_0^2 \rangle$  for a restrictedly random distribution in the form

$$\langle \epsilon_0^2 \rangle = N_0 \cdot \{ \langle \hat{\epsilon}_0^2(0, \mathbf{r}) \rangle - \langle (\overline{\hat{\epsilon}_0(0, \mathbf{r})})^2 \cdot \rangle \} \quad (\text{A.4})$$

with

$$\overline{\hat{\epsilon}_0(0, \mathbf{r})} = \frac{1}{F_p} \int_{F_p} \hat{\epsilon}_0(\mathbf{r}, \mathbf{r}) d^2 \mathbf{r} \quad (\text{A.5})$$

(centre of gravity of the area  $F_p$  in  $\mathbf{r} = 0$ )

For convenience we assume  $F_p$  to be a circular area with radius

$$R_p = \sqrt{\frac{F_p}{\pi}}$$

Now we substitute  $\hat{\epsilon}_0$  in eq (A.4) by  $\hat{\epsilon}_n$  as defined in eq (3.4). If the various integrations are taken in a proper sequence all integrations can be carried out in a closed form. In the volume integration  $\langle \dots \rangle$ , which is appropriately chosen as the first integration, the upper limit of  $r'$  may be set equal to an arbitrary value  $R'_0 \gg R_p$ , which cancels out in the final result when both parts of eq (A.4) are subtracted. Finally, we obtain

$$\langle \epsilon_n^2 \rangle = (b/2\pi)^2 \cdot \pi \cdot \rho \cdot C \cdot f(\xi), \quad \xi = \frac{m}{R_e} \quad (\text{A.6})$$

$f(\xi)$  is easier to express as a function of

$$\eta = \frac{m}{2R_p} = \frac{1}{2} e^{-1/4} \cdot \xi. \quad (\text{A.7})$$

With  $f(\xi) = f^*(\eta)$ , it follows

for  $\eta \leq 1$ :

$$\begin{aligned} f^*(\eta) = & -\log \eta + \left( \frac{7}{4} - \log 2 \right) + \frac{512}{90\pi} \frac{1}{\eta} \\ & + \frac{2}{\pi} \left[ 1 - \frac{1}{4\eta^2} \right] \cdot \int_0^\eta \frac{\arcsin V dV}{V} \\ & - \frac{1}{\pi} \left[ \frac{769}{180} \frac{1}{\eta} + \frac{41}{90} \cdot \eta + \frac{2}{90} \cdot \eta^3 \right] \cdot \sqrt{1 - \eta^2} \\ & - \frac{1}{\pi} \left[ \frac{11}{12} \frac{1}{\eta^2} + \frac{7}{2} + \frac{1}{3} \cdot \eta^2 \right] \arcsin \eta + \frac{1}{6} \cdot \eta^2; \end{aligned} \quad (\text{A.8})$$

for  $\eta \geq 1$ :

$$f^*(\eta) = \frac{512}{90\pi} \frac{1}{\eta} - \left[ \frac{11}{24} + \frac{1}{4} \log 2\eta \right] \frac{1}{\eta^2}.$$

## X. Appendix 2. Calculation of $\langle \hat{\epsilon}_0^4 \rangle$

The comparison of the mean square strain  $\langle \hat{\epsilon}_0^2 \rangle$  for a single dislocation at  $\mathbf{r} = 0$  with  $\langle \epsilon_0^2 \rangle$  for randomly distributed dislocations showed that both expressions diverge logarithmically with the crystal radius  $R_0$ .

On the other hand,  $\langle \hat{\epsilon}_0^4 \rangle$  is (nearly) independent of the outer cutoff radius or crystal radius.

$$\langle \hat{\epsilon}_0^4 \rangle \sim \left( \frac{1}{r_0^2} - \frac{1}{R_0^2} \right) \cong \frac{1}{r_0^2} \quad \text{for} \quad R_0 \gg r_0.$$

In analogy to the second power averages one might assume that also  $\langle \epsilon_0^4 \rangle$  as calculated for randomly distributed dislocations will be independent of  $R_0$ . However, this is not the case (see below). Therefore we consider in the following a restrictedly random distribution. In order to simplify the notation, we write

$$\hat{\epsilon}_0(\dot{\mathbf{r}}_i, \mathbf{r}) \equiv \hat{\epsilon}_i. \quad (\text{B.1})$$

Then, after some re-ordering of the individual terms,  $\langle \epsilon_0^4 \rangle$  may be written in the form

$$\begin{aligned} \langle \epsilon_0^4 \rangle &= \left\langle \left( \sum_{i=1}^{N_0} \hat{\epsilon}_i \right)^4 \right\rangle \\ &= \sum_{i=1}^{N_0} \langle \hat{\epsilon}_i^4 \rangle + 4 \sum'_{i,j} \langle \hat{\epsilon}_i^3 \cdot \hat{\epsilon}_j \rangle + 3 \sum'_{i,j} \langle \hat{\epsilon}_i^2 \cdot \hat{\epsilon}_j^2 \rangle \\ &\quad + 6 \sum''_{i,j,k} \langle \hat{\epsilon}_i^2 \cdot \hat{\epsilon}_j \cdot \hat{\epsilon}_k \rangle + \sum'''_{i,j,k,l} \langle \hat{\epsilon}_i \cdot \hat{\epsilon}_j \cdot \hat{\epsilon}_k \cdot \hat{\epsilon}_l \rangle, \end{aligned} \quad (\text{B.2})$$

with  $\sum' = \sum_{i,j=1}^{N_0} \sum_{i \neq j}$  and similarly for  $\Sigma''$  and  $\Sigma'''$ . In order to substitute the

summations by equivalent integrations, we introduce the following distribution functions (which are to be understood as averages over the distribution functions of an infinitesimal number of equivalent distributions; compare [15, 16]).

$$\bar{P}^{(k)}_{c_1, c_2 \dots c_k} \cdot d^2\dot{\mathbf{r}}_1 \cdot d^2\dot{\mathbf{r}}_2 \dots d^2\dot{\mathbf{r}}_k \quad (\text{B.3})$$

means the probability for finding any one dislocation, which is different from the other  $k-1$ , in the infinitesimal area  $d^2\dot{\mathbf{r}}_i$  at the position  $\dot{\mathbf{r}}_i$ . The subscripts  $c_i$  may accept the following values,

$$c_i = +, \quad c_i = -, \quad c_i = 0. \quad (\text{B.4})$$

$c_i = + (-)$  means that the dislocation in  $d^2\dot{\mathbf{r}}_i$ ,  $\dot{\mathbf{r}}_i$  bears a positive (negative) sign of the Burgers vector  $\mathbf{b}$ . In the case of  $c_i = 0$  the sign of  $\mathbf{b}$  will not be considered.

Using eq (B.3) we define furthermore

$$\begin{aligned}
 \Delta \bar{P}^{(2)} &= \sum_{c_1, c_2}^{(+)} \bar{P}_{c_1 c_2}^{(2)} - \sum_{c_1, c_2}^{(-)} \bar{P}_{c_1 c_2}^{(2)} = \bar{P}_{+,+}^{(2)} + \bar{P}_{-,-}^{(2)} - \bar{P}_{+,-}^{(2)} - \bar{P}_{-,+}^{(2)}; \\
 \Delta \bar{P}^{(3)} &= \sum_{0, c_2, c_3}^{(+)} \bar{P}_{0, c_2, c_3}^{(3)} - \sum_{0, c_2, c_3}^{(-)} \bar{P}_{0, c_2, c_3}^{(3)}; \\
 \Delta \bar{P}^{(4)} &= \sum_{c_1 \cdots c_4}^{(+)} \bar{P}_{c_1 \cdots c_4}^{(4)} - \sum_{c_1 \cdots c_4}^{(-)} \bar{P}_{c_1 \cdots c_4}^{(4)}.
 \end{aligned} \tag{B.5}$$

$\sum_c^{(+)}$  and  $\sum_c^{(-)}$  means summation over the terms with  $c_1 \cdot c_2 \cdots c_k = “+”$  and “-” respectively.

The cylinder cross section is subdivided into  $p^2$  sub-areas of equal size  $F_p$

$$F_p = \frac{F_0}{p^2} \quad \text{or} \quad R_p = \frac{R_0}{p}.$$

The individual sub-areas are denoted by  $U_i$ ,  $i = 1 \dots p^2$ . Those sub-areas containing the dislocation intersection points  $\mathbf{r}_1$ ,  $\mathbf{r}_2$ ,  $\mathbf{r}_3$ ,  $\mathbf{r}_4$  are denoted by  $U_a$ ,  $U_b$ ,  $U_c$ ,  $U_d$  respectively. In order to simplify the following equations we assume

$$N_p^+ = N_p^- = \frac{1}{2} N_p, \rho = \frac{N_p}{F_p}. \tag{B.6}$$

The following five distribution functions will be needed. They can be derived for a restrictedly random distribution by simple counting procedures (see [15])

$$\bar{P}_0^{(1)} = \rho = \frac{N_0}{F_0} \tag{B.7a}$$

$$\begin{aligned}
 \Delta \bar{P}^{(2)} &= 0 \quad \text{for } a \neq b, \\
 &= -\frac{1}{F_p} \cdot \rho \quad \text{for } a = b;
 \end{aligned} \tag{B.7b}$$

$$\begin{aligned}
 \bar{P}_{0,0}^{(2)} &= \rho^2 \quad \text{for } a \neq b, \\
 &= \rho^2 - \frac{1}{F_p} \cdot \rho \quad \text{for } a = b;
 \end{aligned} \tag{B.7c}$$

$$\Delta \bar{P}^{(3)} = -\frac{1}{F_p} \rho^2 \quad \text{for } a \neq b = c,$$

$$= \frac{2}{F_p^2} \rho - \frac{1}{F_p} \rho^2 \quad \text{for } a=b=c, \\ = 0 \quad \text{for all the other cases; \quad (B.7d)}$$

$$\Delta \bar{P}^{(4)} = \frac{1}{F_p^2} \rho^2 \quad \text{for } a=b \neq c=d, a=c \neq b=d, a=d \neq b=c, \\ = \frac{3}{F_p^2} \rho^2 - \frac{6}{F_p^3} \rho \quad \text{for } a=b=c=d, \\ = 0 \quad \text{for all the other cases. \quad (B.7e)}$$

Now we define

$$\bar{\hat{\epsilon}}_a^k = \overline{(\hat{\epsilon}_0(\dot{\mathbf{r}}_a, \mathbf{r}))^k} = \frac{1}{F_p} \int_{U_a} (\hat{\epsilon}_0(\dot{\mathbf{r}}, \mathbf{r}))^k d^2\dot{\mathbf{r}} \quad (B.8)$$

( $\dot{\mathbf{r}}_a$  = centre of gravity of the area  $U_a$ ).

which means the singularity of the  $k$ th power of  $\hat{\epsilon}_0$  is homogeneously distributed over the sub-area  $U_a$ .

If we substitute

$$\sum_{i=1}^{N_0} \langle \hat{\epsilon}_i^4 \rangle = \int \bar{P}_0^{(1)} \cdot \langle \hat{\epsilon}_i^4 \rangle d^2\dot{\mathbf{r}}_1, \\ \sum'_{i,j} \langle \hat{\epsilon}_i^3 \cdot \hat{\epsilon}_j \rangle = \int \int \Delta \bar{P}^{(3)} \cdot \langle \hat{\epsilon}_1^3 \cdot \hat{\epsilon}_2 \rangle \cdot d^2\dot{\mathbf{r}}_1 \cdot d^2\dot{\mathbf{r}}_2, \quad (B.9)$$

and in the same sense for the other sums in eq (B.2) we obtain after some re-ordering

$$\langle \hat{\epsilon}_0^4 \rangle = N_p \cdot \sum_{a=1}^{P^2} \langle \bar{\hat{\epsilon}}_a^4 - (\bar{\hat{\epsilon}}_a)^4 \rangle + 3N_p^2 \sum_{a,b=1}^{P^2} \langle \{ \bar{\hat{\epsilon}}_a^2 - (\bar{\hat{\epsilon}}_a)^2 \} \cdot \{ \bar{\hat{\epsilon}}_b^2 - (\bar{\hat{\epsilon}}_b)^2 \} \rangle \\ - N_p \sum_{a=1}^{P^2} \langle 3\{ \bar{\hat{\epsilon}}_a^2 - (\bar{\hat{\epsilon}}_a)^2 \}^2 + 4\{ \bar{\hat{\epsilon}}_a^3 - (\bar{\hat{\epsilon}}_a)^3 \} \bar{\hat{\epsilon}}_a - 6\{ \bar{\hat{\epsilon}}_a^2 - (\bar{\hat{\epsilon}}_a)^2 \} (\bar{\hat{\epsilon}}_a)^2 \rangle. \quad (B.10)$$

Terms of the kind  $\{ \bar{\hat{\epsilon}}_a^k - (\bar{\hat{\epsilon}}_a)^k \}$  disappear outside  $U_a$  with increasing distance from  $\dot{\mathbf{r}}_a$  faster than  $\bar{\hat{\epsilon}}_a^k$ . This allows the following conclusions:

- (1) In the double sum  $\sum_{a,b}$  the terms with  $a \neq b$  may be neglected.

(2) The volume integration  $\langle \dots \rangle$  of the individual integrands converges very quickly. Therefore the volume-integration may be extended in the  $x$ - $y$ -plane to infinity.

(3) From item (2) follows that the position of  $U_a$  within the cylinder cross section is irrelevant.

(4) Further we conclude from item (2) that we are allowed to use for  $\hat{\epsilon}_0$  the infinite body approximation.

Making use of these conclusions eq (B.10) may be replaced by

$$\begin{aligned}
 \langle \epsilon_0^4 \rangle &= \langle \epsilon_0^4 \rangle_{(1)} + \langle \epsilon_0^4 \rangle_{(2)} + \langle \epsilon_0^4 \rangle_{(3)}, \\
 \langle \epsilon_0^4 \rangle_{(1)} &= N_0 \cdot \langle \hat{\epsilon}_0^4(0, \mathbf{r}) - \overline{(\hat{\epsilon}_0(0, \mathbf{r}))^4} \rangle \\
 \langle \epsilon_0^4 \rangle_{(2)} &= 3N_0 \cdot N_p \cdot \langle \{ \overline{\hat{\epsilon}_0^2(0, \mathbf{r})} - \overline{(\hat{\epsilon}_0(0, \mathbf{r}))^2} \}^2 \rangle \\
 &= -3N_0 \cdot \langle \{ \overline{\hat{\epsilon}_0^2(0, \mathbf{r})} - \overline{(\hat{\epsilon}_0(0, \mathbf{r}))^2} \}^2 \rangle \\
 &\quad - 4N_0 \cdot \langle \{ \overline{\hat{\epsilon}_0^3(0, \mathbf{r})} - \overline{(\hat{\epsilon}_0(0, \mathbf{r}))^3} \} \cdot \overline{\hat{\epsilon}_0(0, \mathbf{r})} \rangle \\
 &\quad + 6N_0 \langle \{ \overline{\hat{\epsilon}_0^2(0, \mathbf{r})} - \overline{(\hat{\epsilon}_0(0, \mathbf{r}))^2} \} \cdot \overline{(\hat{\epsilon}_0(0, \mathbf{r}))^2} \rangle. \tag{B.11}
 \end{aligned}$$

Thus, for a restrictedly random distribution,  $\langle \epsilon_0^4 \rangle$  could be written in a similar form as  $\langle \epsilon_0^2 \rangle$ , compare eq (A4).

Similarly as in Appendix 1 we assume for the integration that the sub-area  $U_a$  is circular with radius  $R_p$  and with its centre  $\mathbf{r}_a = 0$ . Writing

$$\hat{\epsilon}_0 = Q \cdot \frac{\sin \varphi}{r'}, \quad Q = \frac{b}{2\pi} \sin \psi \cos \psi,$$

compare eq (A.3), we obtain from eq (B.8)

$$\begin{aligned}
 \overline{\hat{\epsilon}_0} &= Q \cdot \sin \varphi \frac{r'}{R_p^2}, \quad r' \leq R_p, \\
 &= Q \cdot \sin \varphi \frac{1}{r'}, \quad r' \geq R_p; \tag{B.12a}
 \end{aligned}$$

$$\begin{aligned}
 \overline{\epsilon_0^2} &= Q^2 \frac{1}{R_p^2} \left[ \sin^2 \varphi - \frac{1}{2} + \log \frac{R_p}{r_0} + \frac{1}{2} \log \left( 1 - \frac{r'^2}{R_0^2} \right) \right], \quad r' \leq R_p - r_0, \\
 &= Q^2 \frac{1}{r'^2} \left[ \sin^2 \varphi - \frac{1}{2} + \frac{1}{2} \frac{r'^2}{R_p^2} \log \left( 1 - \frac{R_0^2}{r'^2} \right) \right], \quad r' \geq R_p + r_0; \tag{B.12b}
 \end{aligned}$$

$$\begin{aligned}\bar{\epsilon}_0^3 &= Q^3 \cdot \frac{3}{4} \frac{\sin \varphi \cdot r'}{R_p^2 (R_p^2 - r'^2)}, \quad r' \leq R_p - r_0, \\ &= Q^3 \cdot \left[ \frac{\sin^3 \varphi}{r'^3} + \frac{3}{4} \sin \varphi \cdot \frac{R_p^2}{r'^3 (r'^2 - R_p^2)} \right], \quad r' \geq R_p + r_0.\end{aligned}\quad (\text{B.12c})$$

For  $\bar{\epsilon}_0^4$  in  $\langle \epsilon_0^4 \rangle_{(1)}$  the smearing out according to eq (B.8) may be neglected. Substituting eq (B.12) into eq (B.11) the following results are obtained

$$\langle \epsilon_0^4 \rangle_{(1)} = Q^4 \cdot \rho \cdot \frac{3}{8} \pi \cdot r_0^{-2}; \quad (\text{B.13a})$$

$$\begin{aligned}\langle \epsilon_0^4 \rangle_{(2)} &= 3Q^4 \cdot \rho^2 \pi^2 \left[ \left( \log \frac{R_p}{r_0} \right)^2 - \frac{3}{2} \log \frac{R_p}{r_0} + \frac{5}{4} \right] \\ &= 3\langle \epsilon_0^2 \rangle^2 - 3Q^4 \rho^2 \pi^2 \left[ f_0 - \frac{15}{16} \right]\end{aligned}\quad (\text{B.13b})$$

$$\langle \epsilon_0^4 \rangle_{(3)} = \frac{1}{N_p} \langle \epsilon_0^4 \rangle_{(2)} + \frac{1}{N_p} \frac{3}{2} Q^4 \rho^2 \pi^2 \left[ f_0 - \left( 2 \log 2 + \frac{\pi^2}{6} - \frac{1}{12} \right) \right] \quad (\text{B.13c})$$

with  $f_0$  according to eq (4.5). In  $\langle \epsilon_0^4 \rangle_{(1)}$  the term  $\langle \bar{\epsilon}_0^4 \rangle$  (proportional to  $R_p^{-2}$ ) was neglected.

Finally let us consider a completely random distribution which corresponds in our notation to  $R_p = R_0$ . For this case eq (B.10) must be used with

$$\bar{\epsilon}_0 = 0$$

(for details see [14, 15]).  $\langle \epsilon_0^4 \rangle_{(1)}$  remains unchanged. The other non-vanishing terms degenerate to the form

$$\begin{aligned}\langle \epsilon_0^4 \rangle_{(2)} + \langle \epsilon_0^4 \rangle_{(3)} &= 3Q^4 \cdot \rho \left( \rho - \frac{1}{F_p} \right) \pi^2 \left[ \left( \log \frac{R_0}{r_0} \right)^2 + A \cdot \log \frac{R_0}{r_0} + B \right] \\ A, B &= \text{constants.}\end{aligned}$$

As a result we state that for a completely random distribution  $\langle \epsilon_0^4 \rangle$  diverges logarithmically with the crystal radius  $R_0$ . Since now  $R_0$  appears in  $\langle \epsilon_0^4 \rangle$  it is not allowed to use the infinite body approximation for  $\bar{\epsilon}_0$ . There-

fore the constants  $A$  and  $B$  cannot be calculated with  $\hat{\epsilon}_0$  according to eq (A.3).

### XI. Appendix 3. Calculation of $K_\nu$

Using eqs (A.3) and (3.4) it follows for a screw dislocation

$$\begin{aligned}\hat{\epsilon}_n(0, \mathbf{r}) &\equiv \hat{\epsilon}_n(0, \mathbf{r}'), \mathbf{r}' = [x, y, 0], r' = \sqrt{x^2 + y^2}; \\ &= \mp \frac{b}{2\pi m} \sin \psi \cdot \cos \psi \cdot (\pi - q), \text{ for } r' \leq m/2 \quad (\text{C.1})\end{aligned}$$

$$= \mp \frac{b}{2\pi m} \sin \psi \cdot \cos \psi \cdot q, \text{ for } r' \geq m/2$$

“ $\mp$ ” for  $\sin \varphi \geq 0$

$$q = \text{principal value of } \arctg \left| \frac{2\kappa \cdot \sin \varphi}{(\kappa^2 - 1)} \right|, \kappa = \frac{2r'}{m}. \quad (\text{C.2})$$

We define a function  $F$ ,

$$F = \cos (2\pi g n \hat{\epsilon}_n) - 1 + \frac{1}{2!} (2\pi g n \hat{\epsilon}_n)^2. \quad (\text{C.3})$$

Using  $\nu = |\mathbf{g} \cdot \mathbf{b}| = g \cdot b \cdot |\cos \psi|$ ,  $m = n \cdot \sin \psi$  and eq (A.3)  $F$  may be developed in a power series

$$F_1(q) = \cos \nu(\pi - q) - 1 + \frac{1}{2!} \cdot \nu^2 \cdot (\pi - q)^2 \quad \left. \right\} \kappa \leq 1, \quad (\text{C.4a})$$

$$= \sum_{k=2}^{\infty} (-1)^k \cdot \frac{1}{(2k)!} \cdot \nu^{2k} \cdot (\pi - q)^{2k} \quad \left. \right\} \kappa \geq 1. \quad (\text{C.5a})$$

$$F_2(q) = \cos \nu q - 1 + \frac{1}{2!} \cdot \nu^2 \cdot q^2 \quad \left. \right\} \kappa \geq 1. \quad (\text{C.4b})$$

$$= \sum_{k=2}^{\infty} (-1)^k \cdot \frac{1}{(2k)!} \cdot \nu^{2k} \cdot q^{2k} \quad \left. \right\} \kappa \geq 1. \quad (\text{C.5b})$$

After multiplication with  $N_0$  the spatial average of  $F_1 + F_2$ , eq (C.5), coincides with the wanted expression of eq (5.9).

Since  $\hat{\epsilon}_n$  in eq (C.1) is independent of the  $z$ -coordinate the integration is restricted to the  $x$ - $y$ -plane. Discussing the lines  $q = \text{constant}$  in the  $x$ - $y$ -

plane the differential area  $r'dr'd\varphi$  can be transformed into the form  $f(q)dq$  resulting in

$$N_0 \cdot \langle F \rangle = \rho \cdot \int_0^{R_0} \int_0^{2\pi} Fr' dr' d\varphi \cong \rho \cdot \int_0^{\infty} \int_0^{2\pi} Fr' dr' d\varphi, \\ = \rho \cdot \int_0^{\pi/2} \{F_1(q) \cdot f_1(q) + F_2(q) \cdot f_2(q)\} dq; \quad (C.6)$$

$$f_1(q) = 4 \left\{ \frac{1}{\sin^2 q} - \frac{q \cdot \cos q}{\sin^3 q} \right\}, \quad \kappa \leq 1$$

$$f_2(q) = 4 \left\{ \frac{1}{\sin^2 q} - \frac{(q - \pi) \cos q}{\sin^3 q} \right\}, \quad \kappa \geq 1. \quad (C.7)$$

(Since  $F_2(q)$  decreases for  $r' \gg m/2$  proportional to  $r'^{-4}$  the  $r'$ -integration in eq (C.6) can be extended to infinity.)

Substituting for  $F_1(q)$  and  $F_2(q)$  the corresponding right-hand sides of eq (C.4) all integrations can be carried out analytically. (Some of the integrals diverge for  $r' \rightarrow \frac{m}{2}$  or  $q \rightarrow \frac{\pi}{2}$  respectively. These divergencies, however, cancel each other.) Writing the final result in the form of eq (5.9) we obtain for the constant  $K_\nu$

$$K_1 = \frac{7}{3} - 2 \log 2, \quad K_2 = \frac{3}{2}, \quad K_3 = \frac{91}{27} - 2 \log 2 \\ K_4 = \frac{9}{4}, \quad K_5 = \frac{97}{25} - 2 \log 2, \quad K_6 = \frac{23}{9}. \quad (C.8)$$

## XII. Acknowledgement

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# THERMODYNAMIC PROPERTIES OF SOLIDS CONTAINING DISLOCATIONS

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Using thermodynamics and elasticity theory, a unified treatment of the changes in the thermodynamic properties of solids containing dislocations is given. The results are expressed in terms of temperature and pressure derivatives of the formation energy of the dislocations. The required pressure and temperature dependence of the energy is given by the measured pressure and temperature dependence of the elastic constants appearing in the energy expression found at zero pressure and temperature. The method is not restricted to calculations of volume changes, or to isotropic, static or even elastic systems at zero pressure. Changes in entropy, specific heat, thermal expansion and bulk modulus due to dislocations are easily calculated.

Key words: Bulk modulus; dislocations and thermodynamics; entropy; specific heat; thermal expansion; thermodynamics and expansions.

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Using thermodynamics and elasticity theory, a unified treatment of the changes in the thermodynamic properties of solids containing dislocations is given. The results are expressed in terms of temperature and pressure derivatives of the energy required to form the dislocations. The required pressure and temperature dependence of the energy is given by the measured pressure and temperature dependence of the elastic constants appearing in the energy expression found at zero pressure and temperature. For example, the volume change per defect,  $v$ , of a solid containing defects is given by the thermodynamic relation

$$v = \partial g(p, T) / \partial p \quad (1)$$

where  $g$  is the change in the Gibbs free energy and pressure  $p$  and temperature  $T$  are the independent variables. The Gibbs free energy change per atomic length of screw dislocation in an isotropic medium is given by

$$g = \frac{Gb^2a}{4\pi} \left( \ln \frac{R}{r_0} - 1 \right) \quad (2)$$

where  $G$  is the shear elastic constant,  $\mathbf{b}$  the Burgers vector,  $a$  the atomic spacing, and  $R$  and  $r_0$  are the usual outer and inner cut off radii of the strain field of the dislocation. Equation (2) has the form

$$g = \alpha GV \quad (3)$$

where  $\alpha$  is a constant independent of  $p$  and  $T$ , and  $V$  is the volume of the crystal. Applying eq (1) to eq (3) one obtains immediately

$$\frac{v}{g} = \frac{G'}{G} - \frac{1}{B}. \quad (4)$$

Where the prime signifies a derivative with respect to pressure.

This simple result, found here by a single differentiation has previously been given by Seeger and Haasen [1] who used a result given by Zener [2], and by Toupin and Rivlin [3] as the result of relatively long and involved calculations based upon nonlinear elasticity theory. Equation (4) gives the ratio of the volume change to the energy change of a crystal containing screw dislocations in terms of elastic constants and their pressure coefficients, which may be taken, for example, from ultrasonic measurements.

The thermodynamic method of calculation above depends only on the recognition of the fact that eq (2) with  $G = G(p, T)$ , is the proper expression for the Gibbs free energy change in this case. This method is not restricted to calculations of volume changes. It is also not restricted to isotropic, static, or even elastic systems at zero pressure.

The results for the volume change per unit atomic length of screw dislocation in a number of materials are given in table I, using both the isotropic elasticity expression for the energy, and the anisotropic elasticity expression for cubic materials with  $\langle 110 \rangle$  Burgers vectors.  $\Omega$  is the atomic volume, or, in the case of ionic crystals, the average ionic volume. A few features of the calculations are apparent from the table:

1. The isotropic and anisotropic results do not differ greatly except in the case of the potassium and rubidium compounds. This difference results from the negative pressure derivatives of the elastic constant  $C_{44}$  in those cases. In all cases, the anisotropic results will be more reliable than the isotropic results.

2. The volume changes for some of the materials, notably the sodium and lithium halides, are very large. Such a large volume change could mean the dislocation cores are hollow, and evidence for such hollow cores

in LiF has been found in the measurement of Na ion diffusion along dislocations [4].

3. The volume changes for Si are much larger than those found for Ge, in both the isotropic and anisotropic cases. This is a direct consequence of the relatively high pressure dependence of  $C_{44}$  in Si.

In addition to these results, the changes in entropy, specific heat, thermal expansion, and bulk modulus due to edge and screw dislocations in the isotropic and anisotropic cases, and grain boundaries and pile ups in isotropic materials are easily calculated.

TABLE I. *Elastic strain energy and relative volume changes of a number of solids per unit atomic length of a screw dislocation using isotropic and anisotropic elasticity results*

Material	Isotropic		Anisotropic	
	$g$ (ev)	$v/\Omega$	$g$ (ev)	$v/\Omega$
Al	2.46	1.33	2.44	1.31
Cu	3.35	1.01	2.86	.80
Ag	3.02	1.12	2.61	.92
Au	2.76	.86	2.41	.69
Si	12.0	4.98	11.7	3.86
Ge	11.1	.25	10.7	.12
LiF	7.22	2.58	6.85	3.37
NaF	7.38	2.64	7.32	2.24
NaCl	6.36	2.83	6.25	2.32
KCl	7.84	2.64	6.59	.73
KBr	3.15	3.10	2.76	1.31
KI	6.06	3.28	5.21	1.40
RbBr	6.40	2.64	5.31	.77
MgO	22.0	2.32	21.4	2.82

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## Discussion on Papers by M. Wilkens, and J. Holder and A. V. Granato.

STONEHAM: I would like to make a comment on the paper by Dr. Wilkens. It is often very tempting to calculate the moments of the distribution of internal strains such as the mean square strain which Dr. Wilkens did. I would just like to emphasize that this often leads to problems because of divergencies, and also that it involves the assumption of some inner cut-off radius. When one calculates the proper distribution of the internal strains there is no need to make an assumption for the inner cut-off radius.

BESHERS: This question is for Professor Granato: The non-linearities which you are taking into account by considering the pressure and temperature dependence of the elastic constants also enter in the cut-off radius,  $r_o$ . You have the logarithm of  $r/r_o$ , which you have assumed constant. If you apply a pressure and the body is linear, the ratio  $r/r_o$  will not change, but  $r_o$  is down in the non-linear part and it is not clear that you can assume that the ratio  $r/r_o$  is going to be sufficiently constant for the purpose at hand.

GRANATO: That is true. We have used the usual elastic expression for the energy density; of course, it is only an approximation. One could do better. One could add in something that gives the core dependence if you also knew how it depends on temperature and pressure. Also you could go to higher order by getting the non-linear contribution to the energy density, that would have a third order elastic constant instead of a second order elastic constant and again would give the contribution upon differentiation. But it seems reasonable to suppose that the simple elastic expression will be the main term for the same reasons it is the main term for the energy.

SEEGER: The argument given here seems to be very similar to that given by Zener in his 1942 paper.<sup>1</sup> The really new part, I think, is that you have shown in a general way that this follows from the non-linear elasticity theory. We have convinced ourselves in special cases that the results of the Zener theory and of non-linear elasticity theory are the same.<sup>2</sup> We have used the idea that this is generally true, e.g. for anisotropic problems,<sup>3</sup> where calculations by elasticity theory become so com-

<sup>1</sup> Zener, C., Trans. AIME **147**, 361 (1942).

<sup>2</sup> Pfleiderer, H., Seeger, A., and Kröner, E., Z. Naturf. **15a** 758 (1960).

<sup>3</sup> Seeger, A., Suppl. al. NUovo Cimento, Ser. X, **7**, 632 (1958).

plicated that you have to resort to an argument like that in order to get the generalizations to cubic and non-cubic crystals.

GRANATO: That's right. The Zener theory is more restricted. It applies only for the volume, it cannot be generalized to higher derivatives. It is also very easy to deal with the anisotropic cases here. If you know the energy, you can write it down immediately. Also this works for another case that the Zener formulation would not work for and that is for non-static effects. The Zener formulation holds only in the static case. For example, you can treat phonons by just writing down the energy for a phonon; then for the density of defects,  $N$ , you have just the temperature and that gives the ordinary temperature dependence of the volume and of the elastic constants.

# **IX DISLOCATION-ELECTRON INTERACTIONS**

*Chairman:*

**R. THOMSON**



# CHARGED DISLOCATIONS IN THE DIAMOND STRUCTURE

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The electronic states at dislocations in elemental semiconductors are reviewed in the light of new experimental and theoretical work. Evidence is produced for the existence of a one-dimensional energy band along edge as well as screw dislocations. This explains quantitatively their ability to act as donors as well as acceptors depending on temperature, doping, and dislocation density. The degree of charging has been recalculated from the free energy of a system of charged dislocations screened by free carriers. The dislocation charge limits the Hall mobility in addition to the strain field of the dislocation. Measurements of photoconductivity of deformed semiconductors support the above model of the charged dislocation. The dislocation charge influences the Peierls force and thus the mobility of dislocations in the diamond structure. The occupation limit of the neutral dislocation, measured from the valence band edge, lies at 0.09 eV in germanium, and at 0.3 eV in silicon.

**Key words:** Band structures; charged dislocations; diamond lattice; dislocation-electron interactions; semiconductors.

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## I. Introduction

In 1954 Pearson, Read, and Morin [1] investigated the electrical effects of dislocations in germanium. They found that dislocations introduced by plastic deformation at high temperatures decreased the density of conduction electrons, i.e., that dislocations acted as acceptors. Following suggestions by W. Shockley Read proceeded in a series of well known papers [2, 3, 4] to describe theoretically the properties of a charged dislocation in the diamond structure. The success and elegance of this theory discouraged from further work of similar extent in this field for almost a decade. Whatever was done since Read to determine the energy level of this dislocation acceptor did not, however, fit the earlier results; neither have Read's theoretical assumptions remained unquestioned. It is common

practice now among workers in this field to start a talk like this one by reference to a slide which summarizes all positions of the dislocation acceptor level published so far. They cover the forbidden band of germanium rather uniformly. I will not attempt to review all of this work here which—useful as it has been—suffers from a number of disadvantages:

(a) Deformation has been done mostly by bending which limits the dislocation density  $N$  to values  $\leq 10^7 \text{ cm}^{-2}$  and leads to inhomogeneous dislocation distributions.

(b) The level of chemical doping  $N_c$  of the specimens investigated so far has been rather high ( $\geq 10^{14} \text{ cm}^{-3}$ ) so that dislocation acceptors showed up electrically by partial compensation of chemical donors only.

The high  $N_c$  is necessitated by whatever  $\Delta N_c$  impurities are introduced during deformation, the condition being  $\Delta N_c \ll N_c$ . All of this led to  $N \leq bN_c$  ( $b$  = Burgers vector) in the earlier experiments. We will see, however, that for dislocation effects to become clearly visible  $N \geq bN_c$  must be realized experimentally. Results are now available fulfilling this condition for Ge and Si which lead to a model of the charged dislocation different from Read's in the following qualitative aspects:

- (a) The dislocation acts as a donor as well as an acceptor.
- (b) The dislocation electron states form a one-dimensional energy band rather than discrete levels. Only the limit of occupation of this band is measured electrically.
- (c) Screening of the dislocation is by free carriers rather than by ionized impurities.
- (d) Screw dislocations most probably behave electrically very similar to  $60^\circ$  dislocations.

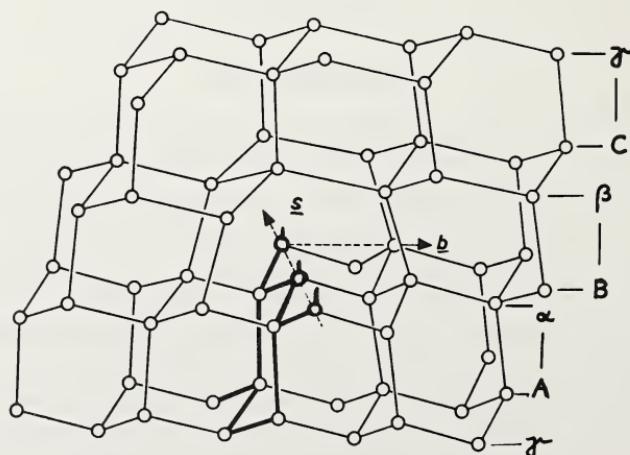


FIGURE 1.  $60^\circ$ -dislocation in the diamond structure.  $A\alpha B\beta C\gamma$  indicate the stacking order of close-packed planes.

The information (d) so far is only preliminary from first Hall data on twisted  $p$ -Ge in addition to indirect information from the change in dislocation mobility in Si with doping level [5]. The mobility changes with the dislocation charge (in the extrinsic range of doping) probably because this changes the core structure and so the Peierls potential. It has been shown [6, 7] that the formation of kinks in the Peierls potential determines the mobility of dislocations in the diamond structure. We will discuss dislocation mobility in section VI below.

Information on the dislocation band outside the limit of occupation may be obtained by optical methods. First results are discussed in section V. In the next section we will describe the structure of dislocations in the diamond structure. Then we turn to the results of electrical measurements to prove the statements (a) to (c) above.

## II. The Electronic Structure of a Dislocation

Figures 1 and 2 recall the structure of a  $60^\circ$  and of a screw-dislocation in the diamond structure, respectively. The former shows a row of "dangling bonds" along the edge of the extra half plane: one bond of the tetravalent atom sitting on this edge has no valence partner. Energy is gained according to Shockley [9] and Read [2] if this dangling electron accepts another electron and thus becomes paired. This leads to an energy level somewhere in the forbidden band. Shockley expected an one-dimensional half-full band of what he calls edge states. Read rejected the idea of a band

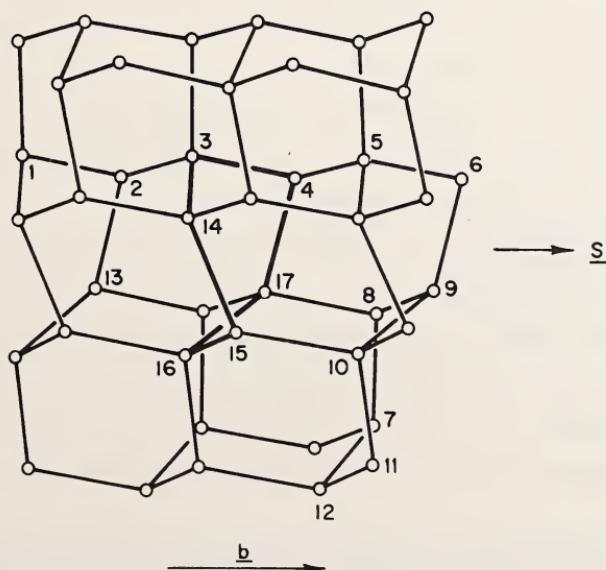


FIGURE 2. Screw dislocation in the diamond structure (according to Hornstra [8]).

that would be highly conducting, a behaviour which has not (yet!) been found. Also such a band would show donor as well as acceptor character. The former was, however, not observed at that time in (strongly doped!) *p*-germanium in which dislocations produced no electrical effect. Read assumed some pairing of the dangling electrons along the 60° dislocation though, as ESR measurements did not show unpaired electrons in dislocated germanium [10]. This is probably due to the strong spin-orbit coupling in the material.

In the meantime an ESR signal of the dislocation in silicon has been found [11]. It is nevertheless not yet clear whether the signal represents unpaired electrons precessing independently or the free electrons of the dislocation band. The temperature dependence of the signal will reveal this. The signal seems to depend sensitively on the orientation of the dislocations. Further work is under way on this point.

The screw dislocation in the diamond structure has no dangling bonds at all (fig. 2). If this dislocation behaves electrically similar to the 60° dislocation as it appears to do then this can only be rationalized in the band model. The model of an one-dimensional dislocation band is in fact a very sensible one. Along the dislocation the translational symmetry of the lattice is maintained while in the two dimensions perpendicular to the dislocation line there is a rather localized disturbance of crystal periodicity.

We assume that the normal band structure is maintained everywhere far outside of the dislocation while the electron states in the immediate environment of the dislocation will be changed. As the periodicity along the dislocation is that of the lattice, the energy levels of these states will form a band. This is also the result of a calculation by Teichler [12] who tries to describe from first principles the electron energies of a neutral screw dislocation in the diamond structure using the pseudopotential method and Wannier functions. He obtains one energy band within the gap for the electron states localized at the dislocation. Its exact position will be the result of further numerical evaluations.

An earlier calculation of the energy level of an electron which is trapped in the shear displacement field of a screw dislocation in a many-valley semiconductor has been done by Celli et al. [13]. With the deformation potential of Ge these authors obtain an acceptor level at 0.08 eV *below the conduction band edge* ( $E_c$ ). A similar calculation for the 60° and edge dislocations yields 0.05 eV below  $E_c$ . Such levels have not been found yet experimentally. The occupation limit of the neutral dislocation band of Ge is observed 0.09 eV *above the valence band edge* ( $E_v$ ) as we will see below.

The band model naturally explains the acceptor/donor behaviour of the dislocation as positive/negative deviations from the half-full, neutral occupation. These deviations will be small as Read [2] has pointed out

since the extra electrons/holes transferred from the crystal or the chemical centers onto the dislocation strongly repel each other there electrostatically. This raises the energy position of the band within the gap until its occupation limit coincides with the Fermi level and no further charge is transferred to the dislocation.

### III. Hall Measurements on Deformed Crystals

We will now describe the Hall measurements of Schröter and co-workers [14, 15] which have led to the conclusions stated in section I.

These experiments were done mostly on weakly *p*-doped germanium and silicon although *n*-type specimens were also investigated. Deformation was by homogeneous single slip in an uniaxial compression creep experiment at 580 °C for Ge, at 770 °C for silicon in an atmosphere of forming gas. Utmost care was applied to keep the specimens clean during deformation and handling: This has been successful within  $\sim 10^{12}$  impurities/cm<sup>3</sup> for Ge, within about 10<sup>13</sup> cm<sup>-3</sup> for silicon. Dislocation densities were determined by etching. The reliability of various dislocation etching solutions was checked against electron transmission microscopy in the case of Ge [16]. It is known [16] that the dislocations produced by this deformation are mostly of edge character with a structure similar to that in figure 1. Thus the dangling bonds have atomic spacing. Hall effect and conductivity were measured between 50 and 250 K ( $\pm 0, 1$  K) for Ge, up to 350 K for Si. The magnetic field was about 6 kG. It was made sure by measurements up to higher fields that the ratio of carrier density to Hall coefficient was constant (assumed to be 3 $\pi/8$ ).

#### A. RESULTS ON GERMANIUM

Figure 3 shows the concentration *p* of free holes in a specimen doped with  $N_{ca} = 7.3 \times 10^{12}$  cm<sup>-3</sup> chemical acceptors as a function of temperature before and after deformation to a dislocation density of  $4.6 \times 10^7$  cm<sup>-2</sup>. The curve of the undeformed specimen is typical for a specimen with chemical acceptors of an energy close to  $E_v$ . The curve of the deformed specimen indicates at high temperatures the presence of additional acceptors of the dislocation type as the curvative changes continuously indicating an energy shift with occupation.<sup>1</sup> At low temperatures the chemical acceptors become inefficient because they become filled from above i.e., dislocations are acting as *donors*.

<sup>1</sup> Additional evidence for dislocations not point defects [17, 18] being the deformation-introduced centers is provided by synchronous annealing studies of Hall effect and dislocation content.

(The other possibility that the chemical acceptors become attached to dislocations during deformation can be excluded by a kinetic argument). It is interesting to follow the changes in the  $\ln p(1/T)$  curve as either dislocation density or doping concentration are changed systematically (figs. 4 and 5). Schröter notes that an *n*-doped specimen (doping  $N_{cd}$ ) fits the general trend which is determined by the parameter  $(bN_{ca}/N)$  if one puts  $N_{ca}^{\text{eff}} = -N_{cd}$  for this specimen.

To understand the measured  $\ln p(1/T)$  curves we notice first that the low-lying chemical acceptors must all be ionized at the temperature of Schröter's measurements so that for charge conservation the degree of occupation of the dislocation

$$f = \frac{p - N_{ca}}{N/b} \quad (1)$$

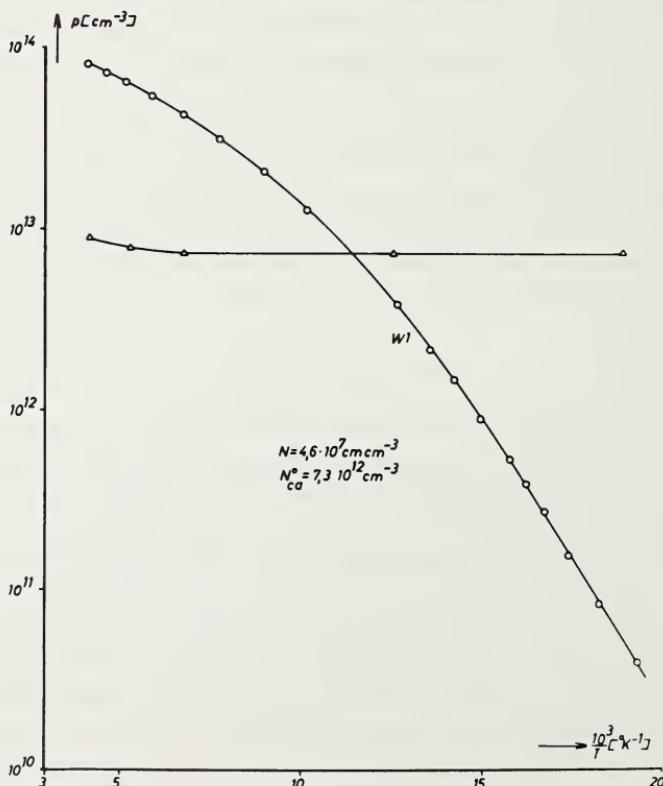


FIGURE 3. Temperature dependence of hole concentration in Ge before and after deformation to a dislocation density  $N$  ( $N_{ca}^0$  = initial density of chemical acceptors) [14].

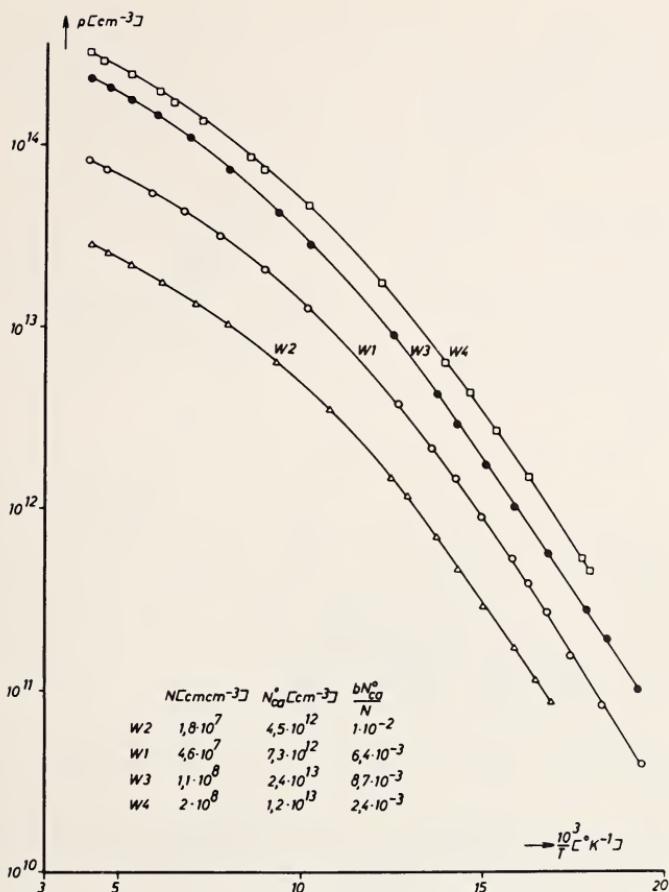


FIGURE 4. Temperature dependence of hole concentration in Ge after deformation to different  $N$  [14].

(At low temperatures  $p \ll N_{ca}$  and  $f = f_0$  is the parameter found experimentally to determine the shape of  $\ln p(1/T)$ .)

The energy  $E$  to excite an electron to the dislocation band (see fig. 6) may depend on  $f$ ,  $p$  (and  $N_{ca}$  which can, however, be eliminated by eq (1)). It is reasonable to put (following fig. 6)

$$E = E_0 + E_i(f, p) + \epsilon(f). \quad (2)$$

$E_0 = E(f=0)$  is the occupation limit of the neutral dislocation (measured from  $E_v$ );  $E_i$  is the interaction energy of an electron on the dislocation with the others already present on this and other dislocations and with the surrounding screen. All energy levels near the dislocation are changed by this electrostatic interaction.  $\epsilon$  is the (small) change with  $f$  in the

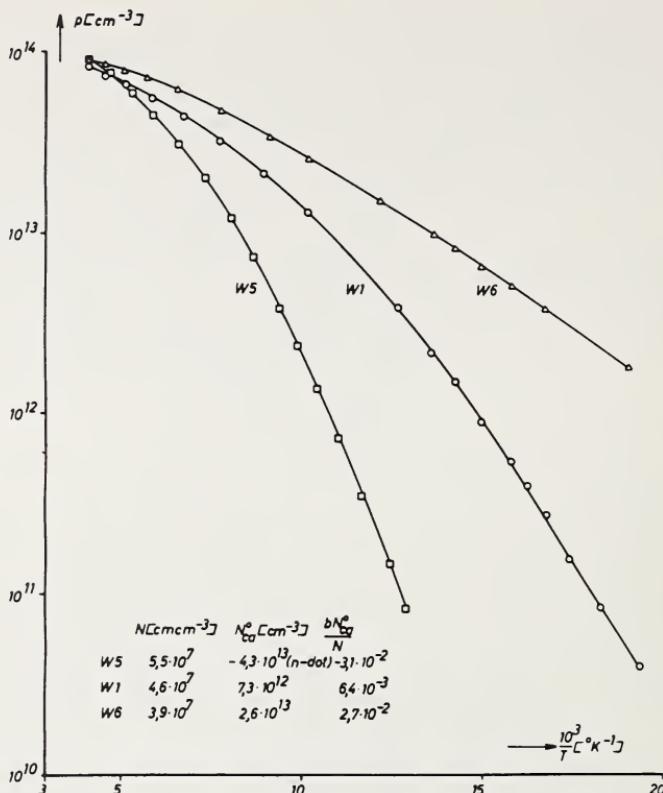


FIGURE 5. Temperature dependence of hole concentration for Ge specimens of about the same  $N$  at different doping levels [14].

occupation limit within the dislocation band. In thermal equilibrium  $E$  must be equal to  $E_F$ , the Fermi energy, which at normal temperatures ( $E_F > kT$ ) is uniquely determined by  $p$  and  $T$  (assuming a standard valence band) according to

$$E_F = kT \ln \left( \frac{CT^{3/2}}{p} \right). \quad (3)$$

(For Ge  $C = 1.17 \times 10^{15} \text{ cm}^{-3} \text{ K}^{-3/2}$ , for Si  $C = 1.95 \times 10^{15} \text{ cm}^{-3} \text{ K}^{-3/2}$ ).

For  $f=0$ ,  $T=T_0$  following eqs (1), (2), (3) one gets

$$p(T_0) = N_{ca}, E_F(T_0) = E_0, \text{ and } E_0 = kT_0 \times \left( \ln \frac{CT_0^{3/2}}{N_{ca}} \right)$$

can be calculated from the neutrality temperature  $T_0$  given e.g., by the

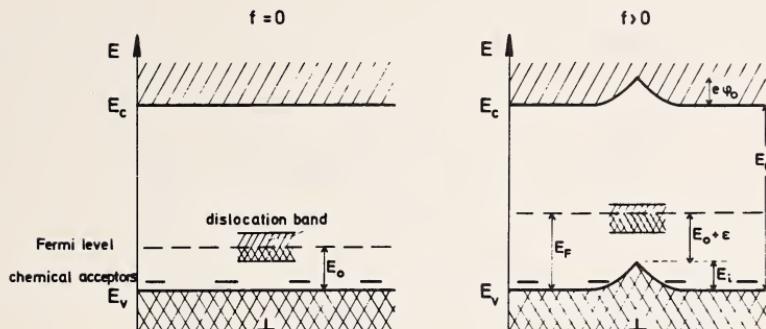


FIGURE 6. Energy level scheme at neutral ( $f=0$ ) and negatively charged dislocation ( $f>0$ ).

intersection of the two curves in figure 3. Schröter finds rather accurately  $E_0 = 0.09$  eV (above  $E_v$ ) for Ge.

The further evaluation of the Hall data on deformed Ge for  $f=0$  requires a calculation of  $E_i$  including a model of screening of the charged dislocation. Read's screening by partial ionization of the doping atoms in the neighbourhood of the dislocation is inapplicable in the range of  $T$  and  $N_{ca}$  under consideration, as figure 3 shows that all (shallow) chemical acceptors of the undeformed specimen are ionized. Bliek [19] has calculated  $E_i$  for a single dislocation in a large crystal using a screened Coulomb potential of fixed screening radius. This results in  $E_i$  being a function of  $f$  alone and suggest plotting eq (2) as  $(E_F - E_0)$  versus  $f$ , where  $E_F$  is calculated from the experimental data via eq (3) and  $f$  via eq (1). The result for Ge is seen in figure 7 (with minor adjustments in  $N_{ca}$  and  $N$ —within their experimental errors—in order to get the data from all the different crystals to overlap as much as possible). There is almost a unique curve  $(E_i + \epsilon)$  versus  $f$  except for the “tails” pointing towards smaller energies. The tails are even larger in silicon and have induced a new calculation of  $E_i$  by Schröter and Labusch [20]. It is interesting to note that at high temperatures ( $T \geq 250$  K) the Hall effect of deformed Ge depends strongly on  $N$  and little on  $N_{ca}$  providing a convenient means of determining the density of (electrically active) dislocations. For Ge (and Si) this agrees rather closely with direct counts of  $N$  [14, 15].

## B. RESULTS ON SILICON

Because of the rather different band structure it was considered worth while to measure the Hall effect also on deformed silicon despite considerable difficulties encountered at the higher deformation temperature and higher specific resistivities of this material [15].

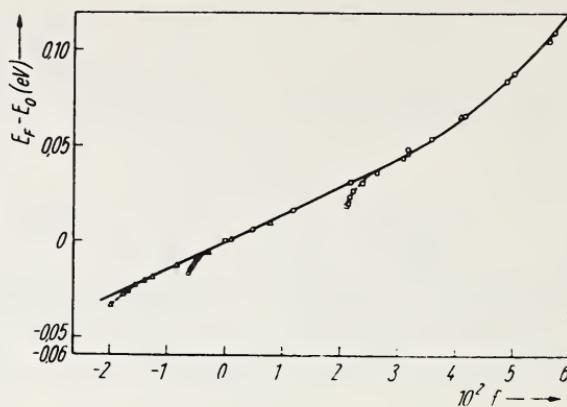


FIGURE 7. Degré of occupation  $f$  of dislocations versus Fermi energy  $E_F$  measured from level  $E_0$  of neutral dislocation in Ge [14].

The measured hole concentration versus temperature for Si again shows acceptor character of the dislocation at high temperatures and donor character at low temperatures. Below 250 K a flat exponential behaviour of  $\ln p$  ( $1/T$ ) is found (fig. 8) which has not been seen in Ge (fig. 3). The change of the curves as a function of  $N$  and  $N_{ca}$  (including  $N_{ca}^{\text{eff}} = -N_{cd}$ ), is qualitatively similar to Ge (fig. 9). The evaluation follows the lines of that in Ge. From the neutrality condition  $f = 0$ ,  $p(T_0) = N_{ca}$  Weber obtains  $E_0 = 0.30$  to  $0.33$  eV (above  $E_v$ ). The  $(E_F(f) - E_0)$  curves, figure 10, calculated from eqs (1) and (3) look rather different from those of Ge, figure 7: Only at high temperatures,  $f > 0$ , a unique  $(E_F(f) - E_0)$  curve is obtained in Si while at low  $T$ , below a certain  $f < 0$ ,  $E_F$  decreases sharply corresponding to the flat range in  $\ln p$  ( $1/T$ ), figure 7. This behaviour excludes a new, second energy level for the dislocation as well as for some point defects, rather shows that  $(E_F - E_0)$  is not a function of  $f$  alone but also one of  $p$ . (Some indication of such a behaviour is visible also in the "tails" of the Ge curves, fig. 7). The reason for this complication is the large screening radius  $\lambda_D \propto p^{-1/2}$  at low temperatures which makes it necessary to recalculate  $E_i$  for a crystal containing *more than one* charged dislocation. This has been done by Schröter and Labusch [20] with the result indicated in figure 10. Only  $N$  has been slightly adjusted with these curves to obtain good fit to the calculated  $(E_F - E_0)$ . The corrected values  $N_{\text{corr}}$  correspond to an electrically active  $N$  slightly higher than the light-optically determined  $N$ . The  $\epsilon$ -term corresponding to a change of the occupation limit within the dislocation band has been neglected.

### C. THEORY OF THE INTERACTION ENERGY $E$

At low temperatures screening of a charged dislocation in a not too strongly doped crystal is rather incomplete and extends beyond the

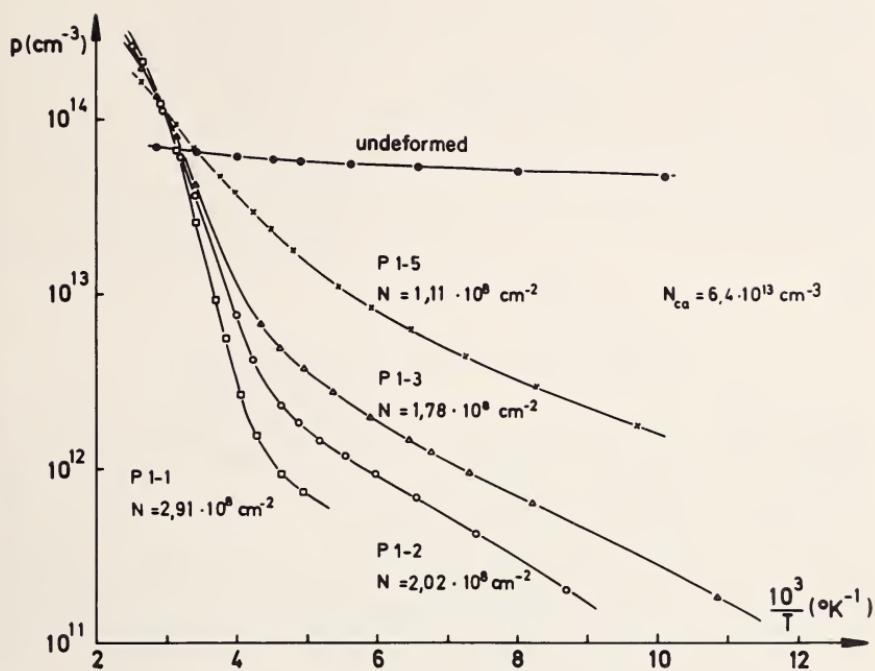


FIGURE 8. Temperature dependence of hole concentration in Si for different dislocation densities [15].

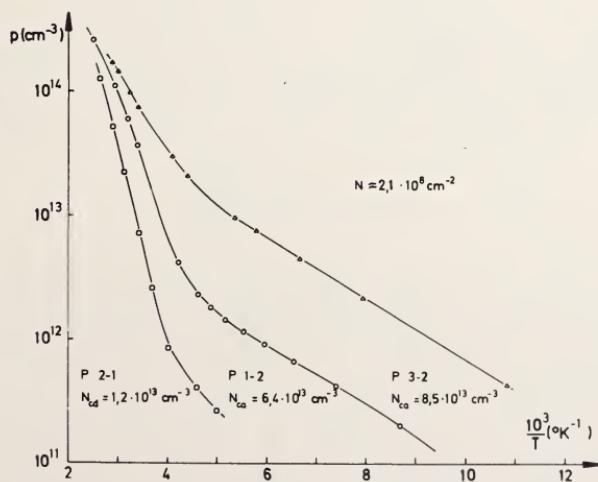


FIGURE 9. Temperature dependence of hole concentration in Si for different doping levels [15].

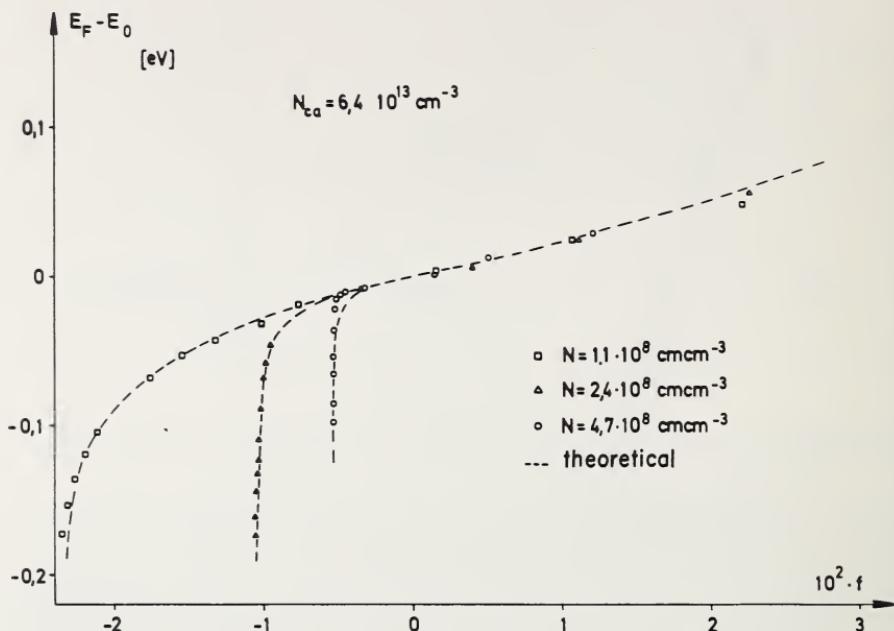


FIGURE 10. Degree of occupation  $f$  of dislocations versus Fermi energy ( $E_F - E_0$ ) for Si [15] together with result of calculation (dotted curve) [20].

next dislocations considering the  $N$ -values obtained in [14, 15]. There is then no longer a large undisturbed crystal reservoir with undeformed energy bands from which electrons can be drawn freely to occupy the dislocation band. The occupation statistics must be reformulated considering changes in the dislocation band as well as in the valence band (the chemical acceptors being completely ionized in the range of interest). This has been done by Schröter and Labusch [20] who obtain two Fermi distributions for these two bands. Variation of the free energy results in

$$E_i = \frac{b}{N} \cdot \frac{\partial E_s}{\partial f} + \frac{\partial E_s}{\partial p}. \quad (4)$$

to be inserted into eq (2) with  $E = E_F$  for thermal equilibrium.  $E_F$  is still to be determined from eq (3).  $E_s$  is the (integral) self energy of the charged dislocation which is calculated now including all the interactions present: with other dislocations, with the free carriers, as well as with the ionized impurities, and among the electrons on the dislocation itself. This is an essential improvement with respect to earlier estimates [2, 19, 21], as is the second term in eq (4) which takes care of the charge balance in the deformed crystal. The explicit calculation of  $E_s$  finally results for  $b \ll \lambda_D f$  in [20]

$$E_i(f, p) = \frac{e^2 f}{2\pi\epsilon b} \left( -\ln \frac{b}{\lambda_D f} + 0.25 + \frac{N_{ca}}{4p} \right) \quad (5)$$

where  $\epsilon$  is the dielectric constant and the Debye screening length  $\lambda_D = \left( \frac{\epsilon kT}{e^2 p} \right)^{1/2}$ . This result is in excellent agreement with experiments as shown in figure 10, the steep rise in  $E_F$  at low  $T$ , small  $p$  being caused by the new, last term in eq (5).

#### IV. Mobility in Deformed Crystals

In addition to the Hall coefficient  $R_H$  the conductivity  $\sigma$  of the deformed Ge- and Si-crystals was measured by Schröter and co-workers [22, 15]. The Hall mobility is then calculated as  $\mu_H = R_H \cdot \sigma$  (and is to be considered as the high field limit). As mostly edge dislocations were introduced by uniaxial compression, the current direction  $\langle 123 \rangle$  formed an angle of  $78^\circ$  with that of the dislocations. The mobility  $\mu_H$  of undeformed, lightly  $p$ -doped Ge below room temperature is determined by the scattering of holes at phonons: One finds  $\mu_H \propto T^{-2.3}$  above 100 K and a somewhat less steep rise below that temperature. Scattering at ionized foreign atoms is unimportant above 50 K for the doping concentrations used here. In the deformed state a very strong additional scattering is observed at low temperatures as figure 11 shows. The combined effect of this defect scattering and of the phonon scattering being still dominant above 120 K leads to a characteristic mobility peak. Figure 12 shows how  $\mu_H(T)$  changes with increasing dislocation density *at constant values* of the old characteristic parameter  $(-bN_{ca}/N) = f_0$ , the degree of charge occupation of the dislocation at low temperatures. A systematic depression of the  $\mu_H(T)$  curves is observed. The identification of the scattering defects with dislocations furthermore is supported by synchronous annealing studies of  $\mu_H$  and  $N$  [22]. The change of  $\mu_H$  with the dislocation charge at constant  $N$  is seen in figure 13. The degree of occupation  $f$  of the dislocations in these specimens is shown in figure 14. At low temperatures holes in  $W_6$  are less mobile than in  $W_1$  corresponding to the stronger positive charging of dislocations in the former.  $W_5$  is an  $n$ -doped specimen ( $N_{ca}^{eff} = -N_{cd}$ ) in which the dislocation charge is always negative (fig. 14). The mobility of the holes, which became dominant after deformation in this specimen too, is very small and does not show the pronounced maximum as the  $p$ -type specimens do: This suggests an explanation of the  $\mu_H$  maximum by the neutral condition of the dislocation as derived from the Hall measurements, see figure 14. In order to isolate the mobility  $\mu_p$  limited by the dislocation charge only, the mobility  $\mu_p$  limited by phonons

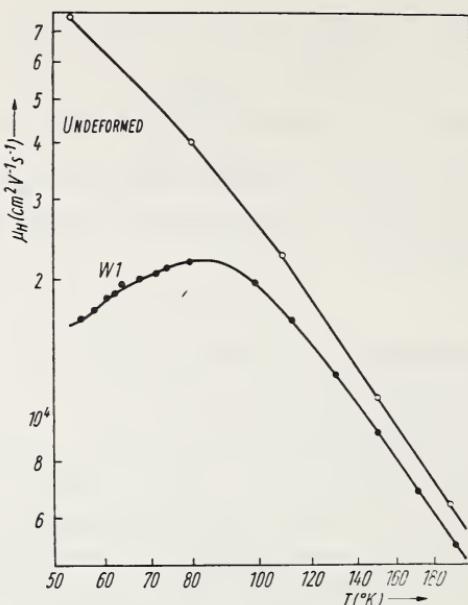


FIGURE 11. Temperature dependence of Hall mobility of *p*-Ge doped with  $7.3 \times 10^{12} \text{ cm}^{-3}$  acceptors before and after deformation to  $N = 4.6 \times 10^7 \text{ cm}^{-2}$  [22].

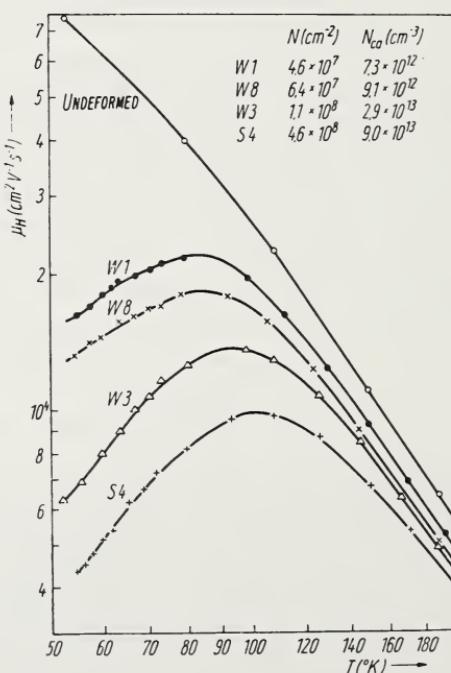


FIGURE 12. Hall mobility versus temperature for constant  $f_0$ . Ge deformed to different  $N$  [22].

(in undeformed specimens) must be separated from the measured  $\mu_H$  according to

$$\frac{1}{\mu_H} = \frac{1}{\mu_p} + \frac{1}{\mu_f}. \quad (6)$$

A  $\mu_f$  maximum results at the temperature  $T_\mu$  which agrees well with the neutrality temperature  $T_0$  (visible in fig. 14) for Ge.

The same also holds for Si some results of which are shown in figure 15. The still finite mobility at  $T_\mu$  indicates the scattering at the displacement field of the dislocation in addition to the carrier scattering at the dislocation charge. The mobility  $\mu_u$  as limited by displacement scattering has been calculated by Dexter and Seitz [23] from the deformation potential with the result  $\mu_u \propto T/N(\mu_p^2 T^{-2.3}$  for Ge was already mentioned above).  $\mu_f$  has first been calculated by Read [3] assuming specular reflection of the carriers at the space charge tubes around dislocations formed by ionized impurities. Broady [21] has modified this scattering mechanism assuming a second hollow cylinder around Read's (of a wall thickness equal to the mean free path) in which the mobility is still reduced. These

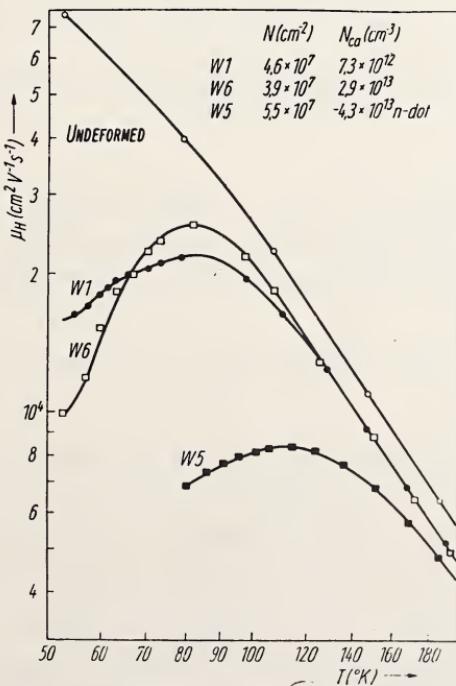


FIGURE 13. Hall mobility versus temperature for Ge specimens of the same  $N$  but different  $f_0$  [22].

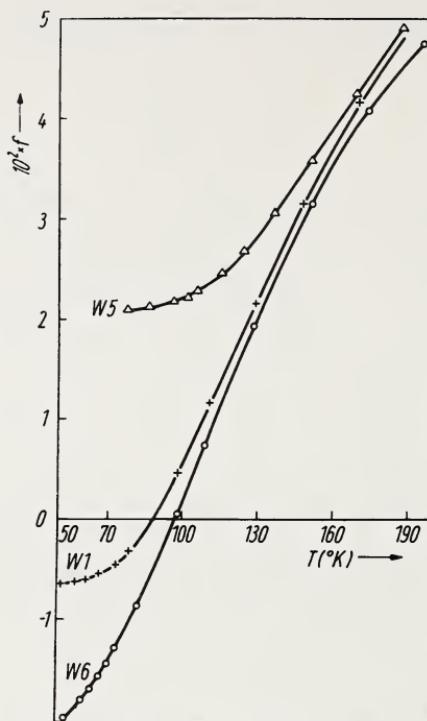


FIGURE 14. Occupation  $f$  of dislocation for Ge crystals of different doping [22] ( $N \sim 5 \cdot 10^7 \text{ cm}^{-2}$ ).

models don't apply for our case  $b \cdot N_c/N \ll 1$  in which all acceptors must be ionized at the temperatures under consideration. Our case of screening by free carriers has been treated by Pödör [24] in Born's approximation with the result

$$1/\mu_f^{\text{th}} \propto \frac{Nf^2\lambda_D}{T^{3/2}} \propto \frac{1}{NT\sqrt{p}} \cdot (p - N_{ca})^2. \quad (7)$$

Figure 16 shows a comparison of the experimental [22] and theoretical [24]  $\mu_f^{-1}$  for Ge after correction with respect to  $\mu_p$  and  $\mu_u$  according to eq (6). The fit to the theoretical parabola is quite good whose nadir corresponds to  $f=0$ . There is numerical factor 5 to 6 multiplied onto Pödör's  $\mu_f^{\text{theor}}$  to fit the experimental results. On the whole the model of the dislocation band describing the donor/acceptor behaviour of the dislocation including the screening calculation [24] fits the measured  $\mu_H$  behaviour quite well if the scattering of the displacement field of the dislocation also is taken into account.

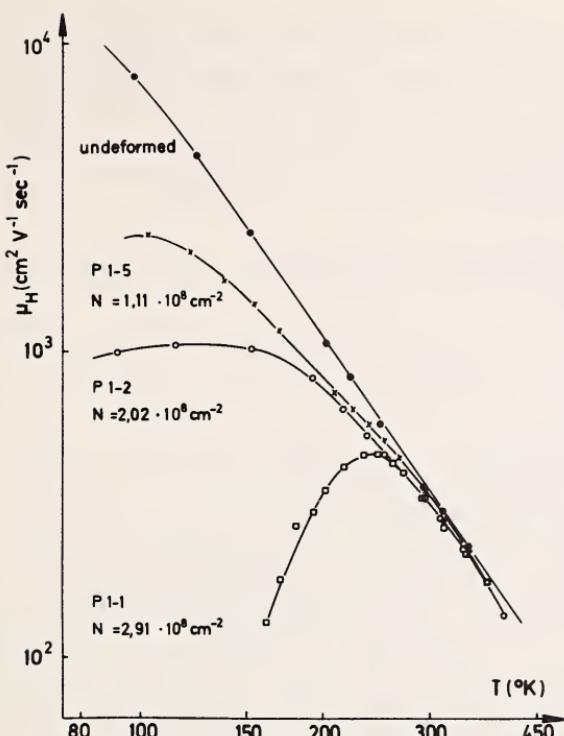


FIGURE 15. Hall mobility versus temperature for deformed Silicon doped with  $6.4 \times 10^{13} \text{ cm}^{-3}$  acceptors [15].

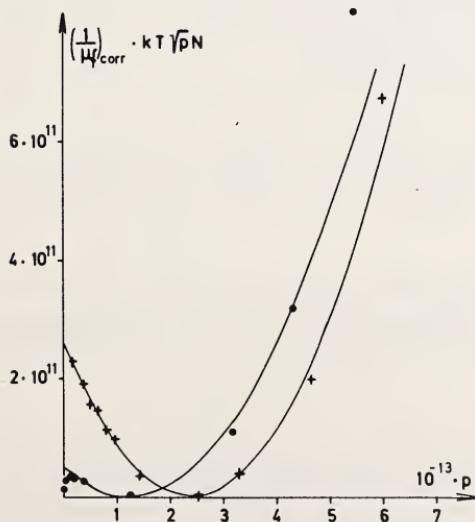


FIGURE 16. Mobility  $\mu_f$  limited by the dislocation charge versus hole concentration. The parabolas are calculated [24]. Experimental results for Ge [22].

## V. Optical Excitation at Dislocations

Since by Hall measurements one obtains information only about the occupation limit of the dislocation band, optical excitation of electrons might become an useful tool to study other states of this band.

Various possible processes of this sort include:

- (a) photo-conductivity—stationary and transient—to study recombination at dislocations;
- (b) optical absorption corresponding to transitions to and from the dislocation band;
- (c) radiative recombination at dislocations of injected carriers.

Recent results on these methods are due to Figielski et al. [25] [26, 27] and due to Güth and co-workers [28]; of these the measurements (a) referring to of the decay of transient photoconductivity by Jastrzębska and Figielski [26] are particularly informative. These authors deformed [26] mostly *n*-type Ge by bending at 650 °C to dislocation densities between  $10^6$  and  $10^7$  cm $^{-2}$ . The extra conductivity following a white light pulse was measured as a function of time after light switch-off at various temperatures. Initially the transient photocurrent decayed in proportion to log time, later on it disappeared exponentially, both with a time constant  $\tau_e$  (of the order 50 s at 150 K).  $\tau_e$  rose at low temperatures ( $T > 160$  K) with an activation energy  $\Delta E = 0.5$  eV (similar to that of the rise of stationary photoconductivity with temperature). The authors showed that the transient photocurrent was due to electrons in the case of *n*-Ge. There the dislocation is negatively charged and captures holes easily while the photoproduced electrons have to overcome a potential  $e\varphi$  to reach the (screened) dislocation (see fig. 6). The rate of electron capture (density  $n$ ) can be described by

$$-\dot{n} = c \cdot Nn \cdot \exp\left(-\frac{e\varphi_0}{kT}\right) \left( \exp \frac{e\varphi_0 \cdot \Delta f}{f_0 \cdot kT} - 1 \right) \quad (8)$$

where  $f_0$ ,  $\varphi_0$  are the barrier height and degree of occupation, respectively, in thermal equilibrium and  $\Delta f$ ,  $\varphi_0 \cdot \Delta f/f_0$  are the changes in these quantities with illumination.  $c$  is a capture coefficient. The change in conductivity then is

$$\frac{\Delta\sigma}{\sigma} \propto \frac{\Delta n}{n} \propto \frac{\Delta p \text{ (trapped)}}{n} \propto \Delta f \frac{N}{bn} \quad (9)$$

It decays according to eq (8) either exponentially or logarithmically with

time (depending on  $\frac{\Delta f \cdot e\varphi_0}{f_0 \cdot kT}$  being small or large compared to one). The decay time is in both cases (independent of  $N$ !)

$$\tau_e = \frac{f_0 kT}{cbn} \exp\left(\frac{e \cdot \varphi_0}{kT}\right) \propto \exp\left(\frac{e \cdot \varphi_0}{kT} + \frac{E_G - E_F}{kT}\right) \quad (10)$$

if  $E_G$  is the gap width,  $E_F$  the Fermi energy (measured still from  $E_v$ ), and eq (3) is applied to electrons instead of holes. Using eq (2) with  $E_i = e\varphi_0$  and the equilibrium condition  $E = E_F$  we obtain

$$\Delta E = d \ln \tau_e / d(1/T) \sim E_G - E_0 - \epsilon,$$

see figure 6 ( $\epsilon$  could be different in this case!). The experimental results therefore yield  $(E_0 + \epsilon) \sim E_0 \sim 0.2$  eV (above  $E_v$ ). Although the concept of this experiment makes no explicit use of  $E_0$  it allows to determine this quantity to some approximation from a measurement of  $(E_i - E_F)$  and from an energy balance, eq (2). Figielksi et al. point out that only the dislocation band model is able to explain the photo-conductivity results on  $n$ -as well as  $p$ -Ge for which results are scarce so far.

In [27] the spectral distribution of the photosensitivity referring to (b) is investigated. In deformed  $n$ -Ge two photosensitive regions are found: one beginning at 0.22 eV and a second one at about 0.42 eV. The latter one decayed logarithmically with time and could be shown to be due to electrons. It is ascribed to excitations of electrons from the dislocation to the conduction band, the rate limiting process being that of recombination analyzed above. Its activation energy agrees with that obtained from the temperature dependence of photoconductivity in deformed  $n$ -Ge. The photoconductivity rise with light of 0.22 eV is followed by a quick decay corresponding to the short lifetime of holes near the negatively charged dislocations. It is therefore ascribed to transitions from the valence band to the dislocation band. The sum of the two excitation energies nearly equals the band gap.

## VI. Dislocation Velocity in Doped Crystals

### A. METHODS

As was mentioned in the introduction the velocity of dislocations in the diamond structure is determined by the rate of formation of kinks in the Peierls potential [7]. This conclusion is supported e.g., by the good agreement between calculations of the kink formation energy [6, 29] and experimental results on the activation energy of dislocation motion [30, 31].

Direct velocity measurements are possible by the double-etch or by x-ray topographical methods [7]. The dislocation velocity can also safely be derived from macroscopic measurements of incubation creep or of pronounced yield [7]. Experimental results are available on pure as well as on strongly doped crystals (in the extrinsic range). Remarkable differences are found as we will see below. This is most likely related to the charge of the dislocation although no theory of the Peierls potential exists for charged dislocations. The matter serves here to demonstrate—in agreement with the foregoing sections—the possibility of negative as well as positive charge effects and the similarity between charged 60° and screw dislocations. Both points support the idea of a dislocation band. The problems of optical charging of dislocations and of dislocations in the sphalerite lattice are also mentioned.

### B. EXPERIMENTAL RESULTS ON DOPED CRYSTALS

Figure 17 shows the velocity of dislocations in Ge at fixed stress  $\tau$  and temperature  $T$  versus concentration  $c$  of doping, either by As, by Ga or by Sn [32]. There is a pronounced dependence of  $v$  on  $c$  in the extrinsic range for this temperature.  $n$ -doping increases,  $p$  decreases  $v$  while tetravalent substitution has no effect. Since the velocity in the intrinsic material is of the form

$$v = B_0 \tau^m e^{-U/kT}, \quad (11)$$

the question arises which of the parameters change with  $c$ .

The result is that  $m$  stays to be about one,  $B_0$  is almost unaffected while  $U$  changes greatly [32].  $n$ -doping is about twice as effective as  $p$ -doping. In the measurements on Ge the dislocation character was not known (probably 60°). With Si by x-ray topography one is sure to investigate screw dislocations [5]. The magnitude of the effect in  $n$ -Si is about the same

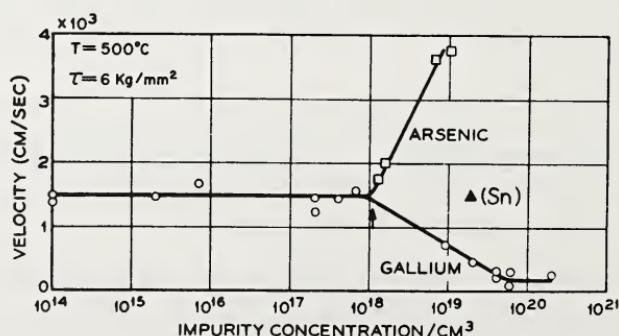


FIGURE 17. Variation of dislocation velocity with doping in Ge. Arrow indicates the intrinsic carrier concentration at 500 °C [32].

as in *n*-Ge at the same relative values of the parameters. In *p*-Si only the effect of relatively small *c* have been studied so far which are similar to those in *p*-Ge. The velocity changes in effect with doping as does the Fermi energy. The effect saturates at  $c \sim 10^{20} \text{ cm}^{-3}$ . It must be of electronic origin as trivial bulk causes can be excluded [7]. An explanation of the doping effect by Frisch and Patel [33] postulates a preferential formation of kinks at certain localized charged dislocation acceptor sites. For their theory which is based on Read's model [1] of the charged dislocation these authors need an acceptor level in Ge fixed above the center of the gap. In silicon they claim that the energy level of the dislocation practically coincides with  $E_c$  [34]. These results are inconsistent with the electrical measurements described above and with the model derived therefrom.

### C. OPTICAL CHARGING

In a recent paper Fortini and deBouard [35] report that the incubation time in bending creep of pure Ge at 380 °C decreases considerably on irradiation with white light (250 W bulb focussed by elliptical mirror). The authors claim that the creep acceleration under light corresponding to a 3.5 percent decrease of the activation energy was not due to a temperature rise of the illuminated specimen which was only 0.24 mm thick. Schaumburg [36] has tried to reproduce this effect by a direct velocity measurement on a 4 mm thick Ge specimen with and without illumination (in this case by a carbon arc). No change in velocity was found at 370 °C and 450 °C within 20 percent (Fortini et al.'s change in activation energy on illumination would result in a factor 4 higher velocity).

On the other hand Schaumburg could show that a thin specimen as used by Fortini et al. [35] would be heated up by illumination easily by 30 to 40 °C enough to explain the whole illumination effect as the result of a simple temperature change. In order to truly excite charge carriers to or from the dislocation the light intensities applied so far don't seem to suffice. Probably the cross section corresponding to the dislocation states is too small or the life time in them is too short. The number of electron-hole pairs created by illumination on the other hand was still a factor of 100 or so too small to change the dislocation charge noticeably.

### D. IN- AND Sb-DISLOCATIONS

Positive and negative 60° dislocations in InSb have different core structures, their extra half planes ending with a row of In- and Sb-atoms respectively [38]. It has been shown now by several experiments [38, 40, 39, 7] that In- and Sb-dislocation also have different mobilities, In dislocations being much faster than Sb dislocations at a given stress and temperature. The In dislocation core is less disturbed by the three-valent edge atoms than that of the Sb-dislocation. On the other hand relative to a tetra-

valent reference lattice the In-dislocation charge corresponds to that of a dislocation in strongly *p*-doped Ge. Whereas an In-dislocation is faster than an Sb-dislocation, however, dislocations in *p*-Ge move more slowly than in *n*-Ge. This demonstrates the inadequacy of this comparison.

## VII. Acknowledgement

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## Discussion on Paper by P. Haasen and W. Schröter.

**BEN-ABRAHAM:** I would like to ask whether you worried about kinks? Just a year ago, Dr. Gilman interpreted the mobility of dislocations in germanium and diamond lattices in terms of charged kinks.

**HAASEN:** It might well be possible that it is the charged kinks which are responsible for changes in mobility with doping. The only thing we know at the moment is that a charge on a dislocation is one possible way to rationalize these effects. Whether the charge is localized at kinks or homogeneously spread in the way we have described it here is not known. Gilman's model really applies to very low temperatures where he uses tunnelling of kinks and things like this. At high temperatures we are sure that it is the formation of kinks which is the process responsible for dislocation movement.

**ASHCROFT:** This is just a point of information. I thought in intrinsic semiconductors, which are what I believe you are using, the surface state electronic density is about an order of magnitude more than the numbers you are dealing with here. My question is, first of all, is that the case, and secondly, how are you sure that you are looking at dislocations and not damage and effects thereof on the surface electronic density?

**HAASEN:** We can follow all the effects we have measured as a function of dislocation density. We can put in various dislocation densities and anneal them out again and get the electrical behavior we expect from this. Surface states would be present in annealed and in unannealed specimens. I think we can completely rationalize our results in terms of a dislocation density. We can count dislocations electrically and as you have seen the result is within 20% of the etched dislocation density.

**MENDELSON:** Did you consider the possibility of an effect on the donors or acceptors from the tendency to separate or dissociate for both  $60^\circ$  and screw dislocations?

**HAASEN:** Do you mean node measurements, or other direct observations, or how else should we believe in a stacking fault separation?

**MENDELSON:** Well, I wasn't thinking whether you would actually make an observation, but how it might affect the electrical properties; that is, how the electrical effects due to donors and acceptors might affect the number of dangling bonds due to a dissociation and how this might tie into the plastic properties—for example, the mobilities of a dissociated dislocation versus a perfect dislocation.

HAASEN: There are only Peierls type calculations for the undissociated dislocation. The mobility of the undissociated dislocation depends on doping as shown in the last slide. You know my negative view about dissociation. I think it's quite a different story. What one still would like to know is the stacking fault energy, say, as a function of doping. But, there is nothing known as far as I can see.

MENDELSON: Well, that would be good if you knew it. Suppose you made the assumption that there is a stacking fault formed and you asked yourself, "What would be the nature of the dangling bonds on both the screw and the sixty degree dislocation and how would these dangling bonds interact with the two types of dopings—the acceptors and the donors?"

HAASEN: There are no dangling bonds with the screw dislocation. That was one of the reasons why we left the dangling bond model and went to the band model, which corresponds to electronic states in the core of the dislocation without making explicit use of bonds and pairing of bonds. The electrical behavior of dislocations in Ge does not seem to depend on the dislocation character.

MENDELSON: Yes, but the dissociated screw would have dangling bonds and that would at least be consistent with your electrical effects of screws.

HAASEN: OK. I still see no theoretical or experimental reason to invoke a split dislocation in the diamond lattice.

MENDELSON: [Written contribution] Dr. Haasen has expressed the belief that dislocations in the diamond lattice are not dissociated whereas various behavior characteristics are consistent with the view that at least the 60° dislocations are dissociated. Amelinckx<sup>1</sup> pointed out that the behavior of dissociated dislocations would be different and by studying extended dislocation nodes concluded<sup>2,3</sup> that the stacking fault energies in Si and Ge are 50-60 ergs/cm<sup>3</sup> and 90 ergs/cm<sup>2</sup> respectively. The validity of this technique for determining the stacking fault energy has been questioned by studies<sup>4,5</sup> which show that nodes could appear to be extended by an anomalous diffraction contrast effect, however the tendency for twins and stacking faults to form during crystal growth of Ge and Si suggests that the energies cannot be very high. Studies of the

<sup>1</sup> Amelinckx, S., Proc. Int. Conf. on Crystal Lattice Defects, Suppl. J. Phys. Soc. Japan **18**, 22 (1963).

<sup>2</sup> Aerts, E., Delavignette, P., Siems, R., and Amelinckx, S., J. Appl. Phys. Letters **33**, 3078 (1962).

<sup>3</sup> Art, A., Aerts, E., Delavignette, P., and Amelinckx, S., Appl. Phys. Letters **2**, 40 (1963).

<sup>4</sup> Booker, G. R., and Brown, L. M., Phil. Mag. **11**, 1315 (1965).

<sup>5</sup> Shaw, A. M. B., and Brown, L. M., Phil. Mag. **15**, 797 (1967).

etching behavior of various twin boundaries and high and low energy stacking faults in epitaxial silicon<sup>6</sup> support the view that twin boundaries and perfect intrinsic twin stacking faults have a low energy. In the studies of Art et al.<sup>3</sup> the screw nodes in Ge were only extended after prolonged annealing. For short anneals most nodes were not extended at all. If anomalous diffraction effects were responsible for their observations, annealing should have no effect. Celli et al.<sup>7</sup> point out that long anneals may be necessary at screw nodes because dangling bonds must be manufactured when the dislocation dissociates.

Shockley partials at dissociated  $60^\circ$  and screw dislocations have free atomic bonds, but due to their small Burgers vector the smaller electron exchange interaction distance for covalent bonding should significantly reduce the "effective" number of free bonds. The result is that free bonds are created when screw dislocations dissociate and are probably reduced when  $60^\circ$  dislocations dissociate. The elastic repulsive force for dissociation of screws is about 1/2 that at  $60^\circ$  dislocations, and when formation of the free atomic bonds is considered, the lack of spontaneous dissociation of screws could be rationalized. On the other hand both elastic and, to a lesser extent, electronic effects favor dissociation of  $60^\circ$  dislocations.

Dissociated  $60^\circ$  dislocations in the diamond lattice are apparently more difficult to move than perfect ones and can account for Kabler's dislocation velocity measurements in germanium;<sup>8</sup> isolated  $60^\circ$  dislocations were found to move more slowly than screws and the activation energy decreases with increasing stress. The behavior is interpreted in terms of constriction and recombination of dissociated dislocations.<sup>9</sup> That similar results are not found by others is probably due to the fact that the scratch-velocity technique is not very reliable because the stress field on the leading dislocation can be several times the applied stress.<sup>10</sup>

The effects on the dislocation velocity of doping with acceptors or donors<sup>11,12</sup> has been attributed to the change of mobility of charged kinks on the dislocation line.<sup>13</sup> In these studies heavy doping with arsenic donors increases the dislocation velocity while gallium acceptors

<sup>6</sup> Mendelson, S., *J. Appl. Phys.* **39**, 2477 (1968).

<sup>7</sup> Celli, V., Kabler, M. N., Ninomiya, T., and Thompson, R., *Phys. Rev.* **131**, 58 (1963).

<sup>8</sup> Kabler, M. N., *Phys. Rev.* **131**, 54 (1963).

<sup>9</sup> Mendelson, S., these proceedings.

<sup>10</sup> Rosenfield, A. R., and Hahn, G. T., in *Dislocation Dynamics*, A. R. Rosenfield, G. T. Hahn, A. L. Bement, Jr., and R. I. Jaffee, Eds. (McGraw-Hill Book Co., 1968) p. 255.

<sup>11</sup> Patel, J. R., and Chaudhuri, A. R., *Phys. Rev.* **143**, 601 (1966).

<sup>12</sup> Patel, J. R., and Freeland, R. E., *Phys. Rev. Letters* **18**, 883 (1967).

<sup>13</sup> Frisch, H. L., and Patel, J. R., *Phys. Rev. Letters* **18**, 784 (1967).

decrease it. An alternative interpretation by Haasen<sup>14</sup> relates the effect to the change in dislocation line energy via the shear modulus. Arsenic concentrations at which the maximum velocity is found in Ge are reported to decrease  $C_{44}$  by 4.4%; this is consistent with the smaller separation of partials. Haasen also suggested that the effects might be related to changes in the electronic structure of dangling bonds at 60° dislocations. The results could also be related to electronic effects at dissociated dislocations. Since the 60° dislocations move slower than screws, their velocity would be controlling. The addition of arsenic donors should enhance acceptor formation by enhancing recombination of dissociated 60° dislocations; the reverse would be the case for additions of gallium acceptors.

ASHCROFT: I have another question about the expression you used for the Fermi energy. If you are in a two-band situation, which I think you have here—a dislocation band in the center of the gap—then I think that the number condition which leads to the Fermi energy should in fact involve an integration of the density of states in the dislocation band. That's one point . . .

HAASEN: A full theoretical explanation of this situation is given in a forthcoming paper by W. Schröter and R. Labusch in *Physica Status Solidi*.

ASHCROFT: Well, the second point is that part of your theories seem to come to grief at low temperatures, and I wonder whether it is because the expression you are using there is for the non-degenerate limit. When you get to very low temperatures you should then use the degenerate limit.

HAASEN: Right! If you go to a temperature at which the chemical acceptors are no longer ionized, then you have to use a different model. But, this temperature is far below our experimental range.

THOMSON: I have a question here. Do you, in your theoretical treatment, have what looks like a single band instead of two bands for the acceptors?

HAASEN: That's right. It's one single band. In the neutral condition it's half filled. The limit of occupation changes with the position of the Fermi level. This corresponds to donor or acceptor behavior of the dislocation, respectively.

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<sup>14</sup> Haasen, P., *J. De Physique, Colloque C3, Suppl. 7-8, 27, 30 (1966).*

# ELECTRONIC EFFECTS ASSOCIATED WITH STACKING FAULTS IN NORMAL METALS

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The authors use a simple pair interaction model to make the following calculations. (1) Stacking fault energy of simple metals. (2) Interaction energy between a stacking fault and an impurity atom or a vacancy, and application to the study of segregation effects. (3) Interaction energy of parallel stacking faults.

Numerical results are given. Consequences of the long range interaction between defects are discussed.

**Key words:** Dislocation-electron interactions; interatomic potentials; stacking faults.

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## I. Introduction

Relatively recent work has shown that, up to the second perturbation order, the total energy of a metal is accurately described by a pair interaction [1, 2, 3, 4, ]

$$E = E_0 + \frac{1}{2} \sum_{ij} E(\mathbf{r}_{ij}), \quad (1)$$

where  $E_0$  is independent of the position of the ions

$E(\mathbf{r}_{ij})$  is an effective interaction potential between ions at sites

$\mathbf{R}_i$  and  $\mathbf{R}_j$

$\mathbf{r}_{ij} = \mathbf{R}_i - \mathbf{R}_j$ .

To describe the effective interaction  $E(\mathbf{r}_{ij})$  we shall suppose that we know the pseudopotential  $w$  created by an ion of charge  $Z$  in a metal whose electronic density is described by the radius  $k_F$  of the Fermi sphere for free electrons, and assume that  $w$  depends only upon the distance  $r$  from the center of the ion. Such a pseudopotential  $w(r)$  has been shown to be the sum of the pseudopotential  $v(r)$  created by the bare ion and by a screening potential  $v_s$ . One has [5, 6]:

$$w(r) = v(r) + v_s(r) \quad (2a)$$

$$w(q) = v(q)/\epsilon(q) \quad (2b)$$

$$\epsilon(q) = 1 + (2k_F/\Pi q^2)g(q/2k_F) \quad (2c)$$

$$g(x) = 1 + [(1-x^2)/2x] \log [(1+x)/(1-x)]. \quad (2d)$$

where  $w(q)$  and  $v(q)$  are the Fourier transforms of  $w(r)$  and  $v(r)$ .

The bare ion pseudopotential can be approximated in different ways, e.g.:

- The point charge approximation where the ion is described as a point charge  $Z$ .
- More elaborate approximations where one takes into account the core electrons wave functions. We shall use here the results of Pick [7]. Although the expression is more elaborate in this case, it has been shown that for most of the applications one can use the same formulas as for the point charge approximation by replacing  $Z$  by an effective charge  $Z^*$ .

The interaction model has been used and thoroughly reviewed by many authors [1-7]. It has the advantage that it does not necessitate the use of adjustable parameters, but it suffers from a number of serious drawbacks which considerably reduce its applicability, in particular:

- Exchange and correlation interactions between conduction electrons are not taken into account; this limits the applicability of formulae 1 and 2 to the comparison of crystalline states with the same electronic densities.
- The wave functions overlap of core electrons is neglected, which limits the model to the case of normal metals. It is to be emphasized that the noble metals cannot be treated within the framework of this approximation.

Formulae (1) and (2), however, have been applied with success to the study of the stability of metals and to the calculation of their total energy [7]. Although less successful, the study of transverse phonon dispersion curves has given results in qualitative agreement with experiment [8, 9].

In this paper we shall make use of the model described by formulae (1) and (2) in the following way: In section II we shall calculate the varia-

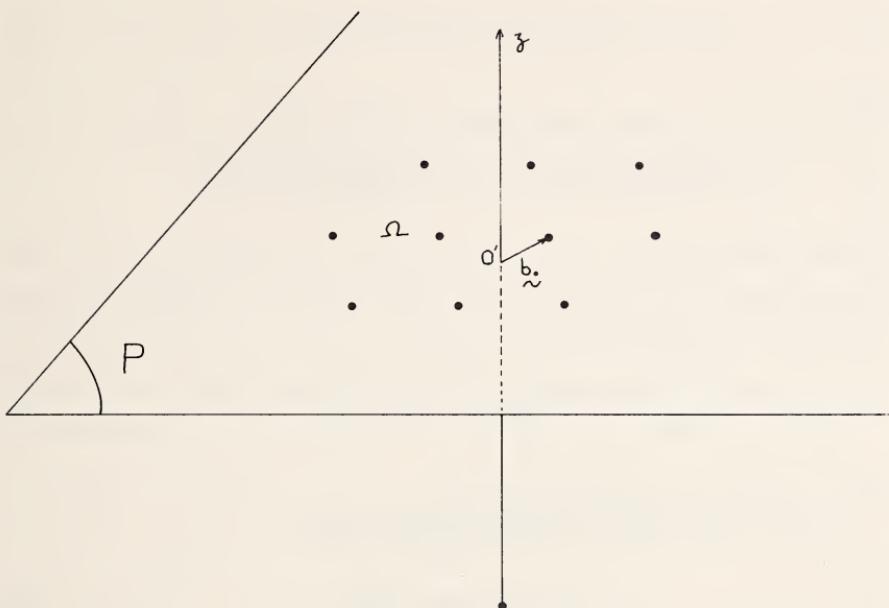


FIGURE 1. Interaction energy between an atom 0 and an atomic plane ( $P$ ). The atoms are the black spheres,  $0'$  is the projection of 0 on  $P$ ,  $\mathbf{b}$  has not been drawn but can be any vector of  $P$ .  $\Omega$  is the average area per atom in  $P$ .  $0'$  is on the  $0z$  axis.  $00' = d$ .

tion in the interaction energy of an atom and a plane lattice of atoms ( $P$ ) which ensues when the latter is shifted of a quantity  $\mathbf{b}$ ,  $\mathbf{b}$  being a vector, but not necessarily a lattice vector, of ( $P$ ) (fig. 1).

The results of this calculation will then be applied to the following cases:

- stacking fault energies of pure normal metals and their alloys (section III)
- Interaction of a point charge and a stacking fault and its relation to the Suzuki effect [10] (section IV)
- Long-range interaction between parallel faults and application to phase transformations (section V)
- An application of these results to loops in quenched Al will be given in section VI and the general conclusions in section VII.

## II. Interaction of an Atom With a Lattice Plane

### II.1. General formulation

It has been shown in a previous paper [11] that the variation of the effective interaction energy between an atom 0 and a plane lattice of atoms when the latter is sheared by a quantity  $\mathbf{b}$  (fig. 1) is given by:

$$\varphi(z) = (4\pi^2/\Omega^2) \sum_{\lambda \neq 0} e^{i\lambda \cdot \mathbf{b}_0} (e^{i\lambda \cdot \mathbf{b}} - 1) \psi(\lambda, z), \quad (3a)$$

$$\psi(\lambda, z) = \int_{-\infty}^{+\infty} e^{ikz} w[(k^2 + \lambda^2)^{1/2}] dk \quad (3b)$$

where  $\Omega$  is the area per atom in the sheared plane

$k$  is the component of the wave vector  $\mathbf{k}$  along  $00'$

$\lambda$  is the reciprocal lattice vector of the *plane* lattice.

From formula (2d) we see that  $g(x)$  has a singularity at  $x=1$  and the asymptotic form of  $\psi(\lambda, z)$  in eq (3b) is then an oscillatory function. This situation arises when

$$k^2 + \lambda^2 = 4k_F^2. \quad (4)$$

There will thus be two distinct cases:

$\lambda > 2k_F$ : the asymptotic form for (3b) is then:

$$\psi \propto z^{-2} \exp - 2k'_0 z \quad (5a)$$

$$4k'_0{}^2 = \lambda^2 - 4k_F^2. \quad (5b)$$

$\lambda < 2k_F$ : then the asymptotic form for (3b) is:

$$\psi \propto z^{-2} \sin 2k_0 z \quad (6a)$$

$$4k_0^2 = 4k_F^2 - \lambda^2. \quad (6b)$$

If one assumes the metal is close packed (f.c.c. or h.c.p., for example), one easily verifies that the first case corresponds to metals of valency smaller than

$$Z_c = 1.14. \quad (7)$$

The second case corresponds to the smallest  $\lambda$  for metals with valency larger than  $Z_c$ .

## II. 2. Monovalent metals and alloys $Z < Z_c$

The asymptotic form of the variation of the interaction energy is easily evaluated:

$$\varphi^*(nd) \simeq \alpha^* a' n^{-2} \exp - n\theta' \quad (8a)$$

$$a' = k_F^2 (2\Pi)^{-3} Z^{-2} [ (Zc/Z)^{2/3} - 1 ]^{1/2} \quad (8b)$$

$$\theta' = 2k_0' d \quad (8c)$$

$$\alpha^* = 2Z^{*2}/\Pi\epsilon^2 (2k_F) \text{ for a pure metal} \quad (8d)$$

$$z = nd, \quad (8e)$$

$d$  being the distance between close packed planes.  $\varphi^*(nd)$  is seen to decrease very rapidly with distance. (In what follows we shall use quantities  $\varphi^*$ ,  $\alpha^*$  corresponding to the use of  $Z^*$ . In all cases where  $Z^*$  is not known we shall make use of  $\alpha$  and  $Z$  corresponding to the value  $Z$  of the ions)

### II.3. Polyvalent metals and alloys $Z > Z_c$

$$\varphi^*(nd) \simeq \alpha^* a n^{-2} \sin n\theta \quad (9a)$$

$$a = k_F^2 (2\Pi)^{-3} Z^{-2} [1 - (Z_c/Z)^{2/3}]^{1/2} \quad (9a)$$

$$\alpha^* = 2Z^{*2}/\Pi\epsilon^2 (2k_F) \text{ for a pure metal} \quad (9c)$$

$$\theta = 2k_0 d \quad (9d)$$

$$z = nd. \quad (9e)$$

$\varphi^*(nd)$  decreases relatively slowly with distance.

## III. Stacking Fault Energies of Pure Metals [11]

### III.1. General formulae

Let  $\Gamma_{p\Delta}$  be the energy per unit surface of a  $p\Delta$  (or  $p\nabla$ ) stacking fault in a h.c.p. structure and  $\Gamma_m$ ,  $\Gamma_i$ ,  $\Gamma_e$  be the energy per unit surface of a twin boundary, an intrinsic fault, and an extrinsic fault respectively in a f.c.c. structure. Simple calculations then give:

$$\Gamma_{1\Delta} = \sum_{n=1}^{n=\infty} n \varphi^*(2nd) \quad (10a)$$

$$\Gamma_{2\Delta} = \sum_{n=1}^{n=\infty} n [2\varphi^*(2nd) - \varphi^*(2nd+d)] \quad (10b)$$

$$\Gamma_{3\Delta} = \sum_{n=1}^{n=\infty} [(2n+1)\varphi^*(2nd) - 2n\varphi^*(2nd+d)] \quad (10c)$$

$$\Gamma_m = \sum_{n=1}^{n=\infty} n [2\varphi^*(3nd) - \varphi^*(3nd-d) - \varphi^*(3nd+d)] \quad (11a)$$

$$\Gamma_i = \sum_{n=1}^{n=\infty} [3n\varphi^*(3nd) - (3n-1)\varphi^*(3nd-d)] \quad (11b)$$

$$\Gamma_e = \sum_{n=1}^{n=\infty} [(3n+1)\varphi^*(3nd) - 3n\varphi^*(3nd+d) - 2\varphi^*(3nd-d)]. \quad (11c)$$

Since the asymptotic form gives except for sodium a good approximation to the accurate value for the second nearest neighbour interaction, one can make use of formulae (8) and (9) to calculate (10) and (11).

### III. 2. Monovalent metals

Equations (8), (10), (11) yield the following results:

- Sums in eqs (11) and (10) can be replaced by their first term
- $\Gamma$  is negative for f.c.c. structures and positive for h.c.p. structure which is in agreement with experiment.

Numerical results are given in table 1.

TABLE 1. *Stacking fault energy for monovalent metals expressed in ergs cm<sup>-2</sup>.  
Stable phase h.c.p.*

The  $\Gamma$  are expressed in ergs cm<sup>-2</sup>

Metal	$\alpha^*$	$\alpha$	$\Gamma_{1\Delta}$	$\Gamma_{2\Delta}$	$\Gamma_{3\Delta}$
Li	0.40	0.39	2	4	6
Na	0.01	0.36	0.03	0.06	0.10
K	0.18	0.32	0.4	0.8	1.2
Ref	[7]	[11]	[11]	[11]	[11]

### III. 3. Divalent metals

For these metals eq (9), (10), (11) yield the following results:

- Sums in equation (10) and (11) must be evaluated up to  $n=20$ . This shows that atoms very far from the stacking fault “feel” its presence
- $\Gamma$  is negative for f.c.c. structure and positive for h.c.p. structure which is in agreement with experiment.

One can then calculate the sums (10) with the help of the following formulae:

$$\gamma_{1\Delta} = \frac{1}{2} \sum_1^{\infty} (2n)^{-1} \sin (2n\theta) \quad (12a)$$

$$\gamma_{2\Delta} = \sum_1^{\infty} [(2n)^{-1} \sin 2n\theta - (2n+1)^{-2} n \sin (2n+1)\theta] \quad (12b)$$

$$\gamma_{3\Delta} = \sum_1^{\infty} [(2n)^{-2} (2n+1) \sin 2n\theta - (2n+1)^{-2} 2n \sin (2n+1)\theta] \quad (12c)$$

$$\Gamma_{p\Delta} = \alpha^* a \gamma_{p\Delta}, \quad p = 1, 2, 3, \quad (12d)$$

— Numerical results are given in table 2. They show that stacking fault energies are rather high. In fact if one assumes that the stacking fault energy as given in table 2 can be used to describe an extended dislocation one sees that its width  $\delta$  would be smaller than  $2a$ .

TABLE 2. *Stacking fault energy for divalent metals expressed in ergs cm<sup>-2</sup>.  
Stable phase h.c.p.*

Metal	$\alpha^*$	$\alpha$	$\Gamma_{1\Delta}$	$\Gamma_{2\Delta}$	$\Gamma_{3\Delta}$	$c/a$	$\delta/a$	$\Gamma$ exp	Ref.
Be	2.38	1.91	390	760	1240	1.633	1.2		[12]
			403			1.856			[13]
Mg	.73	1.63	60	120	195	1.633	1	$280 \pm 100$	[12]
			60			1.625		$125 \pm 25$	[13]
Zn		1.79	195	395	630	1.633	0.5	$300 \pm 150$	[12]
			199			1.567			

However, when the splitting is so small the edge effects of the limiting dislocations must also be taken into account, the model of an infinite fault in an otherwise perfect crystal is inadequate.

The comparison with the experimental results indicated in the last column of table 2 is not in fact very significant, because the experimental values were obtained from measurements on the annealing of quenched vacancies loops [12, 13]. As shown previously [14] these results are difficult to interpret due to the lack of control of the experimental conditions, the dispersion of experimental results given in table 2 indeed confirms this point. In the case of zinc, we used the point charge approximation, the numerical results are, therefore, dubious.

### III. 4. Trivalent metal: the case of aluminum

In the case of aluminum, the stable phase is found to be f.c.c. in agreement with experiment. The sums (11) can be calculated with the help of the following formulae:

$$\Gamma_x = \alpha_a^* \gamma_x \quad x = m(\text{twin}), i(\text{intrinsic fault}), e(\text{extrinsic fault}) \quad (13a)$$

$$\gamma_m = \sum_1^{\infty} [(2/3n) \sin 3n\theta - n (3n-1)^{-2} \sin (3n-1)\theta - n (3n+1)^{-2} \times \sin (3n+1)\theta] \quad (13b)$$

$$\gamma_i = \sum_1^{\infty} [(3n)^{-1} \sin 3n\theta - (3n-1)^{-1} \sin (3n-1)\theta] \quad (13c)$$

$$\gamma_e = \sum_1^{\infty} [(3n+1)(3n)^{-2} \sin 3n\theta - 3n (3n+1)^{-2} \sin (3n+1)\theta - 2(3n-1)^{-2} \sin (3n-1)\theta]. \quad (13d)$$

TABLE 3. *Stacking fault energy of Al expressed in ergs cm<sup>-2</sup>. Stable phase f.c.c.*

$\alpha^*$	$\alpha$	$\Gamma_{in}$	$\Gamma_i$	$\Gamma_e$	$\Gamma_{i \text{ exp}}$
1, 70	4, 20	60	147	132	110
[7]	[11]				[15]

One needs to calculate the sums (13) up to a distance of 30 planes. The results are summarized in table 3. One notes that  $\alpha^*$  is about 0.4 and that the extrinsic stacking fault energy is about 10 percent lower than the intrinsic stacking fault energy. Comparison with experiment leads to comments similar to those developed in III. 2, but one notes that the agreement is quite good for aluminum. These results have been more or less described previously [11].

### III. 5. Alloys

The situation in dilute alloys can be described with the help of a very rough model, i.e., assuming point charges with an effective charge  $Z$  equal to the number valency electrons per atom and [11].

$$\alpha = (1-c)\alpha_{AA} + 2c(1-c)\alpha_{AB} + c^2\alpha_{BB}. \quad (14)$$

Irrespective of the value of  $\alpha$ , curves representing the situations for the sums (12) and (13) can be drawn (see figs. 6 and 7 of ref. [11]) and show

the limits of stability of phases. Assuming  $\alpha > 0$ , one obtains the results given in table 4.

TABLE 4. *Relative stability of f.c.c. and h.c.p. phase in normal alloys*

$Z$	1	1, 14	1, 27	1, 36	1, 66	2, 10	2, 29	3, 53 4
$\theta$ grad		0	100	135	200	270	290	400
H.C.				↔ Instable ↔			↔ Instable ↔	
C.F.C.		↔ Instable ↔		↔ Instable ↔		↔ Instable ↔		

The comments are the following:

- Noble metals base alloys *cannot* be described by the model, as pointed out in the introduction.
- The variation of stacking fault energy as a function of composition in alkali base alloys is not necessarily monotonic; these should be a discontinuity in the stacking fault energy, at least for  $2\Delta(2\Delta)$  and  $3\Delta(3\Delta)$  faults at the concentration  $Z_c$ .
- For divalent metal base alloys the sums 12 decrease with electron/atom ratio. This seems in contradiction with experimental results on the Cd Ag system, but as mentioned previously these alloys cannot be adequately described by the model.

## IV. Interaction of a Stacking Fault and a Point Charge

### IV.1. Interaction energy

We calculate the quantity  $\Delta W_1$ , the difference in energy between the two following cases (fig. 2):

- the energy of a matrix  $M$  of valency  $Z$  containing a stacking fault and a single impurity atom  $I$  of valence  $Z + Z'$ , at a distance  $z$  from the fault.
- the sum of the energy of the impurity atom alone in the perfect matrix and the stacking fault alone in the perfect matrix

$$W_1 = (W_{IM_{2t}} - W_{IM_2}) - (W_{MM_{2t}} - W_{MM_2}) \quad (15)$$

where  $M$  stands for an atom of the matrix lying at the same place as  $I$ .

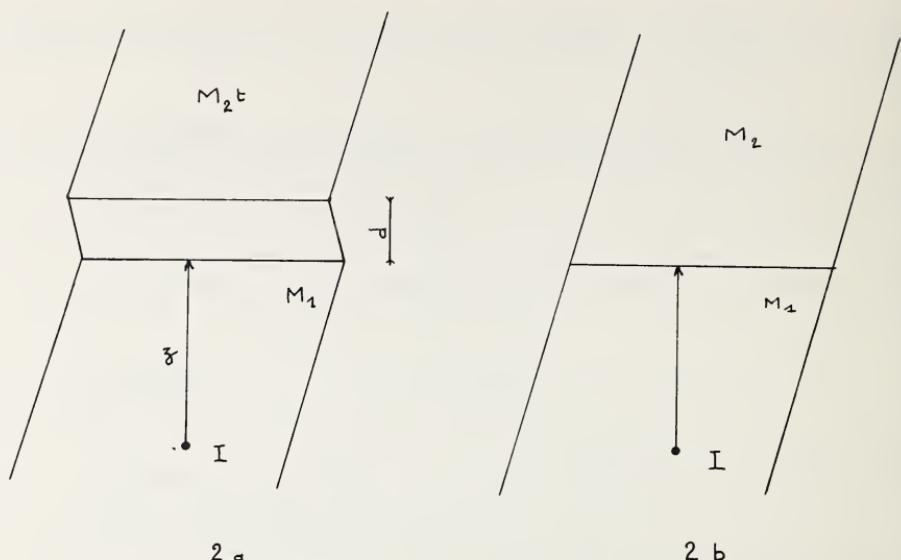


FIGURE 2. Definition of the interaction energy between an impurity atom and a stacking fault. a. The impurity atom I interacts with the part  $M_{2t}$  of the translated matrix. b. The impurity atom I interacts with the part  $M_2$  of the translated matrix. Interaction with part  $M_1$  are the same in both cases and cancel in formula 15.

These calculations are made using the point charge approximation for both the matrix and the impurity atom.

One then obtains the following formulae for the interaction of an intrinsic fault with one impurity atom in f.c.c. crystals:

$$\Delta W_1 = \Omega(Z'/Z) \left[ \sum_{m=k+1}^{m=\infty} \varphi(3md) - \sum_{m=k+2}^{\infty} \varphi(3md-d) \right] z = 3kd + 2d \quad (16a)$$

$$\Delta W_1 = \Omega(Z'/Z) \sum_{m=k+1}^{m=\infty} \left[ \varphi(3md) - \varphi(3md-d) \right] \quad z = 3kd + d \quad (16b)$$

$$z = 3kd$$

( $z$  is the distance between the impurity atom and the fault plane), and similar formulae for the interaction of  $1\Delta$  ( $1\nabla$ ) fault and one impurity atom in h.c.p. crystals:

$$\Delta W_1 = \Omega(Z'/Z) \sum_{m=k+1}^{m=\infty} \varphi(2md) \quad z = 2kd \quad (17a)$$

$$\Delta W_1 = 0 \quad z = 2kd + d. \quad (17b)$$

For hexagonal metals the distance  $z$  is counted from the top of the fault. The results are summarized in table 5. They show a long-range oscillatory interaction, the maximum binding energy  $\Delta E_1$  occurs when the impurity atom is close to the plane, but its value depends on the sign of  $Z'$ .

TABLE 5. *Interaction energy between a point charge and a stacking fault*

$Z' = -1 \quad \Delta E_1 (10^{-2} \text{ eV})$

$z/d$	0	1	2	3	4	5	6	7	8	20
Trivalent	-3.7	-3.7	2.5	-0.2	-0.2	-0.28	0.19	0.19	-0.17	0.03
Divalent $C/a = 1.633$	-4.6	0	0.65	0	0.3	0	-0.22	0	-0.05	0.03

TABLE 6. *Comparison of the binding energy of a solute atom with a stacking fault and the difference in dissolution of the same atom in a f.c.c. and h.c.p. phase ( $Z' = -1$ ).*

	Binding energy ( $10^{-2} \text{ eV}$ )	$\Delta E_2 (10^{-2} \text{ eV})$
Trivalent Al	-3.7	-8
Divalent $C/a = 1.633$	-4.6	-9

The binding energy can be compared with the difference in dissolution energy  $\Delta E_2$  in h.c.p. and f.c.c. planes calculated with the same approximation (see appendix 1). From table 6, one sees that:

$$\Delta E_2 \approx 2\Delta E_1. \quad (18)$$

The case of monovalent non-noble metals leads to no long range interaction.

#### IV. 2. Application

The above evaluations can be used to describe qualitatively the situation in dilute alloys. Let us examine first the case of a dilute alloy con-

taining a very large stacking fault, from the results of IV. 1, one can conclude that:

- Segregation will occur not only on the plane of the fault but on several parallel planes. The so called Suzuki effect [10] cannot therefore be described by simple thermodynamic theories describing the system after segregation as a two-phase system [10, 16, 17, 18]. In fact, one should study a system with an average charge per atom varying with the distance from the fault. Due to the crudeness of the model such a calculation can give only qualitative results and is not worth the effort. Similar conclusions apply for the study of the kinetics of segregation.
- Such a segregation gives an appreciable frictional force (of the order of  $10^{-3} \mu$ ) on dislocations moving on planes which are not parallel to the fault (fig. 3).

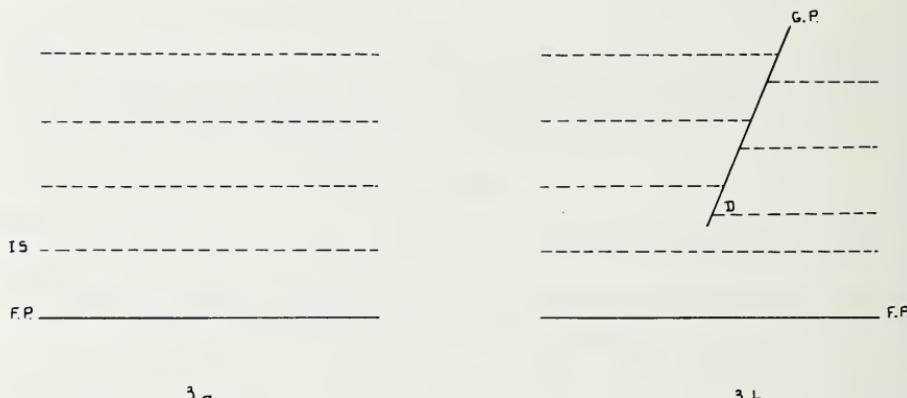


FIGURE 3. a. Stacking fault (F.P.) with segregated impurity atoms I.S. — — —. b. Same situation after a dislocation  $D$  has moved on a glide plane G.P. cutting the fault.

- These results do not apply to extended dislocations of small width. It must be emphasized however, that a long range oscillatory behavior exists even in this case, as will be seen in the conclusion.

## V. Parallel Stacking Faults in Polyvalent Metals (Fig. 8)

Since the electronic perturbation caused by a stacking fault is a long-range one, parallel stacking faults or parallel twin boundaries interact with each other. The formulae are given in appendix 2 and the results calculated in the point charge approximation are shown in figures 4-7 for the following cases:

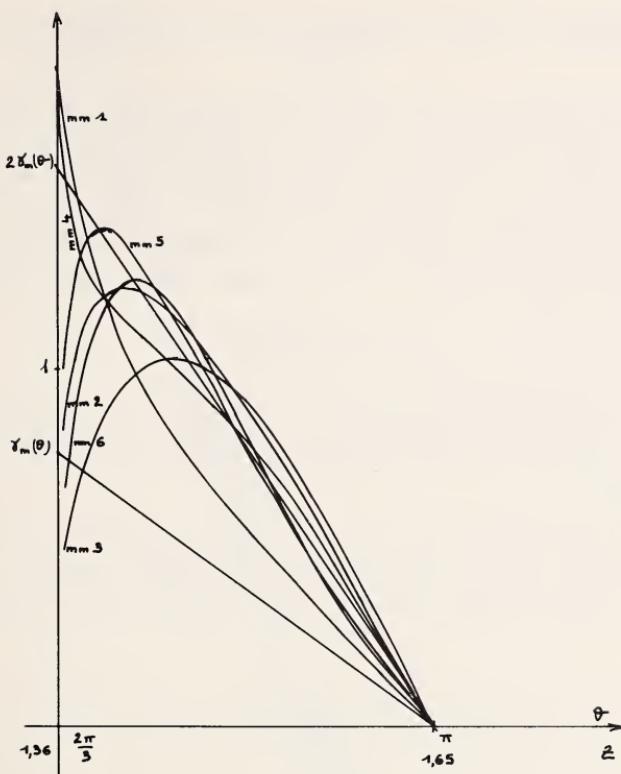


FIGURE 4. Energy of a twin lamella  $\gamma_{mmn}$  of width  $n=1$  to 6 interplanar distances for  $1.36 < Z < 1.65$ . The results for  $1.65 < Z < 2.1$  are obtained by turning the figure upside down, as the energies  $\gamma_m$  and  $2\gamma_m$  of a single twin boundary energy and of two twin boundaries at infinite distance have been plotted. (Arbitrary units).

- parallel twin boundaries in f.c.c. metals and alloys referred to as  $\gamma_{mm}$  (figs. 4 and 5).
- parallel intrinsic faults in f.c.c. metals and alloys referred to as  $\gamma_{ii}$  (figs. 6 and 7).
- parallel in  $1\Delta$  faults in divalent metals.

One can verify that far from the limits corresponding to  $Z = 1.36, 2.09$ , the difference.

$\Delta E_3$  = Energy of a pair of faults — twice the energy of a fault (e.g.,  $\gamma_{ii} - 2\gamma_i$ ) is rather small, of the order of at most 10 percent.

On the contrary, close to the boundaries the interaction energy varies very rapidly with electron per atom ratio, and with the distance this agrees with the fact that such structures are not stable and that structure with periodic stacking faults occur. Calculation shows that periodically faulted structures are more stable in this range of electronic densities [19].

## VI. Application to the Segregation of Vacancies on Stacking Faults

The previous results can be applied to the simple case of superimposed loops appearing in quenched Al [20]. Describing a vacancy in a metal as a point charge  $Z' = -Z$ , one can easily check from table 6 that vacancies will segregate just above the plane of the fault. In that case nucleation of a second stacking fault on the first one is helped by the fact that the extrinsic (double) fault energy is lower than the intrinsic fault energy.

## VII. Conclusion

A simple model for calculating the energy of defects has been shown to give semiquantitative agreement with experiment and describes reasonably well the effects associated with stacking faults in pure normal metals and their alloys.

Although this model, as it is, is too naive to describe the situation in complex metals such as noble metals or transition metals, it must be emphasized that the main physical fact underlying this model is the

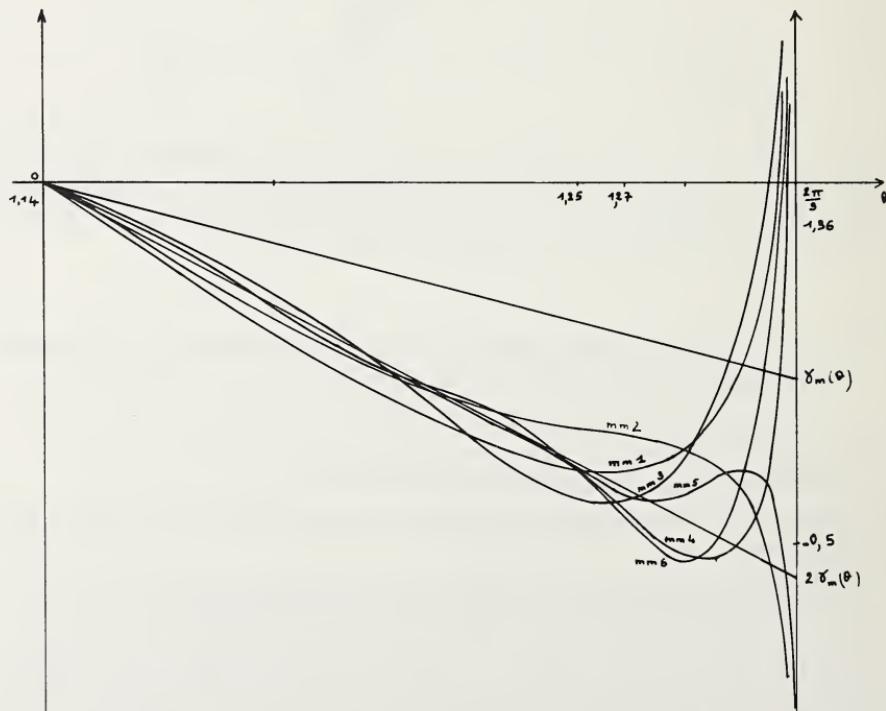


FIGURE 5. Same as figure 4, but with a different scale for  $2.09 < Z < 3.53$  or  $0 < Z < 1.36$ . (Arbitrary units).

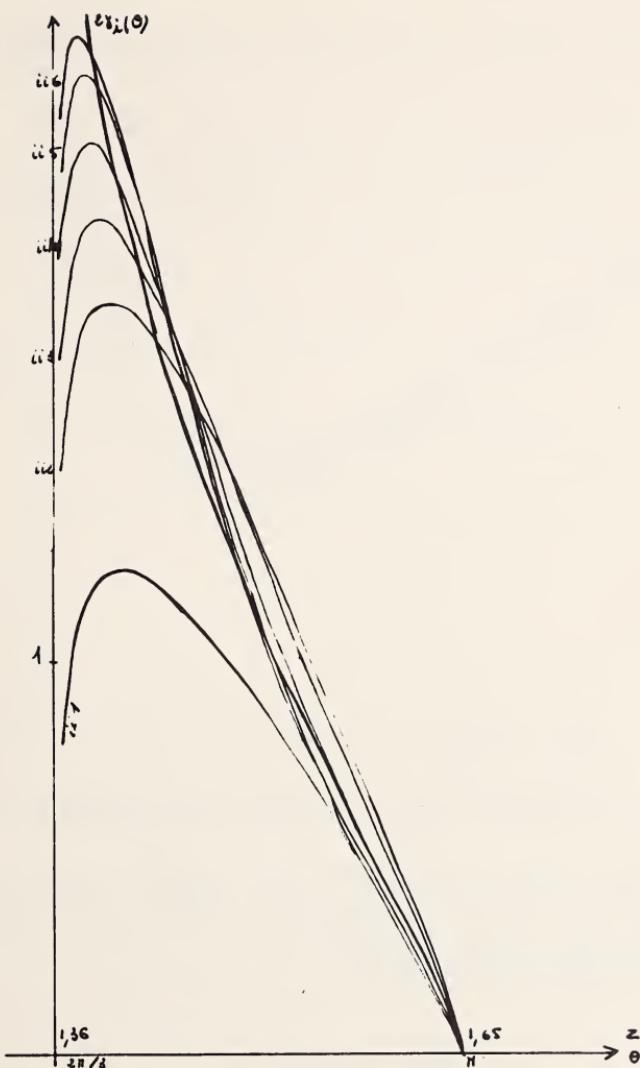


FIGURE 6. Figure for a pair of intrinsic faults in f.c.c. metals. For other data see caption of figure 4. (Arbitrary units).

long-range oscillatory interaction between two perturbations in an electron gas [21]. This interaction results in fact from the existence of a Fermi surface in metals.

Therefore the main qualitative facts analyzed in this paper certainly exist in more complicated metals. Among them we would like to point out that:

- Precipitation of vacancies on an extended fault gives multiple faults as observed in Al or Mg rather than *climb* of the fault, or tetrahedron growth as observed for example in gold, this suggests

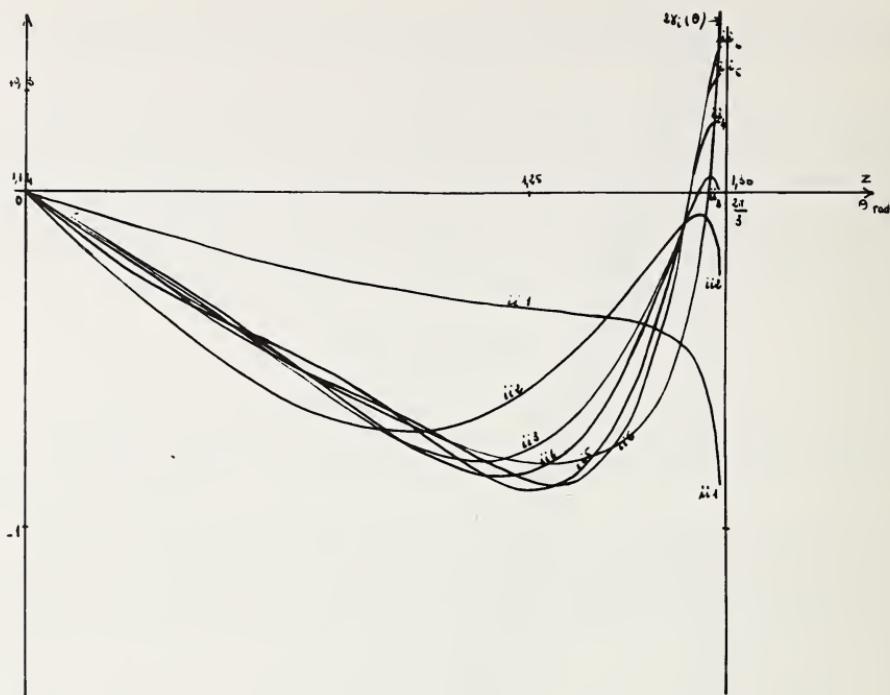


FIGURE 7. Figure for a pair of intrinsic faults in f.c.c. metals. (Arbitrary units).

very strongly that the sign of interaction is different in the latter case.

—strong negative interaction energy between parallel faults will make them easy to nucleate and to propagate. This suggests that such interaction play an important role at least in some case of martensitic transformations.

### VIII. Appendix 1

The difference in dissolution energy  $\Delta E_2$  for an impurity atom in an HCP phase and in a FCC phase is easily shown to be:

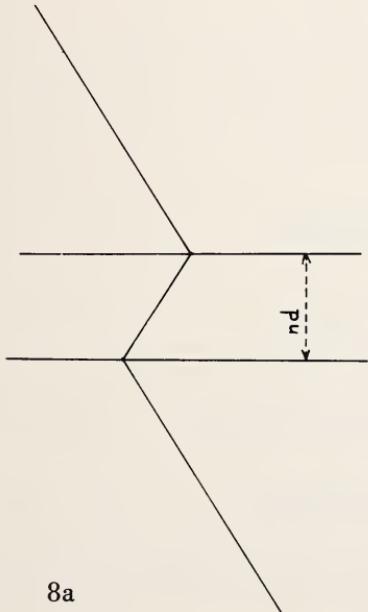
$$\Delta E_2 = 2\Omega(Z'/Z) \sum_{p=0}^{p=00} \left\{ -\varphi[(6p+2)\theta] + \varphi[(6p+3)\theta] - \varphi[(6p+4)\theta] \right\}.$$

### IX. Appendix 2

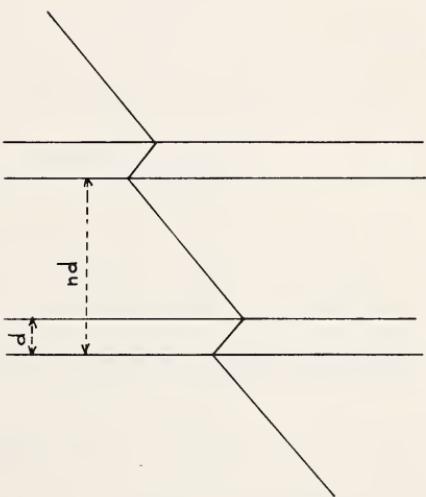
Formulae for the calculations of the sums for the case of FCC metals.  $\gamma_{mm} (nd)$  stands for the energy of a twin lamella of width  $nd$ ,  $\gamma_{ii} (nd)$

stands for the energy of a pair of intrinsic stacking faults whose distance is  $nd$  (see fig. 8).

$$\begin{aligned}\gamma_{mm}(3kd+d) &= \sum_{n=1}^k [(n-k-1)\varphi(3n\theta-\theta) + (n-k)\varphi(3n\theta) - 2(n-k)\varphi(3n\theta+\theta)] \\ &\quad + \sum_{n=1}^{\infty} [-(3n-k-1)\varphi(3n\theta-\theta) + (3n+k)\varphi(3n\theta) \\ &\quad - 2k\varphi(3n\theta+\theta)] \\ \gamma_{mm}(3kd) &= \sum_{n=1}^{k-1} [-2(n-k)\varphi(3n\theta-\theta) + 4(n-k)\varphi(3n\theta) \\ &\quad - 2(n-k)\varphi(3n\theta+\theta)] + \sum_{n=1}^{\infty} [-2k\varphi(3n\theta-\theta) \\ &\quad + 4k\varphi(3n\theta) - 2k\varphi(3n\theta+\theta)]\end{aligned}$$



8a



8b

FIGURE 8. a. Twin lamella of width  $z = nd$  in a f.c.c. structure. b. Parallel stacking faults at a distance  $nd$  in a f.c.c. structure.

$$\begin{aligned}\gamma_{mm}(3kd-d) &= \sum_{n=1}^{k-1} [-2(n-k)\varphi(3n\theta-\theta) + (n-k)\varphi(3n\theta) \\ &\quad + (n-k+1)\varphi(3n\theta+\theta)] + \sum_{n=1}^{\infty} [-2k\varphi(3n\theta-\theta) \\ &\quad + (3n+k)\varphi(3n\theta) - (3n-k+1)\varphi(3n\theta+\theta)]\end{aligned}$$

$$\begin{aligned}
 \gamma_{ii}(3kd+d) = & \sum_{n=1}^k [-(6n-6k-4)\varphi(3n\theta-\theta) + (3n-3k-1)\varphi(3n\theta) \\
 & + (3n-3k)\varphi(3n\theta+\theta)] + \sum_{n=1}^{\infty} [-(6k+2)\varphi(3n\theta-\theta) \\
 & + (3n+3k+1)\varphi(3n\theta) - (3n-3k)\varphi(3n\theta+\theta)] \\
 \gamma_{ii}(3kd) = & \sum_{n=1}^k [-(6n-6k-2)\varphi(3n\theta-\theta) + (3n-3k)\varphi(3n\theta)] \\
 & + \sum_{n=1}^{k-1} (3n-3k+1)\varphi(3n\theta+\theta) + \sum_{n=1}^{\infty} [-6k\varphi(3n\theta-\theta) \\
 & + (3n+3k)\varphi(3n\theta) - (3n-3k+1)\varphi(3n\theta+\theta)] \\
 \gamma_{ii}(3kd-d) = & \sum_{n=1}^{k-1} [-(6n-6k)\varphi(3n\theta-\theta) + (3n-3k+1)\varphi(3n\theta) \\
 & + (3n-3k+2)\varphi(3n\theta+\theta)] + \sum_{n=1}^{\infty} [-(6k-2)\varphi(3n\theta-\theta) \\
 & + (3n+3k-1)\varphi(3n\theta) - (3n-3k+2)\varphi(3n\theta+\theta)].
 \end{aligned}$$

Formulae of the same kind are obtained for two  $1\Delta$  faults in HCP metals:

$$\begin{aligned}
 \gamma_{ii}(2kd-d) = & \sum_{n=1}^{n=k} (n-k)\varphi(2n\theta-\theta) \\
 & + \sum_{n=1}^{n=\infty} [2n\varphi(2n\theta) - (n-k)\varphi(2n\theta-\theta)] \\
 \gamma_{ii}(2kd) = & 2 \sum_{n=1}^{n=k} (n-k)\varphi(2n\theta) + 2k \sum_{n=1}^{n=\infty} \varphi(2n\theta)
 \end{aligned}$$

$z$  being the distance between the mid planes of the faults.

## X. Acknowledgements

The authors are glad to thank Dr. Friedel and Dr. Déplanté for fruitful discussions.

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# **THEORY OF SURFACE STATES ON STACKING FAULTS**

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The Slater-Koster method in the Bloch representation is applied to a model for a stacking fault in an idealized crystal leading to a type of Shockley surface state. A series expansion is obtained for the energy which is worked out for the simplified case of a constant matrix element, with the result that for a tight binding nonoverlapping band, there are surface waves which split off from both the top and bottom of the band. Contrary to Shockley's results for external surfaces, and to the Slater-Koster theory of the localized impurity, localized states occur on the stacking fault for a single nonoverlapping band and for arbitrary potential values. A constant matrix approximation is worked out for the case of the simple metals.

**Key words:** Dislocation-electron interactions; Slater-Koster method; stacking fault.

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## **I. Introduction**

The purpose of this paper is to work out some aspects of a simple model of the surface state on a stacking fault. Previous theoretical attention regarding the stacking fault has centered either on the energy of the fault [1] or its scattering [2].

Our motivation for looking in more detail at the surface state is the realization that for certain types of problems, the surface state and its localized wave function are the important considerations. The first example is in the case of semi-conductors, where speculation about trapping states introduced on dislocations has a long history [3]. Amelynckx and co-workers [4] claim that dislocations in Si and Ge are split, although more recently some workers have disputed this result. Nevertheless, the original dangling band model of this state is very open to doubt since screw dislocations have been shown to possess trapping states also [5]. Thus, the possibility of a stacking fault on the screws makes the stacking fault a possible model for the seat of this bound state.

Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough, Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

The second area of special interest for a surface state lies in the impurity interaction with stacking faults originally proposed by H. Suzuki [6]. Even though a neutral imperfection, if the stacking fault possesses a surface state, the localization of charge will cause local oscillations in charge density similar to those about a charged impurity, and these fluctuations can be the cause of significant impurity interaction with the stacking fault.

The model calculation carried out here will provide qualitative rather than quantitative insight into these problems. Nevertheless, the results suggest that a bound surface state is to be expected quite generally on a two-dimensional break in translational symmetry such as a stacking fault or a twin, and our model calculation serves as point of departure for more detailed numerical work.

In this paper, we shall work from the Slater-Koster theory, according to which a localized or a bound state is expected when the determinantal equation

$$|1 - gV| = 0 \quad (1)$$

has a solution [7]. If  $H_0$  is the hamiltonian of the perfect crystal, and  $H$  is that of the imperfect crystal, then  $V$  is the operator

$$V = H - H_0. \quad (2)$$

The Green's matrix is defined by

$$g = \{E - V_0\}^{-1}, \quad (3)$$

where  $E$  is the total energy of the problem, and in this case, the energy of the bound state. In the usual application of this formalism,  $V$  is a localized perturbation, and the Wannier representation is introduced so that only a few nonzero components  $V_{ik}$  need be considered. However, in our case, the stacking fault is by no means localized, since the long-range order of the crystal has been completely destroyed, and we shall therefore prefer to remain in the Bloch representation.

## II. The Surface States on the Stacking Faults

Our point of departure is to note that, in the face-centered packing arrangement, there is no strain or distortion of an elastic variety at a stacking fault. All the nearest neighbor arrangements around an atom at the stacking fault are correct except for a rotation of atoms from the "C" to "A" positions in the close packed arrangement. The local potential of an electron within its Wigner-Seitz cell should then suffer a negligible perturbation.

Nevertheless, the basic translational symmetry of the crystal at the stacking fault is completely destroyed, and indeed the actual perturbation,  $V$ , is large in every cell on one side of the fault relative to the crystal on the other side as shown in figure 1. Our attention is thus focused on the effect of a change in the basic periodicity of the crystal introduced by the stacking fault, in a rigid ion approximation. For large changes in ion position, some change in the local ion potential occurs, and some elastic distortion is present; however, this restricted model is all we consider here.

According to our model,  $V(x)$  will be zero for  $x < 0$  and is a periodic function of  $x$ ,  $y$ , and  $z$  for  $z > 0$ , with the period of the crystal itself. (See figure 1.) Further, in the standard manner, we assume  $V(x)$  to be composed of a superposition of individual ion pseudo-potentials,  $v(x - R_n)$ , where  $V(x) = \sum_n v(x - R_n)$ , the sum to be evaluated only over the faulted half of the crystal.

We first prove that the diagonal components of this perturbation matrix are strictly zero. The proof follows from an inspection of the rigidly displaced whole crystal (as contrasted with our case where only half the crystal is rigidly displaced). For the whole crystal, the perturbation potential is periodic everywhere; the function for  $z > 0$  is exactly the same as in figure 1, but has now been extended uniformly to  $z < 0$ . In standard fashion, the matrix element between the two Bloch functions  $\psi_k(x)$  is broken into atomic and structure factors, where  $RD$  here stands for rigidly displaced crystal.

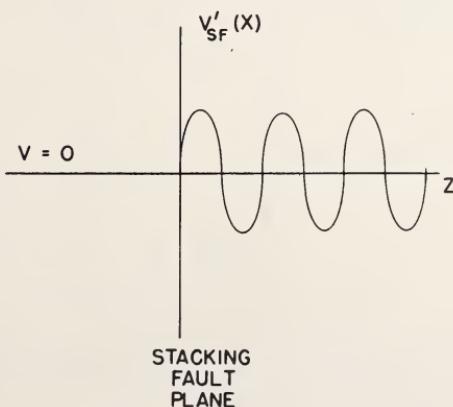


FIGURE 1. Schematic diagram of the assumed form of the perturbing potential for a two dimensional fault in the crystal. The figure shows the potential along a line perpendicular to the fault. It shows a perfectly periodic structure to the right of the fault and a strictly zero value to the left.

$$\begin{aligned}
 (k'|V|k)_{RD} &= \int \psi_{k'}^*(\mathbf{x}) V_{RD}(x) \psi_k(\mathbf{x}) d\mathbf{x} \\
 &= \int \psi_{k'}^*(\mathbf{x}) v(\mathbf{x}) \psi_k(\mathbf{x}) d\mathbf{x} \sum_R e^{-i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}} \\
 &= N v_{k'k} \delta_{k' - k, K}
 \end{aligned} \tag{4}$$

where again  $v(x)$  is the individual pseudo-potential of the atom at the origin. The wave functions in  $v_{k'k}$  are normalized to a single cell, and  $N$  is the number of sites in the (cubic) crystal.  $\mathbf{K}$  is a reciprocal lattice vector. But since the diagonal elements of  $V_{k'k}$  are the first order changes in energy of the crystal system, they must be exactly zero, since the displaced crystal must have precisely the same energy spectrum as the original crystal. Hence  $V_{k'k} = 0$  for  $\mathbf{k}' - \mathbf{k} = \mathbf{K}$ . We have operated for simplicity with a simple cubic system in (4) since our theory will not here be applied to a specific band structure, but the appropriate lattice basis with the corresponding generalization of (4) can easily be supplied in this as well as the following equations.

For the faulted crystal, there is a similar expression,

$$\begin{aligned}
 (k'|V|k)_{SF} &= \int \psi_{k'}^*(\mathbf{x}) V(\mathbf{x}) \psi_k(\mathbf{x}) d\mathbf{x} \\
 &= N^{2/3} v_{k'k} \sum_{z>0} e^{-i(k'_z - k_z)z} \delta_{k'_x - k_x, K_x} \delta_{k'_y - k_y, K_y}.
 \end{aligned} \tag{5}$$

$V(x)$  is the function of figure 1 and the sum is over the half space to the right of the fault, but  $v_{k'k}$  is the same matrix as in (4), and the diagonal elements must be zero as before,  $v_{kk} = 0$ . The only non zero elements are for  $\mathbf{k}' - \mathbf{k} \neq \mathbf{K}$ . For a simple cubic crystal with lattice spacing  $a$ , the sum over the lattice points  $z > 0$  gives the structure factor

$$\sum_{z>0} e^{-k\kappa z} = \Delta_+(\kappa) = \begin{cases} L/2, \kappa = 0, \\ 0, \kappa = \frac{2\pi n}{La}, n \text{ even}, \\ \frac{2}{e^{i\kappa a} - 1}, n \text{ odd}. \end{cases} \tag{6}$$

$$\kappa = k'_z - k_z, \quad L = aN^{1/3}.$$

Since we shall wish to carry out integrations over smooth functions and  $\Delta_+(n)$  is a highly discontinuous function in  $k$ -space, we shall introduce a smoothed counterpart to  $\Delta_+$  and define

$$\begin{aligned}
 \Delta_+(\kappa) &= L/2, \quad \kappa = 0 \\
 &= \frac{1}{e^{i\kappa a} - 1}, \quad \kappa \neq 0.
 \end{aligned} \tag{7}$$

The structure factor,  $\Delta_+(\kappa)$ , is the crystal analogue of the function  $\delta_+(\kappa)$ , as the kronecker  $\delta_{k'k}$  is the discrete analogue of  $\delta(\kappa)$ .

$$(k'|V|k) = v_{k'k} \Delta_+(\kappa) \delta_{k'k} \delta_{k'yk_y} \quad (8)$$

### III. Green's Function Solution of Stacking Fault

The determinantal equation, (1), of the Slater-Koster formalism in the Bloch representation now takes the form

$$0 = D = \begin{vmatrix} 1 & g_1 V_{12} & g_1 V_{13} & \dots \\ g_2 V_{21} & 1 & g_2 V_{23} & \dots \\ g_3 V_{31} & g_3 V_{32} & 1 & \dots \\ \dots & \dots & \dots & \dots \\ \dots & & & \dots \end{vmatrix} \quad (9)$$

As mentioned previously, we shall remain in the Bloch representation. The reason is that even though  $V$  is not limited to a few matrix elements, at least the matrix of  $g$  is diagonal in this representation.

This determinant may be expanded straight forwardly by permutations,

$$D = \sum_p (-1)^p R_1^{j_1} R_2^{j_2} \dots R_N^{j_n}, \quad (10)$$

where  $R_i^{j_i}$  is the element of the first row, etc. In this expansion, the zeroth permutation is simply the product of all the diagonal elements of  $D$ , and is unity. The first permutation gives quadratic terms in the matrix elements,  $V_{ij}$ , and  $g$ , and in general (10) leads naturally to an expansion in various powers of  $V_{ij}$ . If we group together all the terms in the zeroth powers of  $V_{ij}$ , calling that sum  $D_0$ , all the terms quadratic in  $V_{ij}$  together into  $D_2$ , etc., then to fourth order.

$$D = D_0 + D_1 + D_2 + \dots + D_N,$$

$$D_0 = 1,$$

$$D_1 = 0,$$

$$D_2 = - \sum_{i < j} g_i g_j |V_{ij}|^2,$$

$$D_3 = 2 \sum_{i < j < k} g_i g_j g_k \operatorname{Re} \{V_{ij} V_{jk} V_{ki}\},$$

$$D_4 = \sum_{j < k < l} g_k g_l |V_{kl}|^2 \sum_{i < j} g_i g_j |V_{ij}|^2$$

$$- 2 \sum_{i < j < k < l} g_i g_j g_k g_l [\operatorname{Re} \{V_{ij} V_{jk} V_{kl} V_{li} + V_{ik} V_{ji} V_{kl} V_{lj}$$

$$+ V_{ik} V_{jl} V_{kj} V_{li}\}]. \quad (11)$$

Replacing the summations by integrals over  $k_i, k_j, \dots$  —space, and noticing the complete symmetry between the arrangement  $g_1 g_2 |V_{12}|^2$  and  $g_2 g_1 |V_{21}|^2$ , this becomes:

$$\begin{aligned}
 D_2 &= -\frac{1}{2} \int \int g(i)g(j)|V(ij)|^2 didj , \\
 D_3 &= \frac{1}{3} \int \int \int g(i)g(j)g(k)[\text{Re} \{V(ij)V(jh)V(ki)\}] didj dk , \\
 D_4 &= -\frac{1}{4} \int \int \int \int g(i)g(j)g(k)g(l)[1/3 \text{Re}\{V(ij)V(jk)V(kl)V(lj) \\
 &\quad + V(ik)V(ji)V(kl)V(li) + V(ik)V(jl)V(kj)V(li)\}] didj dk dl. \tag{12}
 \end{aligned}$$

The general rule for finding the terms in  $D_n$  can be developed by looking at the partitions or classes of the permutation group in the total determinant expansion, (10).  $D_2$  corresponds to the partition  $(1^{N-2}, 2^1)$ .  $D_3$  corresponds to  $(1^{N-3}, 3^1)$ .  $D_4$  corresponds to two partitions,  $(1^{N-4}, 2^2)$  and  $(1^{N-4}, 4^1)$ . The numerical factors in front of the integrands in (12) are identical to the corresponding numerical factors in the total number of elements in the class or partition concerned. The number of terms in the sums in (11) is exactly the same as the number of permutations in the corresponding partition. In going from the sum, (11), to the integral, (12), we first write the products and integrate without regard to equivalent ways to write the same permutation, then divide by the factor which counts the number of equivalent permutations. This factor is obtained by the same reasoning which leads to the factor dividing  $N$  in the formula for this number of permutations belonging to a given partition. Thus the number of different permutations in the partition  $(1^{N-3}, 3^1)$  is

$$\frac{N(n-1)(N-2)}{3} \simeq N^3/3,$$

the number of terms in the partition  $(1^{N-4}, 2^2)$  is  $N!/(N-4)!2^3 \simeq N^4/8$ , etc.

#### IV. Constant Matrix Approximation

The form of the solution (12) is perfectly general, but will require considerable numerical labor if applied to a specific crystal and band structure. Inspection of (12) shows that the greatest simplification would result if we could simply replace all the matrix elements by their average values. Because it is possible to obtain the results in nearly closed form in this case, we shall work it out in some detail. We leave to later paragraphs a

discussion of how adequate this approximation is. We shall therefore assume

$$V_{k'k} \simeq V, \quad (13)$$

$k' \neq k.$

Combining (13) and (12), (1) then becomes

$$1 - 1/2G^2V^2 + 1/3G^3V^3 - 1/8G^4V^4 = 0 \quad (14)$$

if  $V$  is real and where

$$G = \int g(k) dk = \int \frac{dk}{E - E(k)}. \quad (15)$$

The integration variable,  $k$ , now is the  $z$ -component of the three-dimensional  $k$ -vector.  $G$  is the one-dimensional integrated Green's function and  $E(k)$  depends parametrically on  $k_x$  and  $k_y$ . If a tight binding form is assumed for the density of states in order to get a closed expression,

$$E(k) = E_0(k_x, k_y) + \delta \cos ka, \quad (16)$$

then standard methods give

$$G = \begin{cases} -\frac{1}{\epsilon^2 - \delta^2}, & \epsilon < -\delta, \\ -\frac{i}{\delta^2 - \epsilon^2}, & -\delta < \epsilon < \delta, \\ \frac{1}{\delta^2 - \epsilon^2}, & \epsilon > \delta, \end{cases} \quad (17)$$

$$\epsilon = E - E_0(k_x, k_y). \quad (18)$$

With the substitution  $(\epsilon^2 - \delta^2)/V^2 = y$ , (14) becomes

$$y^2 - 1/2y - 1/3 \sqrt{y} - 1/8 = 0,$$

which has the solution  $y \simeq 0.968$ , or

$$\epsilon = -\sqrt{\delta^2 - 0.968V^2} \quad \epsilon < \delta \quad (19)$$

for the branch of  $G$  for which  $\delta > \epsilon$ . For the branch where  $\epsilon > \delta$ , the same substitutions lead to

$$y^2 - 1/2 y + 1/3 \sqrt{y} - 1/8 = 0,$$

which has the solution  $y \approx 0.30$  and

$$\epsilon = +\sqrt{\delta^2 + 0.30V^2}, \quad \epsilon > \delta. \quad (20)$$

Thus for each value of the pair  $(k_x, k_y)$ , one state is introduced below the sub band, and one state above the band, independent of the sign of  $V$ . This result is general for all orders under the approximation (13). We also note that contrary to the situation for a point defect in a three dimensional crystal, a sub band of bound states *always* appears, independent of the strength of  $V$ , because  $G$  corresponds to the one dimensional Green's function. For the two-dimensional fault, the band of levels corresponds to a bound state which can have various amounts of kinetic energy of translation parallel to the fault.

## V. Metals

We turn now to the question of how valid a constant matrix element approximation might be. Excluding the structure factor, the matrix element is

$$v_{k'k} = \int \psi_{k'} v(\mathbf{x}) \psi_k d\mathbf{x}, \quad (21)$$

where  $v(x)$  is the perturbation potential in a rigid ion displacement of one of the ions of the crystal. In first order in a Taylor series this is

$$v(x) = \mathbf{b} \cdot \nabla u(x), \quad (22)$$

where  $\mathbf{b}$  is the stacking fault displacement, and  $u(x)$  is the one electron potential of one ion of the perfect crystal.

In this form we recognize the close connection to electron transport theory in metals, and can adopt the calculation of the matrix elements from that theory. Following Sham and Ziman [8] (see their equations (10.2) and (14.4)), we have

$$v_{k'k} = i \mathbf{b} \cdot \mathbf{q} \left\{ \frac{-2/3\epsilon_f + U_0(q^2/k_s^2)}{1 + q^2/k_s^2} \right\} J(qr_s),$$

$$J(x) = 3(\sin x - x \cos x)/x^3, \quad (23)$$

$$\mathbf{q} = \mathbf{k}' - \mathbf{k}.$$

$k_s$  is the screening parameter,  $4\pi e^2 \eta(\epsilon_f)$ , which is of the order of a lattice

constant for simple metals. In this equation, we have neglected the orthogonalization of the OPW wave function to the core electrons.  $U_0$  is the difference between the Hartree-Fock potential at the Wigner-Seitz cell radius and the energy at the bottom of the band,  $k=0$ ,

$$U_0 = U(r_s) - \epsilon(k=0). \quad (24)$$

The first point to note is that only "longitudinal" or "umklapp" contributions are permitted. For  $K=0$ , where  $K$  is the reciprocal vector in (4), the "scattering" vector,  $\mathbf{q}$ , must lie normal to the stacking fault plane, and  $q_x = q_y = 0$ . However, the displacement vector,  $\mathbf{b}$ , is in the stacking fault plane, so  $\mathbf{b} \cdot \mathbf{q} = 0$  in (23). Hence only matrix elements corresponding to umklapp in transport theory are allowed. Equation (23) is a decreasing function of  $q$ , so only the smallest reciprocal vectors (in the  $x$ - $y$  plane) need be considered.  $K = \pi/a \{01\}$ . We note that (23) contains a linear factor,  $\mathbf{b} \cdot \mathbf{q}$ . This product is simply the constant,  $\mathbf{b} \cdot \mathbf{K}$ , and is not a function of the  $z$ -component of  $\mathbf{q}$ . Likewise, in (23), although the quantity in braces and  $J$  are functions of the total vector,  $\mathbf{q}$ , the magnitude of this vector is a slow function of  $q_z = \kappa$  through the band of allowed values of  $\kappa$ , because  $q$  already has the large component,  $K$ . Hence the matrix element,  $v_{k'k}$  is zero except for those values of  $q$  on the line in  $k$ -space passing through the nearest reciprocal lattice vectors to the origin in the  $x$ - $y$  plane. For all the points on this line,  $v_{k'k}$  is slowly varying, the function  $J \simeq J(\pi) \simeq 1/3$ , and  $v_{k'k}$  takes the approximate value,

$$v_{k'k} = \frac{i\mathbf{b} \cdot \mathbf{K}}{3} \left\{ \frac{-2/3\epsilon_f + U_0(\pi^2/k_s^2 a^2)}{1 = \pi^2/a^2 k_s^2} \right\}. \quad (25)$$

The total matrix element,  $V$ , of course includes the structure factor,  $\Delta_+$ , from (6), and seems to be singular at  $\kappa=0$ . This is simply the familiar spurious singularity in scattering at a Brillouin zone boundary, and when one takes a proper linear combination of plane waves near the zone boundary, the singularity disappears.

We are thus left with the result that over the range of values,  $\kappa$ , for which  $v_{k'k}$  is non zero, that the approximation of a constant matrix element made in (20) yields a reasonable order of magnitude for the energy of the bound state for simple metals, where the average value of  $v$  is given by (25). The conclusions listed at the close of the last section then appear to be qualitatively correct for the simple metals.

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## Discussion on Paper by C. Nourtier and G. Saada.

SEEGER: I would like to make a comment on Professor Saada's paper. In fact, it's mainly putting it in the record, because I've said it before in other conferences. It is that I have doubt whether the first part of the method—not the summation over the planes—is actually valid, and the reasons why I have this doubt are the following: What you can show by general arguments is that the asymptotic form of the potential around an atom in a Fermi gas is identical with what Professor Saada had on the blackboard, except for the phase factor  $\phi$ . The phase factor is zero if and only if you use second order perturbation theory.

What I want to say is that I think I have strong reasons to believe that  $\phi$  should not be zero in any real case. In fact, it may even be  $\pi$ , which would reverse the conclusions on the stacking fault energies. The argument simply is that in the concept of pseudo-atoms you have to hold the right number of conduction electrons at the atom when you move it around, while on the other hand the potential on the atom—whatever it is—has to be sufficiently localized for it not to interfere with that of a neighbor. Otherwise you can't form a stacking fault simply by shifting the potential rigidly; if the pseudo-potentials strongly overlapped there would be some interference. To me it seems to be very difficult to satisfy these two conditions simultaneously. The case of monovalent atoms is a case where you might argue whether you can do it or not, but my feeling is that in divalent and trivalent metals you cannot do it. That is the main point of my comment.

A small comment is this: I always thought that potassium stayed body centered cubic down to the lowest temperatures. I was surprised to hear that now all alkali metals become hexagonal at low temperatures.

SAADA: Yes, as far as potassium is concerned, I took only the metals for which the method of pseudo-potential was shown to work well from the point of view, for example, of cohesion, phase stability, and so on. So I didn't take potassium because there is a problem for this one. In the case of potassium it is known that it does not have a stable compact phase. Therefore, I didn't make a complete stability of phase calculation. What I say is: You take a given structure and you look whether the h.c.p. or f.c.c. phase is the more stable. Then, what you find is that for monovalent metals it is h.c.p. This doesn't mean in the calculation I worked out that another phase cannot be more stable.

SEEGER: All right.

SAADA: Now, for the first two points. The first one, the  $\phi$  point, I agree

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that there can be a  $\phi$  which can be different from zero, but in our calculation to the second order of perturbation it is all right to take  $\phi = 0$ . What I want to say is that all this work is only valid up to the second order of perturbation. If the development is not valid then all the work goes to water.

SEEGER: My point really is that I believe this treatment is not valid. I think I can give reasons that this  $\phi$  is significantly different from zero.

SAADA: The second point is that for the metals on which I have done the calculation  $\phi$  has been shown by direct calculation to be very small. This is for Al and for Li, for example.

SEEGER: Did you do this with perturbation theory?

SAADA: This has been done with perturbation theory by Pick. See our paper.

# INTERACTIONS OF DISLOCATIONS WITH ELECTRONS IN METALS

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Physical arguments are given to show that the interaction of moving (vibrating) dislocations with conduction electrons in metals is independent of temperature. Calculations based on the assumption that the Fourier components of the displacement field of a moving dislocation can be treated as pseudo-phonons give the same result. These conclusions were confirmed by the results of recent experiments.

**Key words:** Dislocation dynamics; dislocation-electron interactions; phonons.

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## I. Introduction

The interactions are considered in terms of scattering of conduction electrons in metals by moving (vibrating) dislocations. A calculation was carried out following a scheme suggested by Holstein, and the physical implications of the results were discussed in detail [1]. The predictions of this treatment are consistent with the results of an experimental study on the interaction of moving dislocations with conduction electrons in the normal and superconducting states of a metal [2].

The actual treatment of the interaction starts with a Fourier decomposition of the lattice displacements  $u$  (displacement field) associated with a dislocation:

$$u = \sum_q u_q e^{iq \cdot r}$$

Each component  $u_q$  of this decomposition may then be treated as a "phonon" traveling through the lattice with the dislocation velocity  $v_d$  ( $v_d$  is much smaller than the velocity of sound in the solid  $v_s$ ; typically  $v_d \leq 10^{-3} v_s$ ) and the energy lost by these "phonons" to the conduction electrons can be determined using the established formalism of electron-phonon interactions. The interaction so calculated is independent of temperature. In this scheme any dependence of the interaction on temperature would have to come in through the inclusion of effects due to the temperature dependence of the Fermi energy of the conduction electrons

Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough, Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

and the temperature dependence of the components  $u_q$ . That these effects are small and indeed negligible in the context of possible experimental verification by presently available techniques can be seen from the following arguments.

Since the temperature dependence of the Fermi energy is of the order of  $(T/T_F)^2$  (plus higher order terms), the correction is obviously negligible. As far as the temperature dependence of the components  $u_q$  is concerned, it may be noted that the atomic displacements associated with an edge dislocation decrease rapidly with distance from the dislocation core (at a distance from the core of the order of five atomic diameters, these displacements become comparable with the amplitude of thermal phonons near the Debye temperature  $\theta_D$ ), and that they are substantially temperature independent (their temperature dependence is of the order of the thermal expansion of the solid). It follows that the components  $u_q$  dominant in the interaction with electrons have magnitudes of the wave vector  $q$  ranging from approximately the reciprocal of the lattice spacing to the reciprocal of about 10 lattice spacings, i.e.,  $10^7 \leq |q| \leq 10^8 \text{ cm}^{-1}$ . Thus, for most temperatures of interest and certainly in the range  $T \leq \theta_D$  these magnitudes of  $q$  correspond to the condition  $ql_e \gg 1$ , where  $l_e$  is the electron mean free path. It follows that the interaction of dislocations with conduction electrons should be treated in the spirit  $ql_e \gg 1$  and is, therefore, independent of  $l_e$ . Since  $\mathbf{q}$  as well as the dislocation density are also temperature independent, the interaction process is temperature independent. The temperature independent character of the interaction was confirmed experimentally at low temperatures [2].

In addition to the above, the effect of magnetic fields on the dislocation-electron interaction was considered. A simple estimate suggests that such interactions should not be significant for cyclotron radii much larger than a few atomic diameters. It follows that for magnetic fields commonly available such interactions should not be observable. The results of experiments with fields up to 15 kG do not show any indication of an effect of the fields on the interaction [3]. Experiments at much higher fields would have to be carried out in order to reach more concrete conclusions.

## II. Acknowledgement

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# ELECTRONIC ENERGY STATES OF DISLOCATIONS; THE CASE OF COVALENT-IONIC SOLIDS

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It is shown that electronic energy bands are associated with dislocations in wide-band-gap, compound semiconductors. The eigenvalue problem for the dislocation band edge is solved for CdS-type crystals, and the occupation of the band is calculated. The Fermi energy is then determined for crystals containing many deep-lying discrete levels as well as dislocation bands. It is predicted that when a crystal is illuminated with light of appropriate wavelength and increasing intensity, the thermal activation energy governing the electrical conductivity passes through a series of energy plateaus which are equal to the energy of the discrete levels. In a dislocation-free crystal, these plateaus are connected by step changes, while in a crystal with dislocations they are connected by broad transition regions. The above predictions have been verified experimentally.

Key words: Band structure; covalent-ionic solids; dislocation-electron interactions; Fermi energy; semiconductors.

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## I. Introduction

Changes in the energy of an electron in a crystal near a dislocation are usually attributed to lattice dilatation, and in the case of edge dislocations to "dangling bonds." The two readily recognizable consequences of the geometric proximity of the "dangling bonds" are: (1) The wave functions for adjacent sites should overlap significantly, which suggests a band of energy levels. (2) The occupation of an energy level associated with the dislocation edge should be limited by the Coulomb energy associated with the trapped carriers.

In previous treatments of this problem [1-6] one [6] or the other [1-3] of these two properties was emphasized. The resulting theories have, however, adjustable parameters which make it impossible to distinguish between them experimentally.

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In the present treatment a quantum mechanical model was used and it was shown that energy bands are associated with dislocations in wide band gap, CdS type compound semiconductors. This formulation was combined with a statistical treatment of localized energy levels found in such semiconductors. On this basis a test, far more definitive than previous theories allow, has been devised to check the band model of dislocation states [7]. In what follows, for the sake of convenience, reference will be made specifically to CdS, although all the general considerations apply to any solid of the type mentioned. Two reasons have guided the choice of wide band gap compound semiconductors, specifically CdS:

(1) In CdS the dangling bonds are partially ionic rather than entirely covalent. Therefore, the electronic energy states at the dislocation are affected less by charge on the dislocation than they are in an elemental semiconductor such as Ge.

(2) In CdS we often find a high density of deep levels which are associated with various impurities and other point defects. It is shown that these energy levels, which are referred to as *local levels* can be used as a probe of the dislocation bands.

With the above conditions in mind, the band theory for dislocation energy states is formulated for CdS. The resulting eigenvalue equation is solved for the dislocation band edge by using a pseudo-square well approximation for the dislocation potential. The dislocation occupation is then calculated as a function of the Fermi energy. This result, combined with a general description of a wide band gap semiconductor containing many deep levels leads to the following prediction:

In CdS with a low dislocation density the activation energy associated with the temperature dependence of the electrical conductivity will coincide with a local level, whereas in CdS with a high dislocation density the activation energy may fall between two such levels. This prediction has been verified in experiments with undeformed and deformed CdS crystals.

## II. Summary of Calculations

The present derivation is formulated in terms of the electron occupation of donor bands. With simple changes of notation, these results apply to the hole occupation of acceptor bands. In this treatment the charge on the dislocation is accounted for in two ways. First, an explicit correction  $V_q$  is made to the final derived energy levels. This correction is due to the fact that the total Coulomb energy of all captured holes is reduced when an electron is captured.  $V_q$  is essentially the electrostatic energy  $E_s$  defined by Read [1], and it is approximately proportional to the charge on the dislocation. This means that  $V_q$  is related to the dislocation occupation ( $n_D$ ) by

$$V_q = -C(n_D - 1/2 n_s), \quad (1)$$

where  $n_s$  is the number of atomic sites per unit length of dislocation and  $C$  is a positive constant. The second effect of the charge on the dislocation occupation arises because the perturbing potential  $V(r)$ , associated with the dislocation, is charge-dependent. Hence the wave equation involving  $V(r)$  must be solved in a self-consistent manner. However, in CdS the dangling bonds are partially ionic, and  $V(r)$  does not depend strongly on dislocation occupation. It will be assumed that  $V(r)$  can be specified, and that the resulting energy levels are independent of dislocation occupation.

If the energy of an electron in the conduction band is related to its momentum through  $E(p)$ , then in the effective mass approximation the "effective" Hamiltonian for the electron is  $E(-i\hbar\nabla)$ . When this electron is also in the field of a dislocation, the effective wave equation is

$$[E(-i\hbar\nabla) + V(r)]\Psi(r) = W\Psi(r). \quad (2)$$

The eigenvalue  $W$  represents the change of the energy of the entire crystal due to the interaction of a single electron with a dislocation.

An approximate form of eq (2) is obtained by expanding the function  $E(p)$  to quadratic terms about  $(0, 0, p_z)$ . It is assumed that  $E(p)$  has an extremum along this line so the first derivatives in  $p_x$  and  $p_y$  vanish. By choosing a coordinate system in which  $z$  is along the dislocation edge, and the  $x-y$  submatrix of the effective-mass tensor is diagonal the expansion of  $E(p)$  becomes

$$E(p_x, p_y, p_z) = E(0, 0, p_z) + \frac{1}{2m_{xx}} p_x^2 + \frac{1}{2m_{yy}} p_y^2. \quad (3)$$

If the dislocation does not disturb the periodicity of the crystal field along the dislocation edge ( $z$  direction), the wave function and dislocation potential can be written as

$$\Psi(r) = P(x, y)e^{-ikz}, \quad (4)$$

$$V(r) = V(x, y).$$

Combining eqs (2), (3), and (4) and simplifying yields

$$\left[ -\frac{\hbar^2}{2m_{zz}} \frac{d^2}{dx^2} - \frac{\hbar^2}{2m_{yy}} \frac{d^2}{dy^2} + V(x, y)P(x, y) \right] = \lambda P(x, y) \quad (5)$$

where  $\lambda$  is defined by

$$\lambda \equiv W - E(0, 0, \hbar k). \quad (6)$$

Equations (5) and (6) can be interpreted in terms of multiple energy bands. To see this let the zero of energy be at the conduction-band edge.

The function  $E(0, 0, \hbar k)$  then represents the kinetic energy of an electron, in the conduction band, moving in the  $z$  direction with momentum  $\hbar k$ . Since this energy has a quasi-continuum of positive allowed values, the total energy  $W$  can have a quasi-continuum of values above a band edge at  $\lambda$ . For any negative value of  $\lambda$  these energy states constitute a band of allowed states which overlap the forbidden gap. If  $\lambda$  is positive, these states represent the scattering of free electrons by the dislocation.

In order to obtain an approximate solution of eq (5) for the eigen-values  $\lambda$ , it is assumed that, as mentioned earlier  $V(x, y)$  has the form of a rectangular "square well." (This is a crude approximation to the actual potential and its use with the effective-mass approximation is not expected to yield very rigorous results, but it should be helpful in estimating the number of bands which will be bound.) Within the well the potential is  $-|V|$ , and outside it is zero. From the dislocation geometry in CdS [7] it is concluded that 6 Å by 8 Å is a reasonable estimate for the size of the well.

To render eq (5) separable, the "square well" is replaced by the following potential:

$$V(x, y) = U(x/\alpha) + U(y/\beta),$$

$$U(w) = 1/2|V|, \quad |w| > 1 \quad (7)$$

$$U(w) = 1/2|V|, \quad |w| < 1$$

where  $\alpha$  and  $\beta$  are the half-widths of the well in the  $x$  and  $y$  directions. Using this potential, eq (5) can be written in separated form:

$$\left[ -\frac{\hbar^2}{2m_{xx}} \frac{d^2}{dx^2} + U \frac{x}{\alpha} - (\lambda - b) \right] X(x) = 0, \quad (8a)$$

$$\left[ -\frac{\hbar^2}{2m_{yy}} \frac{d^2}{dy^2} + U \frac{y}{\beta} - b \right] Y(y) = 0, \quad (8b)$$

where  $b$  is a separation parameter which is real. With

$$u = x/\alpha, \quad E_u = \lambda - b, \quad \gamma_u^2 = \hbar^2/2m_{xx}\alpha^2; \quad (9)$$

$$v = y/\beta, \quad E_v = b, \quad \gamma_v^2 = \hbar^2/2m_{yy}\beta^2,$$

and after a number of intermediate steps, a set of parametric equations, which specify  $\lambda$  as a function of parameters of the well, are obtained;

$$\begin{aligned}
 V &= \gamma_u^2 (\theta_1 + n_1 1/2\pi)^2 (1 + \tan^2 \theta_1), \\
 0 &\leq \theta_1 \leq 1/2\pi; n_1 = 0, 1, 2 \dots \\
 E_u &= 1/2 \gamma_u^2 (\theta_1 + n_1 1/2\pi)^2 (1 - \tan^2 \theta_1), \\
 V &= \gamma_v^2 (\theta_2 + n_2 1/2\pi)^2 (1 + \tan^2 \theta_2), \\
 0 &< \theta_2 < 1/2\pi; n_2 = 0, 1, 2 \dots \\
 E_v &= 1/2 \gamma_v^2 (\theta_2 + n_2 1/2\pi)^2 (1 - \tan^2 \theta_2), \\
 \lambda &= E_u + E_v.
 \end{aligned} \tag{10}$$

where

$$(1/\gamma) [1/2|V| - E]^{1/2} = (\theta + 1/2n\pi) \tan \theta \quad (1/\gamma) [1/2|V| + E]^{1/2} = \theta + 1/2n\pi.$$

Equations (10) can be solved for the maximum well dimensions ( $d_1, d_2$ ) which give negative values of  $\lambda$ , i.e., dislocation bands as a function of well depth  $V$ . The resulting parametric relationship between  $d_1$  and  $d_2$ , with  $V$  as the parameter, gives the locus of  $\lambda=0$ . An evaluation of the energy shows that at the dimensions assumed for the potential well (6 by 8 Å), the well must be almost 2.5 eV deep for even one dislocation band to exist. For more than one band to exist, the well must be much deeper. An energy of 2.5 eV is close to the band gap in CdS, and corresponds to the minimum energy difference between a bound and a free electron in a perfect lattice. This is a reasonable upper limit for the potential associated with a broken bond. Therefore CdS should contain no more than one dislocation band.

### III. Occupation of Dislocation Bands

To find the occupation of a dislocation band, it is assumed that there is little interaction among the captured electrons, and their distribution is given by a Fermi function

$$f_k(W_T) = \left[ 1 + \exp \frac{W_T - E_F}{k_b T} \right]^{-1}, \tag{11}$$

where

$$W_T = \lambda + E(0, 0, \hbar k) - V_q, \tag{12}$$

and both  $W_T$  and  $E_F$  are measured (positive up) from the conduction-band edge.

To find the average number of captured electrons per unit dislocation length ( $n_D$ ), eq (11) must be summed over all allowed values of  $k$ . As usual, this summation is replaced by the following integration:

$$n_D = \frac{2}{\pi} \int_0^\infty f_k(W_T) dk, \quad (13)$$

where  $E(0, 0, \hbar k)$  is assumed to be a symmetric function of  $k$ . Equation (13) can be integrated by parts; the integrated part vanishes with the result

$$n_D = \frac{2}{\pi} \int_0^\infty k d f_k(W_T). \quad (14)$$

To solve eq (14) the usual free-electron relationship is assumed:

$$E(0, 0, \hbar k) = \hbar^2 k^2 / 2m,$$

where  $m$  is the effective mass for motion in the  $z$  direction. For convenience let:

$$\begin{aligned} f(z) &= (1 + e^2)^{-1}, \\ z &= \frac{W_T - E_F}{k_b T} = \frac{1}{k_b T} [\lambda - V_q - E_F + \hbar^2 k^2 / 2m], \\ B &= \frac{1}{k_b T} (\lambda - V_q - E_F). \end{aligned} \quad (15)$$

The function  $f(z)$  is a conventional Fermi function in which the energy  $z$  is translated to the origin, and the argument  $z$  is expressed in units of  $k_b T$ . The only case considered here is that of the Fermi energy within the dislocation band, i.e., that of positive  $B$ . Combine eqs (14) and (15):

$$n_D = \frac{2}{\pi} \frac{2m}{\hbar^2} k_b T^{1/2} \int_{-B}^\infty (z + B)^{1/2} \left( -\frac{df}{dz} \right) dz. \quad (16)$$

Since the derivative of  $f(z)$  looks like a  $\delta$  function, the value of this integral is determined near the origin. Thus the integral can be approximated by expanding  $(z + B)^{1/2}$  in a power series about the origin, and replacing the lower limit of integration by  $-\infty$ . The integrals in the resulting series can be evaluated explicitly:

$$n_D = \frac{2}{\pi} \left[ \frac{2m}{\hbar^2} k_b T B \right]^{1/2} \left[ 1 - \frac{\pi^2}{25} B^{-2} + \dots \right]. \quad (17)$$

If the Fermi energy is more than a few  $k_b T$  above the band edge, the dislocation occupation can be approximated by the first term in eq (17). Combining this approximation with the definition of  $B$  [eq (15)] gives

$$n_D = \frac{2}{\pi} \left( \frac{2m}{\hbar^2} \right)^{1/2} (E_F + V_q - \lambda)^{1/2}. \quad (18)$$

Using eq (1) to eliminate  $V_q$  in eq (18) gives

$$n_D = K \left[ E_F - \lambda + \frac{1}{2} C_{n_3} - C_{n_D} \right]^{1/2}, \quad K = \frac{2}{\pi} \left( \frac{2m}{\hbar^2} \right)^{1/2}. \quad (19)$$

Equation (19) establishes an implicit relationship between  $n_D$  and  $E_F$ . This equation is analogous to the usual relationship between the occupation  $n_j$  of a local energy level at  $E_j$  and the Fermi energy:

$$n_j = N_j \left[ 1 + \exp \frac{E_j - E_F}{k_b T} \right]^{-1}, \quad (20)$$

where  $N_j$  is the density of these levels. In both eqs (19) and (20), the occupation ( $n_D$  or  $n_j$ ) is determined when the Fermi energy is specified.

In a crystal containing defects the Fermi energy is determined by the temperature and the number and type of defect levels present. An analytical relationship between  $n_D$ ,  $n_j$ , and  $E_F$  can be derived from the equation of charge neutrality, and from continuity equations for the local levels and the dislocation bands

$$n + \sum n_a = p + \sum p_d + N_D p_d, \quad (21)$$

$$n_j + p_j = N_j, \quad (22)$$

$$n_D + p_D = n_s, \quad (23)$$

where  $n_a$  represents electrons occupying acceptor sites,  $p_d$  represents holes occupying donor sites,  $N_D$  represents the density of dislocation lines, and  $n_D$  and  $p_D$  represent the electron and hole occupation of the dislocation bands. After some manipulation the following is obtained

$$\sum N_B + n_j = \sum N_d + N_D (n_s - n_D) + M, \quad (24)$$

where  $\sum N_B$  is the total number of local levels lying below  $E_F$ ,  $\sum N_d$  is the number of donor levels in the crystal, and  $M$  is defined by

$$M = p + \sum p_B - n - \sum n_A. \quad (25)$$

$M$  is the difference between the number of holes in local levels below  $E_j$  and the number of electrons in levels above  $E_j$ . Since  $E_j$  is the local level nearest the Fermi energy, and because of the sharpness of the Fermi function, both of these quantities are small. Therefore  $M$  is small.

An implicit equation for  $E_F$  can be obtained by combining eqs (19), (20), and (24). The Fermi energy can be obtained explicitly by plotting the left-hand and right-hand sides of eq (24) independently, as a function of  $E_F$ , using eqs (19) and (20) to determine how  $n_j$  and  $n_D$  depend on  $E_F$ . The Fermi energy for the crystal is given by the intersection of these two

curves. Because of the steplike nature of the Fermi function, the left-hand side of eq (24) is essentially constant between the local levels, and at  $E_j$  it decreases by  $N_j$  over an energy of a few  $k_b T$ . The right-hand side of eq (24) is dominated by the constant term  $\sum N_d$ ; however, in a crystal containing dislocations, the term  $n_D$  [eq (19)] gives it curvature.

In figure 1, solid and dashed curves represent the left- and right-hand

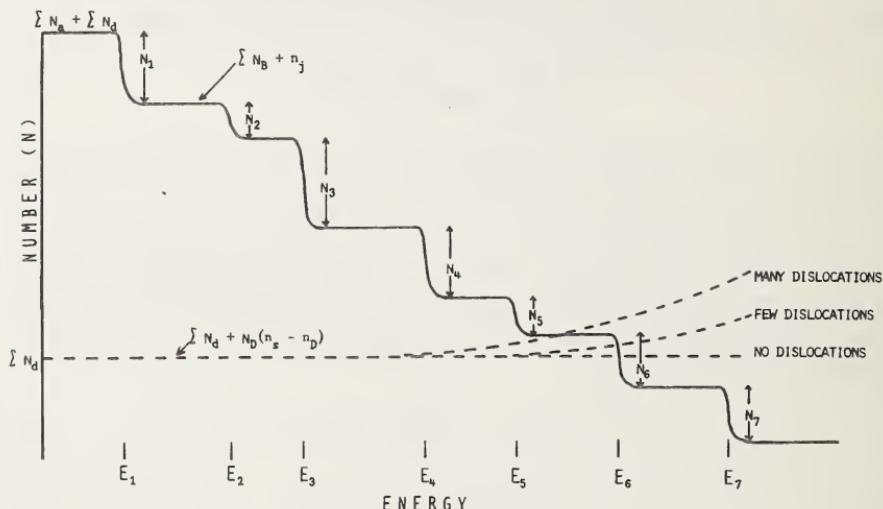


FIGURE 1. Solution to  $\sum N_j + n_j = \sum N_d(n_s - n_D) + M$  for hypothetical crystal.

sides of eq (24) which are plotted for a hypothetical crystal with various dislocation contents. In the dislocation-free case the solid and dashed curves are parallel everywhere except very near the local levels. Thus the intersection must occur very near one of these levels. However, in the crystal with dislocations, the two curves are no longer parallel and intersections can occur between the local levels. For example, in figure 1; the Fermi energy is near  $E_6$  in the dislocation-free case, as well as in the case of few dislocations, but with many dislocations the Fermi energy is between  $E_5$  and  $E_6$ .

With these graphical solutions in mind, appropriate approximations can be made to obtain an analytic expression for  $E_F$ . First, consider the dislocation-free case. Letting  $N_D = 0$ , combine eqs (24) and (20) and solve for  $E_F$ :

$$E_F = E_j - k_b T \ln \left[ N_j / \left( \sum N_d - \sum N_B + M \right) - 1 \right]. \quad (26)$$

Equation (26) can be used to determine the activation energy which governs the temperature dependence of the electrical conductivity. In

the case of CdS, which is an *n*-type, wide-band-gap semiconductor, the electrical conductivity is given by

$$C = nq\mu = N_c q\mu \exp [E_F/k_b T], \quad (27)$$

where  $q$  is the charge on an electron and  $\mu$  is the mobility and the zero of energy is defined at the conduction-band edge. Combine (26) and (27):

$$\ln C = (1/k_b T)E_j + \ln N_c q\mu$$

$$- \ln \left[ N_j / \left( \sum N_d - \sum N_B + M \right) - 1 \right]. \quad (28)$$

By definition [8],  $N_c$  is proportional to  $T^{+3/2}$  and experimentally, [9] between 80 and 700 K, the mobility in CdS is proportional to  $T^{-3/2}$ , hence  $\mu N_c$  is temperature-independent. In addition, as mentioned earlier,  $M$  is small, so its temperature dependence can be neglected in the last term. Therefore, in a dislocation-free crystal, the slope of a plot of  $\ln C$  versus  $1/k_b T$ , i.e., the "activation energy," will be  $E_j$ .

For a crystal containing dislocations, the case in which the Fermi level is near a local level must be distinguished from the case where it is between two local levels. Figure 1 shows that in the former case the exact value of  $E_F$  is determined by the variation of  $n_j$  with energy, and  $n_D$  can be treated as if the intersection were at the local level. In this case  $E_F$  is given by

$$E_F = E_j - k_b T \ln \left\{ N_j / \left[ \sum N_d - \sum N_B + M + N_D n_s - N_D n_D (E_j) \right] - 1 \right\}. \quad (29)$$

By comparing this result to eq (26), we can see that the activation energy is again  $E_j$ .

When the Fermi energy falls between two of the local levels,  $n_j$  is either 0 or  $N_j$ , and it is not a strong function of energy. In this case  $E_F$  can be found by combining eqs (24) and (19):

$$E_F = \lambda + \frac{1}{K^2 N_D^2} \left[ \sum N_d + N_D n_s + M' - \sum N_B \right]^2 + \frac{C}{N_D} \left[ \sum N_d + \frac{1}{2} N_D n_s + M' - \sum N_B \right], \quad (30)$$

where  $M'$  is defined by

$$M' = M - n_j (E), \quad |E - E_j| > k_b T. \quad (31)$$

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In this case the activation energy is equal to  $E_F$  and it will be between two of the local levels.

A scheme was devised [7] to check experimentally these results. The experimental data obtained on undeformed and deformed CdS agree with the above predictions.

### IV. Acknowledgement

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# INTERACTIONS BETWEEN ELECTRONS AND MOVING DISLOCATIONS

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A moving dislocation in a metal induces an electric field which causes currents in the conduction electron gas. The energy dissipation associated with these fields and currents is calculated from the Boltzmann equation in a manner analogous to theories of acoustical attenuation. It is found that the applied stress required for steady motion is proportional to the dislocation velocity divided by the electrical resistivity, in good agreement with low temperature yield and flow stress measurements on bcc metals. The concept of a large electronic component of drag which increases with decreasing temperature is used to give a qualitative explanation of the observed mechanical properties of b.c.c. metals. When one considers electronically damped dislocations impeded by pinning points, it is found that: (1) the dislocation velocity depends only on the mean strength of the pinning obstacles; (2) the stress required to overcome an obstacle dynamically is less than that required statically and is, in fact, the electronic drag stress; and (3) the apparent dislocation velocity should vary rapidly with applied stress. The displacement field of a dislocation is significantly wider and more gradual in a f.c.c. than in a b.c.c. lattice, and this feature can be incorporated into the calculation by assuming that the electronic screening of the positive charge shift of the dislocation is essentially perfect in a f.c.c. lattice. The Boltzmann formulation then gives a temperature independent stress or drag coefficient in agreement with experiment and with Holstein's scattering calculation. The problem of a dislocation moving in an applied magnetic field directed along its length and perpendicular to its direction of motion is also treated. Under suitable conditions it is found that the stress or drag coefficients exhibit oscillations of the cyclotron resonance type which could be as large as 10 to 30% of the zero field values.

Key words: dislocation damping; dislocation-electron interactions; electroresistivity.

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## I. Introduction

In previous work, we have calculated the electronic component of drag on a moving dislocation using a Boltzmann equation approach

Fundamental Aspects of Dislocation Theory, J. A. Simmons, R. de Wit, and R. Bullough, Eds. (Nat. Bur. Stand. (U.S.), Spec. Publ. 317, II, 1970).

analogous to theories of acoustic attenuation [1, 2]. If one assumes that the electronic screening of the positive charge shift associated with the dislocation is perfect, one obtains a drag coefficient or electronic component of yield stress which is temperature independent in good agreement with the scattering calculation of Holstein [3]. In an applied magnetic field, the electronic component of drag is predicted to exhibit oscillations of the cyclotron resonance type, which could be as large as 10 to 30 percent of the zero field drag. However, Brown [4] and others [5] have shown that the positive charge shift is not perfectly screened if one treats the short wavelength components of the dislocation displacement field rigorously. If one uses Brown's result for the deformation potential in the Boltzmann theory, the drag coefficient is found to be inversely proportional to the resistivity. For reasons discussed in section II, the temperature independent result is probably a more accurate description for f.c.c. or h.c.p. metals, while the second, strongly temperature sensitive result may be a correct description of a moving dislocation in a b.c.c. metal. As will be shown, such a result gives a good explanation of the large, markedly temperature dependent yield and flow stresses observed in bcc metals at low temperatures [6-11]. In this case, the previously mentioned magnetic effects are greatly reduced. Such magnetic experiments should thus provide a good test of the theory.

In section II, we outline the Boltzmann theory and give its main results. In section III, the concept of an electronic component of drag which increases strongly with decreasing temperature is utilized to give a qualitative explanation of the mechanical properties of b.c.c. metals. In section IV a short summary and discussion of the results are presented.

## II. Boltzmann Equation Theory and Results

We follow closely the general treatment of Cohen, Harrison and Harrison [12], who use the form of the Boltzmann equation solution given by Chambers [13],

$$f(\mathbf{r}, \mathbf{v}, t) = \int_{-\infty}^t f_s(\mathbf{r}', \mathbf{v}', t') e^{-(t-t')/\tau} dt' / \tau \quad (1)$$

where  $\mathbf{r}' = \mathbf{r}(t')$ , and  $\mathbf{v}' = \mathbf{v}(t')$ . Here  $f(\mathbf{r}, \mathbf{v}, t)$  is the electron distribution function, which gives the probability of finding an electron at point  $(\mathbf{r}, \mathbf{v})$  in phase space at time  $t$ ;  $f_s$  is the distribution function after scattering, and  $\tau$  is the electronic relaxation time. If  $\mathbf{u}(\mathbf{r}, t)$  is the velocity imparted to ions and impurities by the moving dislocation,  $f_s$  has the form of an ordinary Fermi distribution function centered about velocity  $u$ ; i.e.,

$$f_s(\mathbf{r}, \mathbf{v}, t) = f_0(E(r, v - u, t) - E_F), \quad (1a)$$

where  $E_F$  is the Fermi energy. The space time dependence of the single electron energy is chosen to give the correct electron density.

$$\mathbb{E}(\mathbf{r}, \mathbf{v}, t) - E_F = \frac{1}{2} m\mathbf{v}^2 - E_F^0 - \frac{2E_F^0}{3} \frac{\delta n(\mathbf{r}, t)}{N_0} \quad (2)$$

where

$$E_F^0 = E_F - E_0, \quad (3)$$

$E_0$  being the energy at the bottom of the conduction band and  $N_0$  the unperturbed electron density. In the two approximations we eventually use to calculate the drag coefficient or yield stress (perfect screening and a Thomas-Fermi model), eq (2) is identical to

$$\mathbb{E}(\mathbf{r}, \mathbf{v}, t) - E_F = \frac{1}{2} m\mathbf{v}^2 + V_D(\mathbf{r}, t) - E_F^0 = \mathbb{E}_0(\mathbf{v}) + V_D(\mathbf{r}, t) - E_F^0 \quad (4)$$

where  $V_D$  is the deformation potential of the moving dislocation. More generally, however, Brown has shown that eqs (2) and (4) are not identical in a more accurate treatment using the static dielectric function to describe the screening [4]. We retain eq (4) in this treatment, partially because the resulting algebraic equations are simpler, and the results identical in the approximations used, and partially because we feel it may have a more direct correspondence to an eventual scattering theory. We have, however, also carried out the calculation using eq (2) and the more accurate results of Brown for  $\delta n(\mathbf{r}, t)$ , and find that the changes in the main results of the theory are negligible.

The solution to the linearized Boltzmann is found by expanding  $f$  and  $f_0$  to terms which are of first order in  $\mathbf{u}$ .

$$f(\mathbf{r}, \mathbf{v}, t) = f_0(\mathbb{E}_0(\mathbf{v}) - E_F) + f_1(\mathbf{r}, \mathbf{v}, t). \quad (5)$$

Following standard procedure [12, 14], one finds

$$f_1(\mathbf{r}, \mathbf{v}, t) = \left( \frac{-\partial f_0}{\partial \mathbb{E}_0} \right) \int_{-\infty}^t e^{-(t-t')/\tau} \left\{ \mathbf{v}' \cdot \left( e\mathbf{E}(\mathbf{r}', t') \right. \right. \\ \left. \left. - \nabla V_D(\mathbf{r}', t') + \frac{m\mathbf{u}}{\tau}(\mathbf{r}', t') \right) - \frac{V_D(\mathbf{r}', t')}{\tau} \right\} \quad (6)$$

where  $\mathbf{E}$  is the electric field produced by the moving dislocation. Following CHH, we Fourier analyze all quantities and obtain for the electron current,

$$\mathbf{J}_e(\mathbf{r}, t) = \sum_{\mathbf{q}} \boldsymbol{\sigma}_{\mathbf{q}} \cdot \left\{ \mathbf{E}_{\mathbf{q}} + \frac{m \mathbf{u}_{\mathbf{q}}}{e\tau} - \frac{\omega\tau}{(1-i\omega\tau)} \frac{\mathbf{q} V_{D\mathbf{q}}}{e} \right\} e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)} \quad (7)$$

where  $\boldsymbol{\sigma}$  is the conductivity tensor. The simplest form of  $\omega$  which satisfies the requirement of Galilean invariance is simply  $\mathbf{q} \cdot \mathbf{v}_d$ , where  $\mathbf{v}_d$  is the dislocation velocity. We take the deformation potential to have the form

$$V_{Dq} = \frac{2E_F}{3} \Delta_q \Gamma_q = -\frac{2E_F}{3} \frac{qu_{q||}}{\omega} \Gamma_q \quad (8)$$

where  $\Delta_q$  is the Fourier transform of the dilatation,  $u_{q||}$  is the component of  $\mathbf{u}_q$  parallel to  $\mathbf{q}$ , and  $\Gamma_q$  specifies the electronic screening.

Using Maxwell's equations and the charge-current continuity equation one can express the electric field and electron current in terms of  $\mathbf{u}$ . The results have the form

$$\mathbf{E}_{\mathbf{q}} = \mathbf{E}_{\mathbf{q}} \cdot \frac{Ne\mathbf{u}_q}{\sigma_0} \quad (9)$$

and

$$J_{eq} = \mathbf{J}_{\mathbf{q}} \cdot Ne\mathbf{u}_{\mathbf{q}} \quad (10)$$

where  $\mathbf{E}$  and  $\mathbf{J}$  are dimensionless tensors, and  $\sigma_0$  is the d-c conductivity. It is then readily shown [1] that the energy dissipated by electrons when the dislocation moves from one lattice position to an adjacent position is

$$W = -\frac{Nm\tau_DL(cm)^4}{(2\pi)^2\tau} \int d^2\mathbf{q} \mathbf{u}_{-\mathbf{q}} \text{Re} (\mathbf{S}_{\mathbf{q}}) \cdot \mathbf{u}_{\mathbf{q}} \quad (11)$$

where  $L$  is the dislocation length,  $\tau_D$  is the time required for the motion, and the integration extends over the (1-2) plane in figure 1.  $\mathbf{S}_{\mathbf{q}}$  is the dissipation tensor given by

$$\mathbf{S}_{\mathbf{q}} = \mathbf{J}_{\mathbf{q}}^+ \cdot \mathbf{E}_{\text{eff}} \mathbf{u}_{\mathbf{q}} + \mathbf{I} \quad (12)$$

where  $\mathbf{J}^+$  is the adjoint of  $\mathbf{J}$  and  $\mathbf{E}_{\text{eff}}$  is the effective field tensor. The tensors  $\mathbf{J}$ ,  $\mathbf{E}$ ,  $\mathbf{E}_{\text{eff}}$ , and  $\mathbf{S}$  are all given in terms of the conductivity tensor,  $\boldsymbol{\sigma}$ , and the deformation potential. Their exact forms are rather cumbersome and we refer the interested reader to reference [1] where they are given. The Fourier transforms of the ionic velocity functions to be used in eq (11) are also given there.

If there is no applied field,  $\boldsymbol{\sigma}^{15}$  and all of the other tensors are diagonal and the resulting expressions split into longitudinal ( $||$ ) and transverse ( $\perp$ ) components. In particular, one finds that the applied stress required to supply the energy dissipated by the conduction electrons is

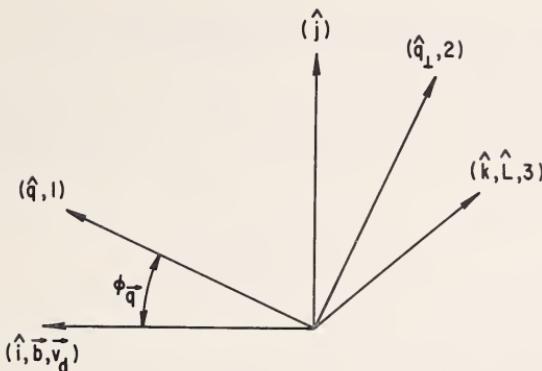


FIGURE 1. Calculations in wave vector space are most easily carried out in the (1, 2, 3) coordinate system specified by the unit vectors  $\hat{q}$ , in the direction of  $\mathbf{q}$ ,  $\hat{L}$ , along the length of the dislocation, and the cross product of these two,  $\hat{q}_\perp$ . The natural coordinate system in real space,  $(i, j, k)$ , is specified by the Burgers vector or glide direction,  $\mathbf{b}$ ,  $\hat{L}$ , and the direction of their cross product  $\hat{j}$ .

$$\begin{aligned}
 S^{(\text{edge})} &= \frac{W}{b^2 L} = S_{||}^{(\text{edge})} + S_\perp^{(\text{edge})} \\
 &= \frac{Nmbv_d}{4\pi^2\tau} \left\{ \xi^2 \int_0^{q_D} dq \int_0^{2\pi} d\varphi \frac{\sin^2 \varphi \cos^2 \varphi}{q} (\text{Re } S_{||}) \right. \\
 &\quad \left. + \frac{1}{4} \int_0^{q_D} dq \int_0^{2\pi} d\varphi \frac{[1 - 4 \sin^2 \varphi]}{q} (\text{Re } S_\perp) \right\} \quad (13)
 \end{aligned}$$

while

$$S_\perp^{(\text{screw})} = \frac{Nmbv_d}{4\pi^2\tau} \int_0^{q_D} dq \int_0^{2\pi} d\varphi \frac{\sin^2 \varphi \cos^2 \varphi}{q} (\text{Re } S_\perp) \quad (14)$$

where  $\mathbf{b}$  is the Burgers vector and  $\varphi$  is the angle between  $\mathbf{q}$  and  $\mathbf{v}_d$ , and  $q_D$  is the Debye wave vector.

One can readily show that  $S_\perp^{(\text{edge})}$  and  $S_\perp^{(\text{screw})}$  are  $\ll S_{||}^{(\text{edge})}$  over the temperature range of interest (0 K to 200 or 300 K) and that the dominant contribution to the  $S_{||}^{(\text{edge})}$  integral comes from the region where  $q$  is large (i.e.,  $q \gtrsim q_{D/10}$ ). In this high  $q$  region,  $q\Lambda \gg 1$ ,  $\Lambda$  being the electron mean free path. If additionally, we assume that  $\omega\tau \lesssim 10^{-1}$ , which should be valid for most materials, we find,

$$\text{Re } S_{||} \approx \left\{ \frac{(q\Lambda)^2}{3} (1 - \Gamma_q) + \frac{\pi q \Lambda}{6} \right\} \left( 1 + \frac{q^2}{q_{TF}^2} \Gamma_q \right) \quad (15)$$

where we have neglected terms of order  $(\omega\tau)^2$  with respect to 1 and terms of order 1 with respect to  $q\Lambda$ .

The simplest approximation is to take  $\Gamma_q=1$ , which assumes that the electrons screen the positive charge shift of the dislocation perfectly. One then finds for an edge dislocation the temperature independent stress

$$S^{(\text{edge})} \approx \frac{Nmbv_d v_F q_D \xi^2}{96}. \quad (16)$$

This is  $\sim 10^6$  to  $10^7$   $\left( \frac{\text{dyne}}{\text{cm}^2} \right)$  for a typical metal. The electron drag coefficient is then

$$B^{(\text{edge})} = \frac{Nmb^2 v_F q_D \xi^2}{96} \quad (17)$$

where

$$\xi = [1 + 2(v_2/v_1)^2], \quad (18)$$

$v_F$  is the Fermi velocity, and  $v_2$  and  $v_1$  are the transverse and longitudinal sound velocities. This result is in good agreement with Holstein's scattering calculation [3]. An earlier, somewhat less general solution of the Boltzmann equation by Kravchenko [16] gives a similar result.

In a more general, quantum mechanical calculation [4], Brown has shown that when the wave vector  $\mathbf{q}$  is not small with respect to  $k_F$  and  $q_{TF}$ , the Fermi and Thomas-Fermi wave vectors, the form of the screening function  $\Gamma_q$  is

$$\Gamma_q = \left\{ (q/q_{TF})^2 + \left[ \frac{1}{2} + \frac{4k_F^2 - q^2}{8k_F q} \ln \left| \frac{2k_F + q}{2k_F - q} \right| \right] \right\}^{-1}. \quad (19)$$

Following Pines [17] and others [18] we replace  $q_{TF}$  by a somewhat smaller screening vector,  $q_s = 0.433 q_{TF}$ , and adopt the approximation

$$\Gamma_q \approx \frac{1}{(1 + q^2/q_s^2)}. \quad (20)$$

Inserting this expression into eqs (15) and (13) one finds for edge dislocations a large, temperature dependent stress which is inversely proportional to the d-c electrical resistivity,  $\rho$ .

$$S \approx \frac{mE_F b q_D^2 \xi^2 \tilde{\mathcal{V}}(x_m)}{24\pi e^2} \frac{v_d}{\rho} = C \frac{v_d}{\rho}. \quad (21)$$

Here  $x_m = q_D/q_s$  and

$$\tilde{\mathcal{V}}(x_m) = \left\{ 1 + \frac{1}{2(1+x_m^2)} - \frac{3}{2x_m^2} \ln(1+x_m^2) \right\}. \quad (22)$$

If we neglect other dislocation drag mechanisms, we can equate  $S$  to the yield stress. More accurately, we mean the flow stress extrapolated back to the elastic line on the stress-strain curve [9]. The term yield stress is used because it represents a fairly well defined point on this curve at which interactions between dislocations (work hardening) should be negligible. For measurements at constant strain rate, as discussed previously [2],  $v_d$  can be assumed to be approximately independent of temperature, so that all of the temperature dependence is contained in  $\rho$ . Separating  $\rho$  into its ideal and residual parts, and inverting eq (21), we find

$$\frac{1}{S} = \frac{1}{C} \frac{(\rho_i(T) + \rho_0)}{v_d}. \quad (23)$$

A plot of  $1/S$  versus  $\rho_i$  should then give a straight line whose slope and intercept determine the dislocation velocity and the residual resistivity, respectively. Several examples are shown in figure 2 and the dislocation velocities and residual resistivities found from these and other such plots are listed in table I. If one now takes these values and uses them in eq (21) one finds the theoretical  $S$  versus  $T$  dependence shown by the smooth curves in figure 3.

TABLE I

Element	$v_d$ (cm/s)	$\rho_0$ ( $\mu\Omega$ - cm)
V	$5.88 \times 10^4$	3.88
Fe	$2.18 \times 10^4$	2.06
Cr	$6.22 \times 10^4$	3.35
W	$1.89 \times 10^4$	1.39
Mo	$2.27 \times 10^4$	2.17
Nb	$7.83 \times 10^4$	5.06
Ta	$6.64 \times 10^4$	3.85
K	11.86	.054

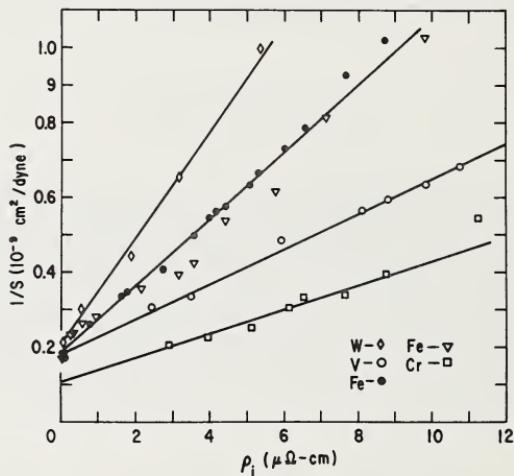
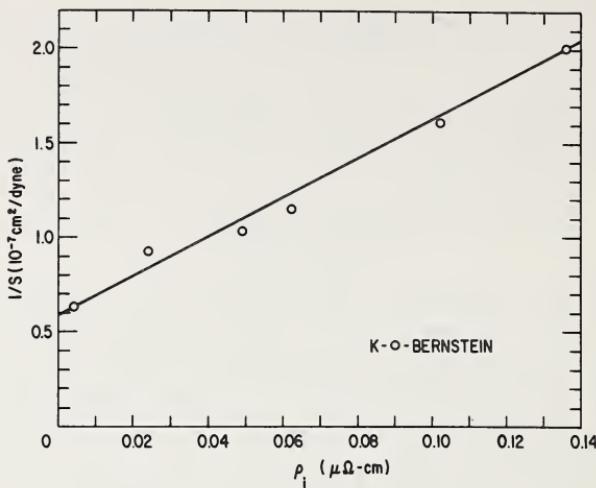


FIGURE 2. The inverse yield stress versus the ideal resistivity for:  
 (a) K<sup>7</sup>; (b) Fe<sup>9, 10</sup>, Cr, <sup>11</sup>V,<sup>8</sup> and W<sup>8</sup>.

It may be noted that theory and experiment are in better accord at low than at high temperatures. This is expected since other dislocation drag mechanisms (phonon drag, impurity and grain boundary pinning, etc.) should become comparable to or greater than the electronic component at higher temperatures. In general the straight line relationship of eq (23) has been found to hold reasonably well up to temperatures of order 150 to 250 K for most b.c.c. metals.

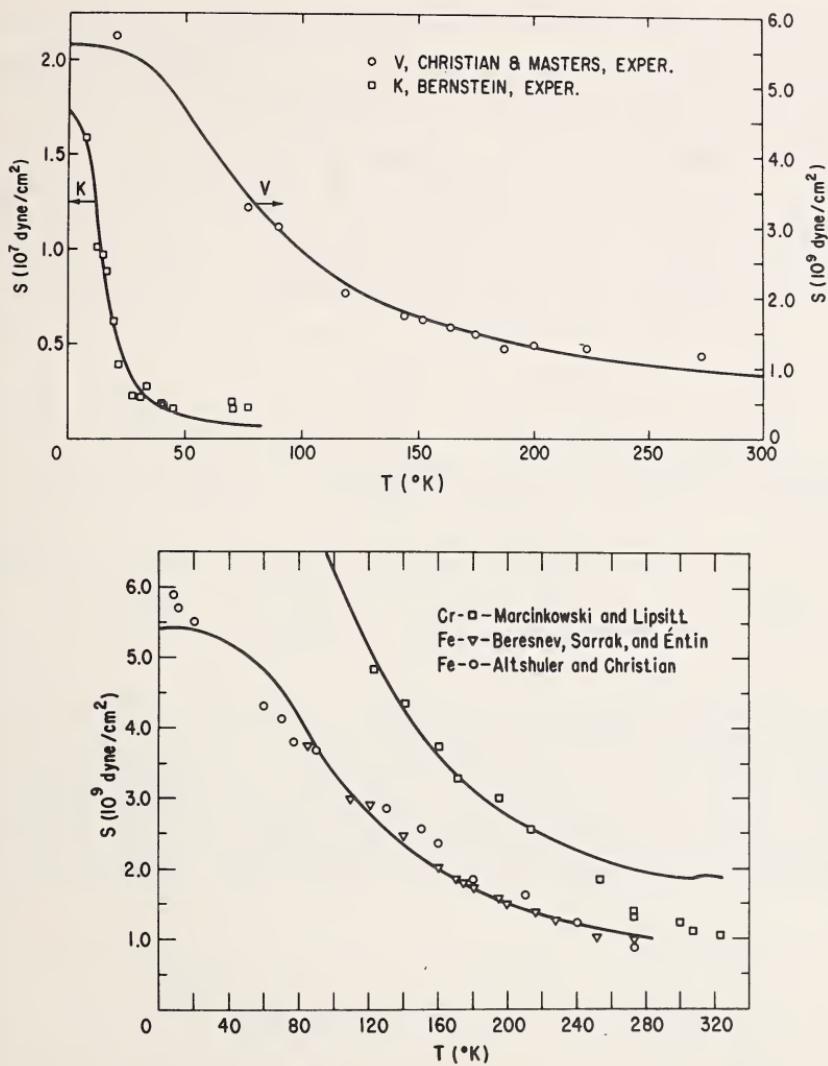


FIGURE 3. Theoretical (smooth curves) and experimental (points) yield stress versus temperature results for: (a) K<sup>7</sup> and V<sup>8</sup>; (b) Fe<sup>9, 10</sup> and Cr<sup>11</sup>.

The dislocation velocities obtained are fairly large, being about 5 to 10 percent of the speed of sound in most cases. This agrees qualitatively with recent experimental measurements [19]. The residual resistance in this theory should be viewed as a parameter which is characteristic of the electronic mean free path in the highly strained region close to the dislocation core. This seems reasonable, since the dominant part of the interaction takes place for large  $q$ ,  $\gtrsim q_D/10$ , so that most of the energy dissipation takes place within a distance of several Burgers vectors from the

dislocation center. This view is supported by the fact that the same residual resistance seems to be appropriate for the Fe data of two different investigators. This was also found to be approximately true for other metals where more than one set of data was available.

In f.c.c. metals, the yield stress shows very little temperature dependence, and the small temperature dependent component which is observed may arise from impurities [1, 20, 21]. Further, ultrasonic experiments show a damping which is essentially temperature independent [22, 23]. It therefore seems likely that the temperature independent drag coefficient of eq (17) is a more accurate description for f.c.c. metals. The difference between f.c.c. and b.c.c. metals can be qualitatively explained by noting that the core distortion should be spread out over a considerably larger region in f.c.c. than in b.c.c. lattices, and the effect of this is to emphasize the contribution of the somewhat longer wavelength components of the Fourier synthesis. Inspection of eq (19) shows that such an emphasis is equivalent to taking  $\Gamma_q = 1$ , which approximation was used in deriving eq (17). We note that an alternative approach, using the concept of dislocation widths yields a similar result [1], at least as regards the temperature dependence.

The electronic drag arising from the transverse components of the field and current, as given by the second term of eq (13) and by eq (14) for a screw dislocation have a more complicated form and we have evaluated these integrals by computer integration.

The transverse component of drag is found to increase with increasing temperature, and this is shown in figure (4) for a screw dislocation in a typical metal. The relatively small magnitude of the stress arises primarily because the displacement field we have assumed for a moving screw dis-

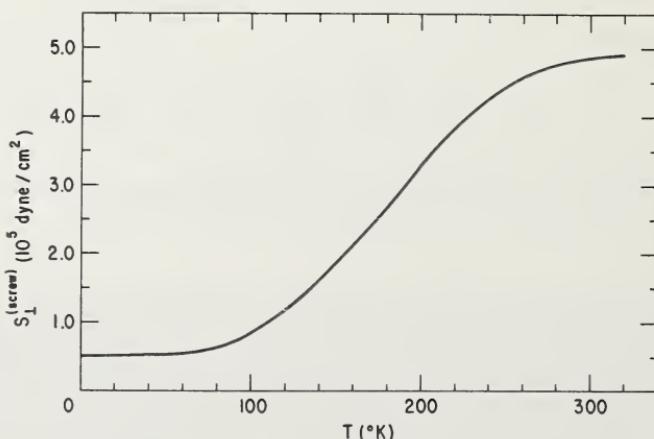


FIGURE 4. Stress versus temperature for a screw dislocation in a typical free electron metal assuming a conduction electron density of  $5 \times 10^{22} \text{ cm}^{-3}$  and a dislocation velocity of  $10^4 \text{ cm/s}$ .  $S_{\perp}^{(\text{edge})}$  has a very similar form.

location has no dilatation. If in fact, this is not the case, this result could be greatly altered.

Next, consider the problem of an applied field  $H$  directed along the length of the dislocation (axis 3 in fig. 1). The conductivity tensor and the dissipation tensor are no longer diagonal. As for the zero applied field case, the dominant contribution to the integral of eq (11) comes from the high  $q$  region  $q \gtrsim q_{D/10}$ . In this region  $S_{11}$  is much greater than either the transverse ( $S_{22}$  and  $S_{33}$ ) or off-diagonal components ( $S_{12}$  and  $S_{21}$ ) of  $S$ . Using the same large  $q$  approximations as CHH for  $\sigma_{11}$ , it can be shown for  $\Gamma_q = 1$  that

$$\text{Re } S_{11} \approx \frac{\pi q \Lambda}{6} \times \frac{\{\text{Re} [(1 - i\omega\tau) \coth Z] (1 + x^2) - \omega\tau \text{Im} [(1 - i\omega\tau) \coth Z] (1 + x^2)^2\}}{[1 + (\omega\tau)^2 (1 + x^2)^2]} \quad (24)$$

where

$$Z = \frac{\pi}{\omega_c \tau} (1 - i\omega\tau), \text{ and } x = q/q_{TF}, \quad (25)$$

$\omega_c$  being the cyclotron frequency,  $(eH/mc)$ . Inserting this result into eq (13) and performing a computer integration, one finds the results shown in figure 5 using parameters appropriate for Cu. Here we have plotted the stress at constant temperature against the ratio  $\omega_m/\omega_c$ ,  $\omega_m$  being the maximum frequency associated with the dislocation wave packet,  $q_D v_d$ . The drag coefficient would, of course, show the same behavior. The oscilla-

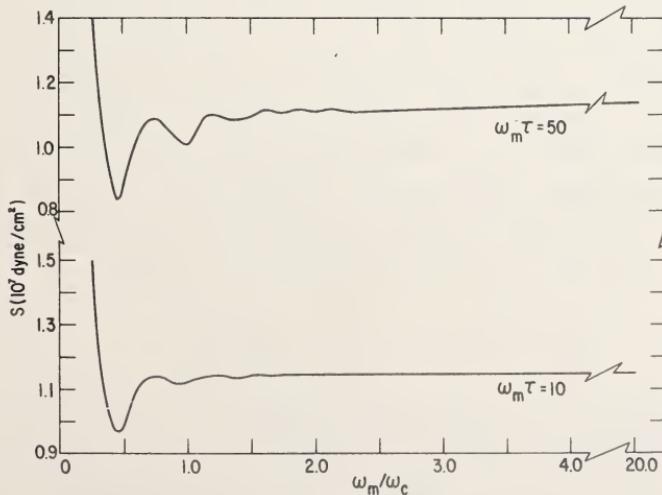


FIGURE 5. Stress versus  $\omega_m/\omega_c$  for Cu parameters ( $v_d = 10^4$  cm/s) assuming perfect screening.

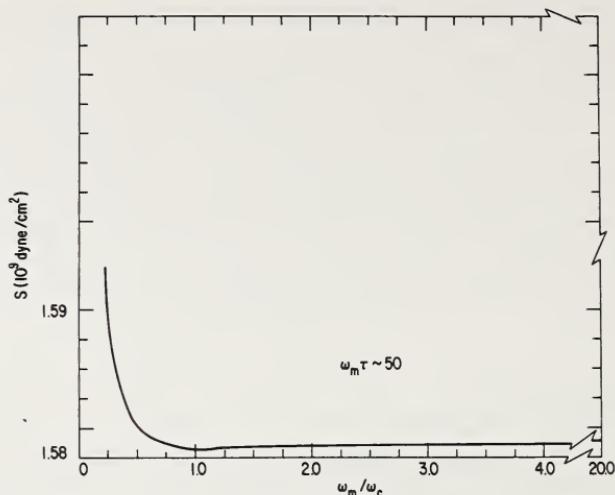


FIGURE 6. Stress versus  $\omega_m/\omega_c$  for a b.c.c. metal, using the screening function of eq (19).

tions are about 10 to 30 percent of the zero field value. Because of the somewhat large residual resistivities associated with the region near the dislocation core, there might be an inherent difficulty in obtaining  $\omega_m\tau$  values even as large as 10. Nevertheless, this problem should be less severe for f.c.c. than for b.c.c. metals, and it seems likely that some oscillatory behavior should be observable for f.c.c. metals. The locations and separations of such oscillations could be used to determine the primary velocity of a dislocation moving between adjacent lattice positions.

If one does not take  $\Gamma=1$  but uses eq (19), which is presumably a better description for b.c.c. metals, one finds that the magnetic effects are drastically reduced, due to the fact that the large, temperature dependent part of the stress is rather insensitive to the magnetic field. A typical result is shown in figure 6. It is clear that magnetic experiments of this type on b.c.c. and f.c.c. metals should be crucial in clarifying the situation.

In addition to the drag coefficients one can also derive electric fields, currents, and charge densities from the Boltzmann formalism [1]. Using the complete screening function of eq (19) and the integration techniques of Brown, one finds for the charge density, for example,

$$\begin{aligned}
 \rho(\mathbf{r}') = & -Ne \left( \frac{k_F b \xi}{2\pi} \right) (2\pi k_F a_0 C_0) \left\{ \frac{\sin \varphi \sin (r'_F + \pi/4)}{(r'_F)^{5/2}} \right. \\
 & + (2k_F v_d \tau) \cos \varphi \sin \varphi \frac{\cos (r'_F + \pi/4)}{(r'_F)^{5/2}} \\
 & \left. - (2k_F v_d \tau)^2 \cos^2 \varphi \frac{(4k_F^2 + q_{TF}^2)}{q_{TF}^2} \frac{\sin \varphi \sin (r'_F + \pi/4)}{(r'_F)^{5/2}} \right\} \quad (26)
 \end{aligned}$$

where  $a_0$  is the Bohr radius,  $C_0$  is a dimensionless constant  $\sim 1$ , and  $r'_F = 2k_F|\mathbf{r} - \mathbf{v}_d t|$ . All electromagnetic quantities exhibit the Friedel oscillations characteristic of a Fermi gas.

### III. Mechanical Properties

We now consider a new theory for the temperature dependence of the flow stress of b.c.c. metals. The observed temperature dependence of the flow stress and that calculated for the electron damping of dislocation motion are the same over the relevant range of temperature. Since it would seem improbable that this could be coincidental we shall, as implied earlier, equate the energy dissipated as heat by moving dislocations to the work of plastic deformation.

The question as to how the work of plastic deformation is dissipated seems largely to have been neglected. Nicholas [24] examined this matter and concluded that if, as experiment seemed to indicate, dislocations do not move rapidly with speeds approaching that of sound, the dissipated energy could be accounted for by the formation of point defects through the motion of jogs. However, it was pointed out later by Louat and Johnson [25] that jogs of the same sign are apt to accumulate leading to the formation of dislocation dipoles rather than point defects. Nicholas' results are then seen to overstate significantly the energy dissipated in this way. Accordingly, it seems necessary to suppose that dislocations do move rapidly.

To resolve the resultant contradiction of experiment we have only to postulate that dislocations move in a series of jerks so that their mean speed is much less than that of sound whereas their maximum speed may approach it. This view finds support from Fisher and Lally's [26] observation of noise induced in a plastically deforming material. It would also seem inescapable from the realization that in the situation with which we are concerned the forces on a dislocation through an applied stress field are large compared with the effective dissipative force when a dislocation moves at a speed very much less than that of sound.

Allowing that dislocations do move rapidly we still have to explain why the speed is essentially constant as required from our earlier considerations.

When preparing a new theory it is advisable to indicate some shortcomings of the old. Accordingly, before discussing these above ideas further, we shall examine briefly two current theories severally based on the ideas of large Peierls forces and the dissociation-association of screw dislocations (Hirsch, 27).

## A. PRESENT THEORIES

Basic to the formalism of both the Peierls and dissociation-association models is the postulate that the flow stress ( $S$ ) is the sum of two components, thus

$$S = S_i + S(T) \quad (27)$$

where  $S_i$  is independent and  $S(T)$  a function of temperature. Furthermore,  $S_i$  is identified with the resistance to dislocation motion consequent on the presence of internally induced stress fields. It is an essential assumption of these models that the lateral speed ( $V_k$ ) of kinks produced through thermal activation is much greater than the forward speed ( $V_D$ ) of the dislocation as a whole. Concomitantly, the dislocations are envisaged in the analysis as essentially straight. In view of later considerations it is now appropriate to examine the validity of this assumption.

It is clear that the activation energy for kink motion ( $E_k$ ), if it be activated, must certainly be less than  $\sigma_p b^3$  where  $\sigma_p$  is the Peierls' stress. This quantity is to be compared with that for double kink nucleation ( $E_n$ ) namely,  $30 kT$  (Dorn and Raynak, [28]). In the case of iron (28), for example,  $\sigma_p \sim 4 \times 10^9 \text{ dyn/cm}^2$  so that  $E_k < \sigma_p b^3 \sim 6 \times 10^{-14} \text{ erg}$  which is almost certainly a gross upper limit. Even so this limit is less than  $10 kT$  at all temperatures above  $\sim 60 \text{ K}$ .

Now, since the speeds of these motions are determined by exponential functions of the activation energies, it is clear that  $V_k \gg V_D$  at all temperatures above 60 K, as a gross upper limit. We conclude therefore that  $V_k \gg V_D$  over much, if not all, of the relevant temperature range. This result vindicates the assumption that on double-kink models the dislocations are essentially straight.

We now remark that internal stress fields are random in direction and thus that the local value of internal stress at some point on a *straight* dislocation is equally apt to be in such a sense as to aid as they are to retard the dislocation motion. In fact the sum of such forces exerted on the dislocation must tend to zero with increasing dislocation length. A little consideration now indicates that one might there expect a flow stress

$$S = S(T) - S_i \quad (28)$$

rather than that of eq (27).

Seemingly, this difficulty may only be obviated by supposing that kink speeds are comparable with the forward speed of the dislocation so that the dislocation may bend. But as we have seen this position is untenable.

Finally, we note that while it is possible to envisage particular configurations of obstacles such that the dislocations are indeed bent and so are

everywhere acted on by internal stresses which tend to oppose their motion this is irrelevant since it is required that eq (27) be valid in general.

We conclude then, that eq (27) is invalid for both the Peierls and dislocation models and, since this equation appears to be critical, that one should seek alternative processes.

We now return to a consideration of the ideas introduced in section III.

### B. DISLOCATION MOTION FOR A SQUARE ARRAY OF OBSTACLES

Consider a dislocation to move through a lattice containing point imperfections which impede its motion. Suppose for simplicity that these imperfections form a square array of side  $l$  in the slip plane of the dislocation. Suppose further that at a given instant the dislocation adopt the configuration indicated in figure 7 and that the dislocation is then on the point of breaking away from the restraints. Neglecting interactions, the elastic energy of a circular arc of dislocation in equilibrium under an applied stress  $\sigma_s$  is

$$E = \sigma_s^2 l^3 / 24\mu \quad (29)$$

where  $\mu$  is the shear modulus. If breakaway occurs this potential energy

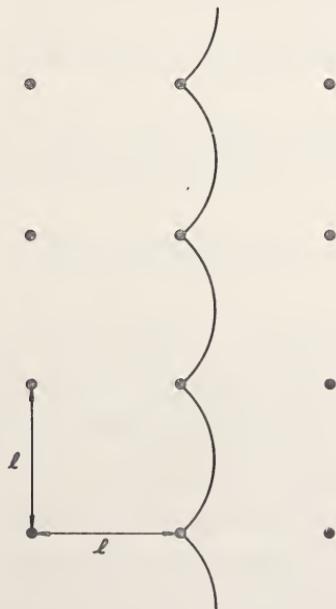


FIGURE 7. A dislocation traversing a square array of imperfections.

will in the main be converted into kinetic so that we may write

$$\frac{1}{2} \frac{\mu b^2 l V^2}{c^2} \cong \frac{\sigma_s^2 l^3}{24\mu} \quad (30)$$

where  $\frac{\mu b^2}{c^2}$  is the mass per unit length of dislocation,  $\mathbf{b}$  is the Burgers vector,  $c$  is the speed of sound and  $V$  the dislocation speed. We then find

$$V \cong \frac{\sigma_s l c}{2\sqrt{3}\mu b}. \quad (31)$$

We now write

$$\sigma_s = \alpha \frac{\mu b}{l} \quad (32)$$

where  $\alpha$  is a constant which denotes the specific strength of the locking process. In these terms we have

$$V \cong \frac{\alpha c}{2\sqrt{3}}. \quad (33)$$

It is of particular interest to note that  $V$  is independent of  $l$ , thus of the concentration of pinning points. Furthermore, for reasonable values of  $\alpha$ , e.g.,  $\alpha = 0.1$ ,  $V$  is a few percent of the speed of sound.

We now observe that there should exist a stress  $S$  such that the energy dissipated in motion between one set of pinning points and the next is just made up by the work done on the dislocation, namely  $Sb^2$  per unit length.

A solution to the relevant differential equation seems intractable even for the simplified case in which one considers a sinusoidally varying potential energy,

$$E = E_0 \left( \sin \left( \frac{2x\pi}{l} \right) + 1 \right) / 2.$$

Recourse was accordingly made to the use of a digital computer. The results of such calculations showed that  $S \propto B \sqrt{E_0} \propto BV_{\max}$ , provided the damping force  $BV_{\max}$  was small compared with that due to the potential gradient. It may be noted that  $V_{\max}$  has the same significance as does  $V$ . In cases where this proviso was not met it was found that with increasing  $B$ ,  $S$  approached a characteristic value equivalent to  $\sigma_s$ .

To recapitulate, we have seen that if a dislocation could be put in motion so as to overcome a barrier to its motion then that motion would continue using stresses smaller than those required to overcome the barrier in a static manner. We have also seen that the magnitude of the stress

required is  $BV$  where  $V$  is determined by the specific strength of the individual pinning processes and not at all on the separation of those points. These results are thus in accord with eq (21). In particular dislocation speeds determined in this way agree essentially with those found by fitting this equation to the experimental results.

An array of locking points such as we have considered will not occur in a real material and we shall now consider dislocation behavior for a more realistic arrangement of obstacles.

### C. DISLOCATION MOTION FOR A RANDOM ARRAY OF OBSTACLES

Unresolved in our considerations of the square array is the question of how the dislocation first gets into motion. This problem vanishes when we consider a random array. Thus, prior to motion the distances between recessive pinning points along the length of a dislocation are distributed at random about some length  $l_s$ . We suppose breakaway of some such length  $l$  when a stress

$$S = \frac{\alpha \mu b}{l} \quad (34)$$

is applied, provided the dislocation does not encounter a new obstacle before bending the required amount. The probability of finding such a length  $l$  is readily shown to be (cf Kocks, [28])

$$p = e^{-\frac{\alpha}{6} \left(\frac{l}{l_s}\right)^2} = e^{-\frac{\alpha}{6} \left(\frac{\sigma_s}{\sigma}\right)^2} \quad (35)$$

Whence we see that for  $\alpha = \frac{1}{10}$ ,  $l/l_s = 10$

$$p = \exp(-1.6)$$

so that such lengths should be relatively common. Accordingly, we may suppose that at stresses small compared with  $\sigma_s$ , dislocations will break away from their pinning points and once this has occurred our earlier considerations should apply in so far that motion should continue provided the applied stress is sufficient to make up for the damping losses.

The stress necessary for continued motion is not here so readily defined as for the square array. Thus, following the initial breakaway, the moving dislocation is apt to encounter a new pinning point so that we then have two moving lengths. The criteria for continued motion of either of these lengths is influenced by the angle turned by the dislocation at the outer pinning points. Sometimes this angle will be such as to make breakaway easier, sometimes harder.

For small stresses, in which case the probability of breakaway from all three pinning points is small, continued deformation implies that one or the other of these lengths breaks free and the whole dislocation line advances piecewise so that the mean velocity of the dislocation is very much smaller than the instantaneous velocity of a particular element of it. The analysis of this behavior is complicated by the presence of random internal stresses and this matter has not been resolved.

When the applied stress is large enough, the dislocation will tend to advance as a whole. One may then compute an average dislocation velocity for a dislocation surmounting a series of potential hills. Since such averages are necessarily dominated by the dislocation behavior near the top of those hills one must anticipate results which will fit the form

$$V \propto S^m \quad (36)$$

where  $m = m(S)$  and  $m(S)$  is a function which decreases monotonically to 1 with increasing  $S$ .

We have finally to remark that we have taken no account of thermal activation. Clearly, this process will be important in the initial activation of dislocation motion. However, in these considerations it has no influence on the temperature dependence of the flow stress since its role is simply that of a trigger and is not involved in the general process of deformation.

#### IV. Summary

We have seen that the Boltzmann equation theory gives a good account of the energy dissipated by a dislocation moving through a metal arising from its interaction with conduction electrons. If one assumes that the conduction electrons screen the positive charge shift associated with the dislocation perfectly, the drag coefficient for an edge dislocation is found to be temperature independent and is in good agreement with Holstein's scattering calculation [3], and with low temperature ultrasonic [22, 23] and yield stress [20, 21] measurements on f.c.c. metals. When one uses the static dielectric screening function of eq (19) or the approximation to it given by eq (20), a large temperature dependent drag is found which is proportional to the d-c conductivity of the metal. It is suggested that this may be the origin of the large temperature dependent yield and flow stresses observed in b.c.c. metals. The difference in the electronic screening is thought to occur because the core distortion of an f.c.c. dislocation is spread out over a considerably larger region of the lattice than in the b.c.c. case. The drag on a screw dislocation via this mechanism is found to be small compared to the edge dislocation drag, and increases with temperature.

The problem of a dislocation moving in an applied magnetic field parallel to its length and perpendicular to its velocity is also considered. In the perfect screening approximation, oscillations of the cyclotron resonance type in the stress or drag coefficient are predicted which could be as large as 10 to 30 percent of the zero field value. If one uses the screening function of eq (19), these effects are found to be drastically reduced. Such experiments should therefore be quite useful in clarifying the situation as regards the difference between f.c.c. and b.c.c. metals.

A verification of the temperature dependent electronic drag of eq (21) by an improved scattering theory would be highly desirable. It seems clear that a modification of Holstein's (4) calculation to include a more general deformation potential such as Brown's will make little change in his result. It also seems unlikely that the desired result will be obtained by carrying the calculation to second order in perturbation theory to include the effect of thermal vibration on the deformation potential. Perhaps a better approach would be to try to justify the use of a screening function like eq (19) in eqs (2) or (4) and subsequently in eq (1a), by following a procedure similar to that of Holstein and co-workers [30, 31]. They have shown that for long wavelength acoustic phonons the energy conservation laws in the scattering expression for  $(\partial f_k / \partial t)_{\text{coll.}}$  are modified to a form which corresponds to a delta function,

$$\delta[(E_{\mathbf{k}'-\mathbf{mu}/h} + V_{D\mathbf{k}'}(\mathbf{r}, t)) - (E_{\mathbf{k}-\mathbf{mu}/h} + V_{D\mathbf{k}}(\mathbf{r}t) \mp h\omega_{qn})] \quad (37)$$

where  $V_{D\mathbf{k}}(\mathbf{r}, t)$  is similar to the usual deformation potential, and  $h\omega_{qn}$  is a phonon energy. This is the quantum mechanical justification of eq (1a). Whether or not some procedure similar to this can be carried out for short wavelength disturbances remains to be seen.

Turning to mechanical matters we have seen that if dislocations surmount obstacles in a dynamic manner we can anticipate a flow stress  $BV$  in which  $V$  is characteristic of the obstacles and is quantitatively a few percent of the speed of sound. We have also seen that there will exist a range of stress in which the average dislocation velocity behaves as  $S^{m(S)}$  where  $m(S)$  decreases monotonically with increasing stress to the limiting value 1.

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## Discussion: Closing Comments by R. M. Thomson

THOMSON: Listening to the papers of this session has brought to mind a few final thoughts with regard to the situation in semiconductors:

We seem to have finally come full circle on the original Shockley proposal that the presence of dangling bonds on dislocations implies both acceptor- and donor-like states. Another, very obvious point, which was again discussed some in the early days, is the mobility of charge on dislocations. If there is some kind of band state associated with the dislocations, the carriers should be mobile. Some early search was made for mobile carriers with negative results, but I believe both the possibility for device applications and the basic physics demand that one bring up this question once more. Limitations to the mobility will be produced by impurities trapped at the dislocations and various types of inhomogeneities such as nodal points, etc., but one should be able to design experiments to minimize these effects. On the other hand, if the band is narrow, then the electron state on the dislocation may have suffered a Mott-like transition to a non-conducting Heitler-London state. Also, the one-dimensional character of the charge distribution gives a very high effective mass due to correlation effects.

These are obviously interesting theoretical questions, but at this stage we probably need some guidance from the experimentalists.

In a somewhat different vein, is the question, how difficult will it be to work out a one-electron theory of the state on the dislocation? There still seems to be controversy about the ability to treat a large perturbation in the semiconductors. Callaway and Hughes claim to have had good results for the vacancy with the use of the Slater-Koster technique. In addition, one suspects it should be possible to combine the dislocation structure factor with some sort of pseudo-potential method for a first calculation. To the proposition that the Slater-Koster technique could be applied, A. M. Stoneham has made the following observation:

"The Slater-Koster method does not involve a perturbation expansion, but the problem it solves is only realistic at small perturbations. Experiment indicates the small perturbation assumption is not valid for the vacancy in silicon, and this is probably why Callaway and Hughes have been unable to reproduce any of the experimental results with the use of arbitrary parameters. I should emphasize that the corresponding difficulty does not arise in Green's function approaches to lattice dynamics in crystals with defects, except possibility in highly anharmonic crystals. Also, I should mention that there may be difficulty in defining the perturbing potential. It is well known, for example, that empirical pseudo-

potential fits to band structures are not unique, and usually involve arbitrary assumptions—e.g. spherical point symmetry. In short, whilst the Slater-Koster technique is an important tool, it is neither as fundamental nor as general as is often asserted."

Thus one suspects there is considerable room for some hard theoretical work on the electronic structure of dislocations in semiconductors.

# X PANEL: FUTURE DIRECTIONS FOR DISLOCATION THEORY

*Chairman:*                   **A. SEEGER**

*Panel Members:*           **N. W. ASHCROFT**

**A. C. ERINGEN**

**E. KRÖNER**

**J. LOTHE**

**A. A. MARADUDIN**

**J. A. SIMMONS**



## Questions Submitted to the Panel— “Future Directions for Dislocation Theory”

1. What more can be done with classical continuum dislocation theory?
  - a. static *vs* dynamic formalisms
  - b. discrete *vs* continuous distributions
  - c. linear *vs* nonlinear theories
2. What fruitful interactions can we expect between the ideas of dislocation theory and modern continuum mechanics?
3. What is the future for lattice calculations?
  - a. static theories
  - b. dynamic theories
4. Given an interatomic description, what is the best continuum approximation to it? For instance: If a long-range two-body potential suffices in the atomic system what is the appropriate continuum formalism? Or how may many body interactions be incorporated into a continuum framework?
5. Are there experimental techniques which can be employed to measure such microscopic phenomena as couple-stresses, non-local effects, disclinations, and incompatibilities, . . . . Perhaps high resolution microscopy, . . . ?
6. What are the prospects for our further understanding of thermally activated processes?
7. What quantum effects are likely to be important in dislocation theory? Conversely, what is the hope of doing more meaningful quantum calculations in dislocation theory?
8. Can we extend old analogies or uncover new analogies between dislocation theory and other field theories, particularly electromagnetism, hydro-dynamics, general relativity, quantum mechanics . . . ?
9. What are the prospects of producing a macroscopic plasticity theory based on meaningful microscopic parameters? How soon will we be able to contribute to technologically important subjects, such as fatigue, fracture, etc.?



# REPORT ON THE PANEL DISCUSSION: “FUTURE DIRECTIONS FOR DISLOCATION THEORY”

A. Seeger

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The chairman opened the discussion by comparing the assignment of the panel to that of “futurologists” who have the difficult task of predicting the further developments in the field of dislocation theory.

Fortunately, at present this task appears not to be nearly as delicate as it would have been some twenty years ago, when doubts about the existence of dislocations were wide-spread and when the first obstacle to overcome in talking to a large audience was to convince them that dislocations might exist at all. The chairman expressed the view that nowadays the main problem is the development of new methods and techniques for doing practical and reliable calculations rather than discovering new fundamental ideas.

In making dislocation theory a powerful tool in crystal physics, one should be aware of the progress made in neighbouring fields. For instance, the measurements of single crystal higher order elastic constants have rapidly improved during recent years. This progress makes possible numerical calculations on non-linear problems involving dislocations in *anisotropic* media. Further, it is to be expected that the development of dislocation dynamics proper and the theory of the interactions between dislocations and other fields in crystals (electrons, phonons, magnons, etc.) will play an important role in the near future. Another problem, which has been waiting for a solution since 1934 when dislocations were first applied to crystal plasticity, is the construction of a *macroscopic* theory of plasticity based on dislocation theory.

For the scientists attempting to make further progress in dislocation theory, the chairman recommended warmly the perusal of recent books on dislocation theory, such as those by Nabarro and by Hirth and Lothe in which the present status of the dislocation theory is recorded. This may help to avoid re-solving problems already solved and to concentrate on the outstanding open questions.

Before the panel and the audience was a list of nine questions prepared by J. Simmons, R. Bullough, and R. de Wit. Opening the discussions on these questions the chairman asked E. Kröner and J. Simmons to express their views about “What more can be done with classical continuum dislo-

cation theory." Kröner pointed out that the alternative between "discrete or continuum description" of dislocation arrangements (to which he referred as field and continuum dislocation theories) is somewhat analogous to the alternative between Lorentz's and Maxwell's theories of electromagnetism. However, this analogy is restricted by the fact that the dislocation lines are in general rather far apart, i.e., that the distances between them are usually much larger than the interatomic distance. As a consequence the average dislocation density is not a sufficient macroscopic measure of dislocation arrangements. Kröner proposed that a more satisfactory continuum description may be achieved by introducing point correlation functions in the sense of statistical mechanics. A further complication compared with electromagnetism arises from the irreversibility of the thermodynamic processes accompanying dislocation motion. This calls again for the use of statistical mechanics.

Comparing linear to non-linear dislocation theories Simmons emphasized the great advantage of the linear superposition principle valid in the linear theory. He recommended extended calculation of Green's functions and their use for solving dynamic and inhomogeneity problems in dislocation theory. Referring to a recent paper by Indenbom and Orlov, Simmons expressed doubts about the possibility of reducing general three-dimensional problems to two-dimensional problems and asked the audience for comments on this point. J. Lothe, A. Head, and K. Malén expressed the opinion that the basic result of the Indenbom-Orlov paper is correct and that it should be used to solve definite problems in order to check the practical usefulness of the method.

In reply to Simmons, Seeger stressed the importance of non-linear continuum theories for investigating those effects which vanish in the linear approximation, for instance the phonon scattering from dislocations. The theory has been developed to the extent that the handling of such problems is not much more complicated than that of linear problems, provided that the calculations are restricted to the first non-vanishing terms contributing to the effects to be investigated. Simmons remarked that when treating singular dislocations some lattice calculations are necessary anyway so that it is questionable whether the non-linear theory should be applied in such a case.

B. von Turkovich asked whether it is possible to demonstrate the uniqueness of the solutions of non-linear problems. Seeger answered that it is very difficult to prove uniqueness theorems for general non-linear problems. He mentioned that the recent treatise by Noll and Truesdell on non-linear field theories in the *Encyclopedia of Physics* contains existence and uniqueness theorems only for very restricted cases. In practice the relevance of a "solution" may often be judged by physical intuition when the non-linearity is small and the linear solution is known.

R. Thomson raised the question of the usefulness of continuum theories for solid state physics except when treating boundary-value problems. S. I. Ben-Abraham argued that continuum theories provide the simplest tool to deal with measurable quantities. N. Fox compared the present situation in the continuum theory of dislocations with that existing 10 years ago at the initial stage of the continuum theory of liquid crystals, when no definite solutions had yet been obtained. The recent successes of the latter theory justify an optimistic outlook for the future of the continuum theory of dislocations.

The chairman turned to the second question for the panel: "What fruitful interaction can we expect between dislocation theory and continuum mechanics" and invited E. Kröner and C. Eringen to comment on this subject.<sup>1</sup>

E. Kröner emphasized that one of the main objects of this interaction is the construction of a better continuum theory of plasticity, which is needed by people doing practical calculations on plasticity problems. To this end a closer co-operation between scientists working in dislocation theory and in continuum mechanics is necessary.

A. C. Eringen remarked that if in a precise continuum theory the phenomenological or constitutive coefficients can be determined experimentally or by theoretical considerations, the continuum theory holds promise of being a useful tool for materials science. Moreover by providing internally consistent theoretical frameworks, continuum theories may help to eliminate physically meaningless results obtained sometimes from statistical considerations, as for instance happened in the case of some statistical theories of liquids. He also stressed the importance of constructing dislocation theory as a boundary and initial value problem.

A. Head added that another important connection between micro- and macro-theories could be the prediction of the constitutive properties of new materials starting from the micro-phenomena that the metallurgist is going to put into these materials.

The chairman went on to propose discussing simultaneously the related third and fourth questions "What is the future for lattice calculations?" and "What is the best continuum approximation to a given interatomic description?"

A. Maradudin predicted a bright future for lattice calculations with the aid of high-speed computers in both static and dynamic theories. He admitted, however, that certain difficulties have to be overcome in picking suitable interatomic potentials and in imposing the boundary conditions, especially if a non-linear lattice theory is used. He remarked that from this point of view harmonic lattice calculations as done by Bullough, Hardy, and himself may be advantageous. Maradudin suggested that either the zero-temperature energy or the Helmholtz free energy of a crystal containing a dislocation could be calculated by the lattice dynamics theory, in

<sup>1</sup> See also below for the chairman's comments on this question.

order to get information about the Peierls barriers. Along the same line one could obtain the equation of motion of a dislocation loop which takes into account interactions with lattice vibrations.

J. Lothe asked if it would not be better to consider physical objects that are less sensitive to the choice of the interatomic potentials, such as jogs and kinks, even though their configurations are more complicated than those of a singular dislocation or a stacking fault. The chairman replied that such studies were in fact performed by F. Granzer and his group in Frankfurt am Main (Germany) for ionic crystals, the only class of crystals for which the interatomic potential is at present fairly well known.

N. Ashcroft expressed the opinion that recent work on the higher elastic constants is incredibly valuable for getting information about the pair potential of a perfect crystal. He wondered if similar information could be obtained about the structurally dependent part of the potential of a dislocated crystal provided the dislocation arrangement is known. The chairman answered that this procedure cannot be applied, since dislocation arrangements are far from thermodynamical equilibrium. Maradudin suggested that for the treatment of many problems, as, for instance, the phonon dispersion from dislocations, it is easier to avoid the use of pair potentials by doing all quantum-mechanical calculations in reciprocal space. A. Seeger supported this view and added that the pair potential formalism is only correct if second-order perturbation theory is sufficient to handle the problem.

R. Bullough doubted the applicability of Fourier transform methods for the study of the dislocation core and the stacking fault. He also expressed the opinion that the repulsive potential of ionic crystals is not sufficiently known and, therefore, the formation energy of defects is not accurately determined. Seeger replied that the Fourier transform methods have already been successfully applied for stacking faults. Concerning ionic solids he remarked that recent work by Lidiard and his group and by his own group furnished repulsive potentials in very good agreement with the measured elastic constants. With these potentials the formation energy of a vacancy in sodium chloride can now be calculated with an accuracy that presumably exceeds the accuracy of the experimental value. A. Maradudin wondered how non-central forces have been taken into account in the potential. A. Seeger answered that three-body forces were considered, but their contribution to the cohesive energies turned out to be merely about 1% or even less.

J. Hardy noted that when one works in reciprocal space for the static lattice theory the equations obtained in the long wavelength limit go over to the continuum equations. In this case there is no difficulty of matching a continuum to a discrete region. With regard to the formation energy of defects in ionic crystals Hardy mentioned that one should better calculate the

formation energies of the separate constituents of a Schottky pair rather than the total energy, as is usually done.

A. Seeger recommended the use of non-local theories to supplement the lattice description when these involve long-range forces and interactions of non-mechanical origin. Examples are electro- and magneto-strictive effects, for instance in calculations on defects in piezoelectric crystals.

F.R.N. Nabarro suggested that it would be worthwhile to study *exactly* the behavior of the dynamical Peierls force as the velocity tends to zero as well as the interaction between dislocations and phonons within the framework of the Frenkel-Kontorova model.

The chairman proposed to discuss the fifth question "Are there experimental techniques which can be employed to measure such microscopic phenomena as couple-stresses, non-local effects, disclinations, and incompatibilities?"

A. Maradudin pointed out two methods for the determination of the elastic constants describing non-local effects. The first method is the comparison of the frequencies of continuum vibrations with the results obtained by means of neutron spectroscopy. The second technique, applicable only to crystals without a centre of inversion, such as tellurium or calcite, is to measure the speed of propagation for right- and left-circularly polarized sound waves along the polar axis. The rotation angle of the polarization plane of the sound wave propagating along this axis is determined by the fifth-rank tensor which is the first-order correction term to the elastic constants when expanded in powers of the wave vector.

The chairman raised the question whether acoustical measurements justifying the introduction of additional elastic constants such as those required in theories with a non-symmetric stress tensor and couple-stresses have already been done. A. Granato answered that up to now there are no accurate experimental results requiring additional "elastic" constants.

R. deWit asked if the stresses around a singular dislocation given by the linear theory of elasticity have been checked experimentally.

A. Head answered that the strains around dislocations measured by electron microscopy are in agreement with the anisotropic linear theory of elasticity. In addition, it should be possible to determine uniquely the displacements around the dislocations on the atomic scale by high-resolution electron microscopy, without implying the validity of a continuum theory. J. Eshelby mentioned some other older photoelastic experiments done on gelatine cylinders by Volterra's pupils.

The time allotted to the panel discussion had now elapsed. Accordingly, the chairman thanked the organizers, the panel members and the audience, and underlined the good future prospects of various branches of dislocation theory. He appealed once more to a stronger co-operation

between scientists with different backgrounds, e.g., in crystal physics and continuum theories, for the future development of the theory.

At the request of the organizing committee, the panel chairman has added some written comments on questions not—or only briefly—treated in the discussions.

Question 2: What fruitful interactions can we expect between the ideas of dislocation theory and modern continuum mechanics? In the writer's opinion, dislocation theory has itself contributed substantially to the development of modern continuum mechanics, so that the two fields do not represent antitheses. Nevertheless, it may be said that in its narrower field the development of new ideas and, even more so, of methods useful for doing calculations in dislocation theory has on the average been far ahead of the approach known as "rational mechanics" despite statements to the contrary that may be found in the literature. With the present activity in theories of tearing and folding in connection with dislocation and disclination theory this situation is likely to continue for some time. Nevertheless, in the interest of uniformity and of the interchange of ideas the writer recommends to make use of the notations and some of the concepts that have emerged from the rational mechanics approach, as has been done in the paper submitted to this conference by Teodosiu and Seeger.

Question 6: What are the prospects for further understanding of thermally activated processes? Almost a complete session has been devoted to this important subject at this conference, and two review papers and the subsequent discussions have given a survey of the present situation. It appears that the additional complexities of thermally activated processes involving dislocations above and beyond those of thermally activated processes in gases or involving point defects in crystals have now been recognized. Considerable progress has been made to solve the specific difficulties associated with the extended nature of the dislocations, and certain simple general results have emerged. The open problems of thermally activated processes of point defect in crystals, e.g., those associated with the nature and the exact description of the transition state, remain in the dislocation problems *a fortiori* and should be attacked in the future. In the course of such refinements it will presumably be necessary to pay more attention to the detailed processes and rearrangements in the dislocation cores during the activation process than has been done hitherto. Such refined considerations will presumably also be required if one wants to obtain a better understanding of the temperature dependence of activation energies and entropies.

Question 7: What quantum effects are likely to be important in dislocation theory? Conversely, what is the hope of doing more meaningful quantum calculations in dislocation theory? Quantum effects will presumably be most important in problems of thermal activation. At low temperatures, the harmonic oscillators which are introduced in order to describe the vibrations of the dislocation lines should be treated by quantum statistics and not, as usually done, by classical statistics. This will lead to an additional temperature dependence of activation entropies and energies, and, if properly done, include the effects of zero-point motion. In addition, at very low temperatures there should be tunneling effects, which have been alluded to several times in the experimental literature on dislocations, for which a convincing treatment appears to have not yet been given.

The writer considers the prospects for doing meaningful quantum mechanical calculations, say on the structure of dislocations, as not very good as long as the present emphasis on the use of pseudo-potentials and second order perturbation theory in the electron theory of crystals continues. The disturbance of the regular crystalline arrangement in the dislocation core is much too large to be treated in a meaningful way by the methods which are at present used to describe, e.g., the phonon spectra of metals. A quantum mechanical calculation of the dislocation core in, say, a simple metal appears feasible with the present computer facilities, but requires theoretical concepts and methods different from those which are in vogue at present.

Question 8: Can we extend old analogies or uncover new analogies between dislocation theory and other field theories, particularly electromagnetism, hydrodynamics, general relativity, quantum mechanics . . . ? During the panel discussions the analogies of the continuum theory of dislocations to electromagnetism and hydrodynamics have already been commented on. Very fascinating appears the possibility of analogies to the general theory of relativity and cosmology. Several writers, including E. Kröner and his associates, and J. Brinkman, have commented on these questions. Unfortunately, the rather detailed considerations by J. Brinkman have so far appeared only in a very condensed form (IUTAM Symposium Freudenstadt/Stuttgart). They are particularly interesting at the present time when there is a widespread tendency to search for modifications, generalizations, or even supplantations of Einstein's theory of 1916. J. Brinkman belongs to those who believe that the conceptual foundations of the general theory of relativity ought to be revised, and he is of the opinion that the continuum theory of dislocations may serve as a useful guideline. It may be appropriate to remark that, as shown by the continuing work of Kondo and his school and that of Anthony, the general continuum description of dislocations and disclinations is itself a rapidly developing subject.

Question 9: What are the prospects of producing a macroscopic plasticity theory based on meaningful microscopic parameters? How soon will we be able to contribute to technologically important subjects, such as fatigue, fracture etc.? If one extrapolates from the past, the answer to the first of these questions can only be: "poor." This is deplorable, since the open problems are both intellectually challenging and technologically important. It should be recalled that these problems have been one of the principal incentives in the early developments of dislocation theory. In the writer's personal opinion the almost complete standstill in this area is due to not a small degree to the confusion that has been created during the last decade by poorly founded theories of work-hardening and preliminary but overemphasized experimental work on dislocation observation, which have brought the whole field into a state of disrepute. It is to be hoped that this state will soon end, so that good scientists will be attracted to the field in large numbers and that substantial progress can be made again.

#### **Acknowledgement**

The author wishes to thank C. Teodosiu and W. Frank for their assistance in condensing the oral discussion.

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