ANISOTROPIC ELASTICITY WITH APPLICATIONS TO DISLOCATION THEORY*

J. D. ESHELBY,† W. T. READ,‡ and W. SHOCKLEY‡

The general solution of the elastic equations for an arbitrary homogeneous anisotropic solid is found for the case where the elastic state is independent of one (say x_3) of the three Cartesian coordinates x_1, x_2, x_3. Three complex variables $z_{(l)} = x_1 + p_{(l)} x_2$ ($l = 1, 2, 3$) are introduced, the $p_{(l)}$ being complex parameters determined by the elastic constants. The components of the displacement (u_1, u_2, u_3) can be expressed as linear combinations of three analytic functions, one of $z_{(1)}$, one of $z_{(2)}$, and one of $z_{(3)}$. The particular form of solution which gives a dislocation along the x_3-axis with arbitrary Burgers vector (a_1, a_2, a_3) is found. (The solution for a uniform distribution of body force along the x_3-axis appears as a by-product.) As is well known, for isotropy we have $u_3 = 0$ for an edge dislocation and $u_1 = 0$, $u_2 = 0$ for a screw dislocation. This is not true in the anisotropic case unless the $x_1 x_2$ plane is a plane of symmetry. Two cases are discussed in detail, a screw dislocation running perpendicular to a symmetry plane of an otherwise arbitrary crystal, and an edge dislocation running parallel to a fourfold axis of a cubic crystal.

L'ÉLASTICITÉ ANISOTROPE ET SON APPLICATION À LA THÉORIE DES DISLOCATIONS

La solution générale des équations de l'élasticité pour un solide anisotrope, homogène est trouvée dans le cas où l'état élastique est indépendant d'une (mettons x_3) des trois coordonnées cartésiennes x_1, x_2, x_3. Trois variables complexes $z_{(l)} = x_1 + p_{(l)} x_2$, ($l = 1, 2, 3$) sont introduites, les $p_{(l)}$ étant des paramètres complexes déterminés par les constantes d'élasticité. Les composantes du déplacement (u_1, u_2, u_3) peuvent être exprimées comme des combinaisons linéaires de trois fonctions analytiques, une de $z_{(1)}$, une de $z_{(2)}$, et une de $z_{(3)}$. Une forme particulière de solution est trouvée, elle donne une dislocation le long de l'axe x_3 avec un vecteur de Burgers arbitraire (a_1, a_2, a_3). (En même temps apparait, comme sous-produit, la solution dans le cas d'une distribution uniforme de la force interne le long de l'axe x_3). Dans le cas d'isotropie, $u_3 = 0$ pour une dislocation-coin et $u_1 = 0$, $u_2 = 0$ pour une dislocation-vis. Ceci n'est pas vrai dans le cas d'anisotropie, à moins que le plan $x_1 x_2$ soit un plan de symétrie. Deux cas sont discutés en détail, une dislocation-vis perpendiculaire à un plan de symétrie d'un cristal, qui est d'autre part quelconque, et une dislocation-coin parallèle à un axe quaternaire d'un cristal cubique.

ANISOTROPE ELASTIZITÄT MIT ANWENDUNGEN AUF DIE THEORIE DER VERSETZUNGEN

Die allgemeine Lösung der Elastizitätsgleichungen für einen willkürlichen anisotropen Festkörper wird für den Fall angegeben, in dem der Elastizitätszustand von einer (zB. x_3) der drei Cartesischen Koordinaten x_1, x_2, x_3 unabhängig ist. Es werden drei komplexe Veränderliche $z_{(l)} = x_1 + p_{(l)} x_2$ ($l = 1, 2, 3$) eingeführt, wobei die $p_{(l)}$ komplexe Parameter sind, die durch die Elastizitätskonstanten bestimmt sind. Die Verschiebungskomponenten (u_1, u_2, u_3) können als lineare Kombinationen von drei analytischen Funktionen, nämlich als eine von z_1, eine von z_2 und eine von z_3, ausgedrückt werden. Eine spezielle Form der Lösung wurde für eine Versetzung in der x_3-Achse mit willkürlichem Burgers-Vektor (a_1, a_2, a_3) gefunden. (Als Nebenresultat ergibt sich die Lösung für eine gleichförmige Verteilung der Kraft entlang der x_3-Achse.) Bekanntlich gilt im isotropen Fall für eine Stufenversetzung $u_3 = 0$ und für eine Schraubenversetzung $u_1 = 0$ und $u_2 = 0$. Im anisotropen Fall trifft das nicht zu, ausser wenn die $x_1 x_2$ Ebene die Symmetrieebene ist. Zwei Fälle werden eingehend diskutiert: (1) Eine Schraubenversetzung, die senkrecht zu einer Symmetrieebene eines sonst willkürlichen Kristalles verläuft, und (2) Eine Stufenversetzung, die parallel einer der vierfachen Achsen eines kubischen Kristalles verläuft.

1. Introduction

This paper develops the general theory of anisotropic elasticity for a three-dimensional state of stress in which the stress is independent of one Cartesian coordinate. The general theory is applied to the dislocation theory of metals, which has reached a state where the refinement of allowing for anisotropy is sometimes justified. However, many other practical applications of the general elasticity results are possible, particularly in engineering stress analysis where the anisotropy of the material is important. The application in the present paper, however, is restricted to dislocation theory.

The problem has already been considered for edge dislocations in a previous paper [1].§ Unfortunately the assumption there that the problem can always be treated as one of plane strain is not justified unless the dislocation line runs perpendicular to a symmetry plane. In general the solutions given in [1] represent an edge dislocation plus a concentrated force at the origin along the dislocation line.

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†Department of Physics, University of Illinois, Urbana, Illinois, U.S.A.

‡Bell Telephone Laboratories, Murray Hill, New Jersey, U.S.A.

§We take the opportunity to correct some errors in [1]. On p. 904, line 5, *for* s'_{41} *read* s_{41}; p. 905, line 6 from below, *for* f_n *read* f'_n; p. 906, equation (8), *for* y^2 *read* $\lambda^2_1 y^2$, $\lambda^2_2 y^2$ respectively in the arguments of the first and second logarithms; p. 907, lines 4, 2 from below *for* (6) or (8) . . . (10) *read* (7) or (9) . . . (11); p. 910, line 8 from below, *for* case *read* ease.

In the following sections we determine successively:

(i) The most general three-dimensional state of stress in an elastically distorted region when the stress is independent of one Cartesian coordinate.

(ii) The most general analytic (continuous, continuously differentiable and single valued) distribution of stress in the region surrounding a cylinder parallel to the axis of constant stress. The excluded region may be a hole through the crystal or a line imperfection, i.e. a bad region in the sense used by Read and Shockley [2] and Frank [3].

(iii) The state of stress around a dislocation.

2. Notation and Basic Relations

Unless the coordinate axes are simply related to the axes of a crystal of high symmetry, the stress-strain relations will involve a large number of non-vanishing elastic constants. In the general case, which we shall treat, there are twenty-one elastic constants relating the six stress components and the six strain components. Clearly, unless some short-hand notation is employed, the formulas become hopelessly cumbersome and the meaning is obscured. We shall use the simple three-dimensional Cartesian tensor notation as a means of expressing lengthy relations in a concise and easily comprehended form.

Calling the rectangular coordinates x_1, x_2, and x_3 instead of x, y, z, we suppose that the elastic state is independent of x_3. Let u_i be the ith component of displacement where i can be 1, 2, or 3. *Italic subscripts* $i, j, k, \ldots$ will take the range 1, 2, 3 and *Greek subscripts* α, β, the range 1, 2. The component of stress acting in the ith direction on the plane normal to the jth axis is τ_{ij}. The strains e_{ij} are related to the partial derivatives of displacement by

$$e_{ij} = \tfrac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]. \tag{2.1}$$

The components of the strain tensor (2.1) are to be distinguished from the usual engineering strains which are not tensor components; they are equal to e_{ij} for $i = j$, but have twice the value (2.1) for $i \neq j$.

We shall use the customary summation convention, according to which summation is understood to be carried out over repeated ("dummy") subscripts.

The most general linear relation between stress and strain involves a fourth-order tensor C_{ijkl} and is given by

$$\tau_{ij} = C_{ijkl}\, e_{kl}. \tag{2.2}$$

Considerations of symmetry and energy conservation require that

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{klij}, \tag{2.3}$$

these relations being responsible for the fact that there are only twenty-one different elastic constants. The constants can be transformed from one set of axes x_i to another set x'_i by the relation

$$C'_{pqrs} = \cos(x_i, x'_p)\cos(x_j, x'_q)\cos(x_k, x'_r)\cos(x_l, x'_s)\, C_{ijkl}. \tag{2.4}$$

When the coordinate axes are along the axes of a cubic crystal all but three of the different elastic constants vanish.

3. Equilibrium Conditions

We shall first determine the most general solution for an equilibrium state of stress in a region of elastic distortion. In the present section the conditions of equilibrium will be investigated and formulas derived for the force on an internal surface. In the following section the equilibrium equations will be expressed in terms of displacement and the most general solution for both displacement and stress obtained. (By formulating the problem in terms of displacement we avoid having to deal with the compatibility conditions.) The expression for the force on an internal surface will be needed in section 5 in interpreting the general expression for an analytic distribution of stress.

We begin by considering the equilibrium of an element of material in the crystal. Since nothing varies with x_3 we take a cylindrical element with axis parallel to the x_3-axis. Let A be the cross section of the cylinder in the $x_1 x_2$ plane and let C be the closed curve bounding A. The force (per unit length) exerted across C by the material outside the cylinder is

$$F_i = \int_C \tau_{i\beta}\, n_\beta\, dc. \tag{3.1}$$

where n_1 and n_2 are components of the normal to C.

For the material inside C to be in equilibrium, it is necessary that an external force $-F_i$ should be exerted on the cylinder. We now distinguish two cases:

1. The curve C is a reducible circuit; that is, C can be shrunk to a point without passing outside the material or cutting through a singularity in the stress distribution.

2. The curve C is not a reducible circuit; instead it encloses either a hole through the material in which external forces could be applied, or a bad

region where the theory to be developed does not apply.

In case 1, clearly the resultant force F_i must vanish, since there is no physical mechanism for applying an external force in the interior of a crystal. Thus for any choice of the circuit C which does not enclose a hole or singularity, the line integral in (3.1) vanishes. This implies the existence of a vector having components ϕ_i defined throughout the good region by

$$\frac{\partial \phi_i}{\partial x_1} = \tau_{i2}, \quad \frac{\partial \phi_i}{\partial x_2} = -\tau_{i1}, \tag{3.2}$$

from which the equilibrium conditions for stress

$$\frac{\partial \tau_{i\beta}}{\partial x_\beta} = 0 \tag{3.3}$$

are readily obtained.

Conversely, if we begin with the equilibrium equations (3.3), we can prove that the functions ϕ_i exist and that $F_i = 0$ for any reducible circuit.

We now consider case 2 above, where C encloses a hole or singularity. Assume that C does not pass through any singular points, so that the equilibrium equations are satisfied and the ϕ_i exist at all points on C. Then (3.1) gives

$$F_i = \int_C d\phi_i = \Delta\phi_i \tag{3.4}$$

where $\Delta\phi_i$ is the change in $\Delta\phi_i$ in going once around the curve C. When $\Delta\phi_i \neq 0$, ϕ_i is multiple valued. Alternatively we may make a mathematical cut in the $x_1 x_2$ plane; ϕ_i is then single valued and has a discontinuity $\Delta\phi_i$ across the cut.

To summarize: every equilibrium state of stress can be represented by a vector with components ϕ_i, every set of three functions ϕ_i represents an equilibrium state of stress, and the discontinuities in the functions ϕ_i correspond to a resultant force on an internal surface.

Rather than derive the differential equations for the ϕ_i (which would involve the compatibility conditions), in the next section we shall formulate the problem in terms of displacement, which has a more direct physical meaning, and use the equations of equilibrium (3.1). The ϕ_i are then obtained by integration.

However, there are some special cases in which it is convenient mathematically to represent the state of stress in the $x_1 x_2$ plane by a function ϕ called the Airy stress function, which is related to ϕ_1 and ϕ_2 by

$$\frac{\partial \phi}{\partial x_2} = -\phi_1, \quad \frac{\partial \phi}{\partial x_1} = \phi_2. \tag{3.5}$$

The relations (3.5) and the existence of ϕ follow from (3.2) and the condition $\tau_{12} = \tau_{21}$.

Only in special cases can ϕ be treated independently of ϕ_3. In such cases it is sometimes more convenient to express the state of stress in the $x_1 x_2$ plane in terms of the single function ϕ rather than in terms of the two functions u_1 and u_2.

4. General Solution

In this section we shall determine the most general solution for the displacement and thence for the stress in a region of elastic distortion. The condition of elastic distortion necessarily excludes singularities in stress, so that at all points in the elastic region the equations of equilibrium (3.1) hold. By expressing stress in terms of displacement in the three equilibrium equations, we obtain three equations for the three components of displacement.

First substituting (2.1) in (2.2) we have

$$\tau_{ij} = \tfrac{1}{2} C_{ijkl} \frac{\partial u_k}{\partial x_l} + \tfrac{1}{2} C_{ijkl} \frac{\partial u_l}{\partial x_k}. \tag{4.1}$$

However, by (2.3) the third and fourth subscripts of the elastic constants can be interchanged so that

$$\tau_{ij} = \tfrac{1}{2} C_{ijkl} \frac{\partial u_k}{\partial x_l} + \tfrac{1}{2} C_{ijlk} \frac{\partial u_l}{\partial x_k}, \tag{4.2}$$

where the two terms on the right are seen to be equal since the dummy subscripts k and l go through the same set of values. Therefore, taking account of the fact that nothing varies with x_3, we have

$$\tau_{i\beta} = C_{i\beta k\alpha} \frac{\partial u_k}{\partial x_\alpha} \tag{4.3}$$

and equation (3.3) becomes

$$C_{i\beta k\alpha} \frac{\partial^2 u_k}{\partial x_\alpha \partial x_\beta} = 0. \tag{4.4}$$

This is a set of three second-order linear partial differential equations, the solution of which is given by an arbitrary function of a linear combination of the variables x_1 and x_2. Thus,

$$u_k = A_k f[p_1 x_1 + p_2 x_2] = A_k f[p_\alpha x_\alpha] \tag{4.5}$$

where the A's and p's are determined by substituting into (3.7) which gives

$$A_k p_\alpha p_\beta C_{i\beta k\alpha} = 0. \tag{4.6}$$

This equation has a solution for the vector A_1, A_2, A_3 only if the determinant of the coefficients vanishes. This determinant is a sixth-order polynomial in p_1 and p_2. It is obvious that in (4.5) we can always take $p_1 = 1$; (4.6) is then a sixth-order equation for p_2. It is shown in the appendix that since the energy density is always positive the roots are necessarily complex, and since the coefficients are real they occur in conjugate pairs. The vector $A_{(l)k}$ corresponding to a given root $p_{(l)}$ is in general complex. The condition that the displacements be real requires that the imaginary parts of corresponding pairs of solutions shall cancel. Thus we take only three roots $p_{(1)}$, $p_{(2)}$, and $p_{(3)}$, no two of which are complex conjugates, and set

$$u_k = \sum_{l=1}^{3} A_{(l)k} f_{(l)}[z_{(l)}] \tag{4.7}$$

where

$$z_{(l)} = x_1 + p_{(l)} x_2 .$$

It will be understood throughout that where complex expressions are used only the real part is to be taken. The subscripts in parentheses distinguish the three individual solutions corresponding to the three different values $p_{(1)}$, $p_{(2)}$, $p_{(3)}$ and are not to be confused with the subscripts denoting coordinate axes.

From (4.3) and (4.7) we find that the most general equilibrium distribution of stress in the elastic region is

$$\tau_{ij} = \sum_{l=1}^{3} [C_{ijk1} + p_{(l)} C_{ijk2}] A_{(l)k} \frac{df_{(l)}}{dz_{(l)}} [z_{(l)}] \tag{4.8}$$

and the corresponding functions ϕ_i, obtained by substituting (4.8) in (3.2) and integrating, are

$$\phi_i = \sum_{l=1}^{3} [C_{i2k1} + p_{(l)} C_{i2k2}] A_{(l)k} f_{(l)}[z_{(l)}] . \tag{4.9}$$

Alternatively we may verify directly that (4.9) agrees with the first of equations (3.2); that it also satisfies the second of (3.2) follows from (4.6) which now takes the form

$$A_k[C_{i1k1} + p_{(l)} C_{i1k2} + p_{(l)} C_{i2k1} + p_{(l)}^2 C_{i2k2}] = 0.$$

We shall find below that particular solutions of (4.7) can be found which represent dislocations lying on the x_3-axis or localized forces applied to the x_3-axis. In general to express any such situation it is necessary to combine terms arising from all three values of l. Thus in the subsequent analysis, solutions will be represented as sums over the three roots.

5. Continuous Distribution of Stress Surrounding a Singularity

In the previous sections we obtained a general solution valid at all points in a region where the distortion is elastic, i.e. in a good region. No restrictions were placed on the shape of the good region, nor was it assumed that the stresses were continuous. Actually the equilibrium equations, which hold in a good region, require that the tractions be continuous across any surface but leave open the possibility of a discontinuity in the normal stress on a plane perpendicular to the surface of discontinuity.

In the present section we shall assume that the distortion is elastic everywhere in the crystal except in a cylindrical region along the x_3-axis. This excluded region may be either a hole through the crystal or a line imperfection, or bad region, of the type discussed in section 1. The good region is therefore bounded by two cylindrical surfaces, the outer one being the external surface of the crystal.

In this section we shall also introduce the requirement that the stress in the good region be continuous, single valued and have continuous derivatives. We then investigate the conditions imposed on the arbitrary functions $f_{(l)}$ $[z_{(l)}]$ of the last section by the above conditions ((ii) of section 1) on the stress in the good region, and the shape of the good region. We shall reserve for the appendix the discussion of the most general solution consistent with these requirements, and use expressions for $f_{(l)}$ sufficient for the needs of physical dislocation theory.

From (4.8) we see that if τ_{ij} is to be analytic and single valued in a region of the crystal, it is sufficient (though not necessary, see the appendix) that $df_{(l)}$ $[z_{(l)}]/dz_{(l)}$ be an analytic single-valued function in the corresponding region of the complex $z_{(l)}$ plane, which will be bounded by two closed curves corresponding to the inner and outer boundaries of the actual region in the $x_1 x_2$ plane. Therefore by Laurent's theorem $df_{(l)}[z_{(l)}]/dz_{(l)}$ can be expressed as a power series with both positive and negative powers of $z_{(l)}$. Hence

$$f_{(l)}[z_{(l)}] = \frac{D_{(l)}}{\pm 2\pi i} \ln z_{(l)} + \sum_{n=-\infty}^{\infty} C_{(l)n} z_{(l)}^{\,n} \tag{5.1}$$

where for convenience in connection with (5.2) below the sign of $2\pi i$ is taken to be same as the sign of the imaginary part of $p_{(l)}$.*

It is at once seen that $f_{(l)}[z_{(l)}]$ is not a single-valued function since it changes by $D_{(l)}$ per revolution about the x_3-axis, the circuit being taken in the positive direction. Thus if we make a cut joining the

*A positive circuit around the origin of the $x_1 x_2$ plane is a $\pm$ circuit in the $z_{(l)}$ plane depending on the sign of the imaginary part of $p_{(l)}$. Note that there is no summation over l. Such a summation will always be indicated explicitly.

inner and outer boundaries there will be a discontinuity

$$\Delta u_k = \sum_{l=1}^{3} A_{(l)k} D_{(l)} \tag{5.2}$$

in the displacement across it.

All the other terms in (5.1) give single-valued displacements.

It is also seen, from (3.4) and (4.9), that the logarithmic term in (5.1) is the only one which contributes to the resultant force on the internal boundary

$$F_i = \Delta \phi_i = \sum_{l=1}^{3} [C_{i2k1} + p_{(l)} C_{i2k2}] A_{(l)k} D_{(l)}. \tag{5.3}$$

From (4.8) the stress corresponding to (5.1) is found to be

$$\tau_{ij} = \sum_{l=1}^{3} [C_{ijk1} + p_{(l)} C_{ijk2}] A_{(l)k}$$

$$\left\{ \frac{D_{(l)}}{\pm 2\pi i} \frac{1}{z_{(l)}} + \sum_{n=-\infty}^{\infty} n C_{(l)n} z_{(l)}^{\,n-1} \right\}. \tag{5.4}$$

From (5.4) it is seen that each value of l corresponds to two linearly independent stress distributions (two because the constants are complex) each giving a discontinuity in displacement and a force. In general all three l's are required to represent any state of stress, solutions for individual l's having no simple physical meaning. We shall later consider a simple case where two l's can represent the state of stress in the $x_1 x_2$ plane, the third l giving the stress components in the x_3 direction.

In the next section we shall discuss the terms in $D_{(l)}$ which represent dislocations and uniform distributions of force along the x_3-axis. The terms in $C_{(l)\pm n}$ enable us to satisfy arbitrary boundary conditions on the inner and outer cylindrical surfaces. The C's will not give a net force on a boundary (this is provided for by the D's) but in general the $C_{(l)-1}$ give a net couple on it.

For certain values of the elastic constants equation (4.6) may give multiple roots for p_2. Such cases are most easily dealt with by passing to the limit from a neighboring set of elastic constants for which this is not so (cf. [1]).

6. Dislocations

In this section we shall assume that the excluded cylindrical region is a line imperfection, or bad region. This requires the vanishing of the resultant force F_i exerted across the boundary between the good and bad regions since there is no mechanism whereby an external force could be applied to the bad region to maintain equilibrium.

In the previous sections we have found that for stress fields independent of x_3 the discontinuity in displacement is a constant. As is well known, in an actual crystal this constant must either vanish or be equal to a *lattice translation or slip vector* defined as *the shortest vector connecting two atoms in the crystal structure which have identical surroundings.* In a face-centered cubic metal, there are six possible slip vectors, one in each of the six [110] directions; in a body-centered cubic structure there are four possible slip vectors corresponding to the four [111] directions.

When the discontinuity in displacement vanishes, the bad region is either an extra row of atoms or a missing row. Since such a situation would be unlikely to occur unless two unlike dislocations on adjacent slip planes ran together we shall consider this as a special case of a dislocation array and proceed to investigate the stress field around a dislocation.

If the slip vector is a_k, the conditions for a dislocation are

$$\begin{aligned} \Delta u_k &= a_k\,, \\ F_i &= 0\,. \end{aligned} \tag{6.1}$$

We should also see whether there is a net couple on the inner boundary. It may be shown to vanish however we choose the $D_{(l)}$ (cf. [1]).
From (5.2) and (5.3), conditions (6.1) become

$$a_i = \sum_{l=1}^{3} A_{(l)i} D_{(l)} \qquad (i = 1, 2, 3), \tag{6.2}$$

$$0 = \sum_{l=1}^{3} A_{(l)k} D_{(l)} [C_{i2k1} + p_{(l)} C_{i2k2}] \qquad (i = 1, 2, 3). \tag{6.3}$$

Equations (6.2) and (6.3) are a system of six linear equations for the determination of the real and imaginary parts of $D_{(1)}$, $D_{(2)}$, and $D_{(3)}$. Thus in general all three l's are required to represent any simple dislocation. Similarly all three l's are required in the general case to represent a concentrated internal force at the origin.

In [1] it was assumed that a solution could always be found by taking $u_3 = 0$, that is, $A_3 = 0$. This is allowable in the sense that it will certainly represent some state of stress. For an edge dislocation it is then possible to prescribe the conditions $\Delta u_1 = a_1$, $\Delta u_2 = a_2$, $F_1 = 0$, $F_2 = 0$. F_3 is then determined and in general does not vanish unless $C_{\alpha\beta k3} = 0$. Hence, except when the $x_1 x_2$ plane is a symmetry plane, the expressions in [1] represent the dislocations they purport to, plus a force along the x_3-axis necessary to maintain a state with $u_3 = 0$. The presence of F_3 was overlooked in the original paper.

In an infinite body with the requirement that the stresses shall vanish at infinity, the $C_{(l)n}$ with $n > 0$ are excluded and so also is the more general type of dislocation considered in the appendix. Then along any straight line through the origin the stresses can be expressed as a series of inverse powers of $r = (x_1^2 + x_1^2)^{\frac{1}{2}}$. The term in r^{-1} is fixed by the $D_{(l)}$ and the higher terms by the $C_{(l)n}$, $n < 0$, that is, by conditions at the inner boundary. Thus at large distances from the origin the state of stress is determined solely by the Burgers vector.

By adjusting the $C_{(l)\pm n}$ we can make the outer surface of the cylinder stress-free. If we cut out a cylinder of finite length there will be a distribution of stress on the ends. This will have zero resultant, but not in general zero moment [4]. When these end stresses are removed the cylinder will thus be twisted and the u_i will not be independent of x_3 even if end effects are neglected.

7. Dislocations in Special Cases

In this section we consider the case where the $x_1 x_2$ plane is a plane of symmetry. Then the problem is considerably simplified in that the components of stress in the $x_1 x_2$ plane can be expressed in terms of derivatives of u_1 and u_2 only, and the stress components in the x_3 direction in terms of u_3 only; that is, $C_{\alpha\beta k3} = 0$. This means that the matrix expression for A_k splits so that A_3 does not mix with A_1 and A_2, or in other terms, $A_{(3)1} = A_{(3)2} = A_{(1)3} = A_{(2)3} = 0$.

We shall treat u_3 first for the general case where $x_1 x_2$ is a plane of crystal symmetry and then deal with u_1 and u_2 together for the more specialized case where the x_3-axis is a crystal axis in a cubic crystal. The latter results are implicit in [1], but we here carry the calculations out explicitly and reach an expression for the shear stress on any plane parallel to the slip plane of the dislocation. A knowledge of this quantity is sufficient for many problems; for example, determination of the possible stable arrangements of two-dimensional arrays of dislocations or calculation of the energies of single dislocations [1] and grain boundaries [5].

(a) *Screw Dislocation in a Simple Case*

It is convenient here to adopt a conventional notation, replacing the fourth-order tensor C_{ijkl} by the elastic constants $c_{11}, c_{12}, c_{13}, \ldots, c_{66}$, where the pair of subscripts 11 is replaced by 1, 22 by 2, 33 by 3, 23 by 4, 13 by 5, and 12 by 6. Then in the present symmetrical case where $c_{14} = c_{15} = c_{16} = c_{24} = c_{25} = c_{26} = 0$, we have

$$(7.1) \qquad \tau_{23} = c_{44}\frac{\partial u_3}{\partial x_2} + c_{45}\frac{\partial u_3}{\partial x_1}, \qquad \tau_{13} = c_{54}\frac{\partial u_3}{\partial x_2} + c_{55}\frac{\partial u_3}{\partial x_1}.$$

Substituting these into the equilibrium equation in the x_3 direction

$$(7.2) \qquad \frac{\partial \tau_{13}}{\partial x_1} + \frac{\partial \tau_{23}}{\partial x_2} = 0$$

gives an equation corresponding to (3.9) of the general case:

$$(7.3) \qquad c_{55}\frac{\partial^2 u_3}{\partial x_1^2} + 2c_{45}\frac{\partial^2 u_3}{\partial x_1 \partial x_2} + c_{44}\frac{\partial^2 u_3}{\partial x_2^2} = 0,$$

the solution to which is an arbitrary function of $x_1 + px_2$ where p is complex and is a root of

$$(7.4) \qquad c_{44}p^2 + 2c_{45}p + c_{55} = 0.$$

The two roots of (7.4) are complex conjugates and the condition that u_3 be real requires that the two solutions also be complex conjugates. We therefore take either root and set

$$(7.5) \qquad u_3 = f(x_1 + px_2),$$

where it is understood that only the real part of the complex right-hand side is to be taken. The condition that the stress be analytic requires that the arbitrary function be of the form (4.2) where only the logarithmic term need be considered here. We therefore express u_3 in terms of the complex constant D,

$$(7.6) \qquad u_3 = \frac{D}{\pm 2\pi i}\ln(x_1 + px_2).$$

If a_3 is the component of the slip vector in the x_3 direction we have: real part of $D = a_3$. From (4.9) the stress function ϕ_3 is

$$\phi_3 = [C_{3231} + p\, C_{3232}]f(x_1 + px_2),$$

or in the present notation

$$(7.7) \qquad \phi_3 = [c_{45} + p\, c_{44}]f(x_1 + px_2).$$

Therefore the vanishing of the net force $F_3 = \Delta\phi_3$ in the x_3 direction gives

$$(7.8) \qquad D(c_{45} + p\, c_{44}) = 0$$

which is the third of equations (6.3) for the present case and determines the imaginary part of D.

The stresses are then readily determined from (7.1).

When the axis of the dislocation is parallel to a crystal axis in a cubic crystal, $c_{45} = 0$ and $c_{55} = c_{44}$, so that equation (7.3) reduces to the Laplace equation, and u_3 and the associated stresses are given by the same formulas as in the isotropic case, the constant c_{44} being used for the shear modulus [6]. This leads to $z = x_1 + ix_2$ so that $\ln z = \ln r + i\theta$ in cylindrical coordinates. The first term represents a concentrated force along the x_3-axis, the second a screw dislocation. Another simple example of practical interest is a pure screw dislocation parallel to a $\langle 110\rangle$ direction in face centered cubic. Taking the x_1- and x_2-axes parallel to [110] and [011] respectively and using the elastic constants c_{11}, c_{12}, c_{44} referred to cube axes, we have $-p^2 = 2\, c_{44}/(c_{11} - c_{12}) = \beta^2$. It is convenient to express the two non-vanishing stress components in cylindrical coordinates:

$$\tau_{\theta z} = \frac{c_{44}}{2\pi\beta}\frac{a_3}{r}, \qquad \tau_{rz} = \frac{c_{44}}{2\pi\beta}\frac{a_3}{r}\frac{(1-\beta^2)\sin\theta\cos\theta}{\cos^2\theta + \beta^2\sin^2\theta}. \tag{7.9}$$

(b) *Edge Dislocation in a Simple Case*

We now consider the state of stress in the x_1x_2 plane when the axis of the dislocation is along the axis of a cubic crystal. As we have seen in the last section, u_3 can be treated independently and is the same as in the isotropic case. We thus have only two equations for the determination of the displacement and stress in the x_1x_2 plane, and there are two independent terms in the general solution which is of the form (3.8). The constants A_1, A_2, and p are given by (3.9) which in this case becomes

$$(C_{1111} + p^2C_{1212})\,A_1 + (C_{1122} + C_{1221})pA_2 = 0,$$
$$(C_{2211} + C_{2121})p\,A_1 + (C_{2112} + p^2C_{2222})A_2 = 0, \tag{7.10a}$$

or in terms of the small c's,

$$(c_{11} + p^2c_{44})\,A_1 + (c_{12} + c_{44})p\,A_2 = 0,$$
$$(c_{12} + c_{44})p\,A_1 + (c_{44} + p^2c_{11})\,A_2 = 0. \tag{7.10b}$$

The determinant vanishes for the four values of p given by

$$p_{(1)} = e^{i\alpha},\ p^*_{(1)} = e^{-i\alpha},\ p_{(2)} = -e^{i\alpha}, \qquad p^*_{(2)} = -e^{-i\alpha}, \tag{7.11}$$

where α is given by

$$\alpha = \tfrac{1}{2}\cos^{-1}\left[\frac{2c_{12}\,c_{44} + c_{12}^2 - c_{11}^2}{2c_{11}\,c_{44}}\right], \tag{7.12}$$

and is real for the common cubic metals (see the appendix). The corresponding eigenvectors A_k may be chosen with $A_1 = 1$ so that the values of $A_{(l)2} \equiv A_{(l)}$ are

$$A_{(2)} = -A_{(1)} = \frac{c_{44}\,e^{i\alpha} + c_{11}\,e^{-i\alpha}}{c_{12} + c_{44}}. \tag{7.13}$$

The general solution for the displacement is therefore

$$u_1 = f_{(1)}[z_{(1)}] + f_{(2)}[z_{(2)}]$$
$$u_2 = A_{(1)}f_{(1)}[z_{(1)}] + A_{(2)}f_{(2)}[z_{(2)}], \tag{7.14}$$

where $z_{(1)} = x_1 + e^{i\alpha}x_2$ and $z_{(2)} = x_1 - e^{i\alpha}x_2$. For an analytic distribution of stress the f's, as we have seen, are of the form (4.2) where only the logarithmic term need be considered. Expressing these functions in the form (6.1), we have to determine the two complex constants $D_{(1)}$ and $D_{(2)}$. These are given by (6.3) for the slip vector and (6.4) for the vanishing of the net force. For the present case (6.3) becomes

$$a_1 = D_{(1)} + D_{(2)},$$
$$a_2 = A_{(1)}\,D_{(1)} + A_{(2)}\,D_{(2)} = A_{(2)}[D_{(1)} - D_{(2)}]. \tag{7.15}$$

(6.4) becomes

$$0 = D_{(1)}[C_{1221}\,A_{(1)} + C_{1212}\,p_{(1)}] + D_{(2)}[C_{1221}\,A_{(2)} + p_{(2)}\,C_{1212}]$$
$$0 = D_{(1)}[C_{2211} + p_{(1)}\,C_{2222}\,A_{(1)}] + D_{(2)}[C_{2211} + p_{(2)}\,C_{2222}\,A_{(2)}]$$

which may be expressed in terms of c_{11}, c_{12}, c_{44} and α as

$$0 = [A_{(1)} + e^{i\alpha}][D_{(1)} - D_{(2)}]$$
$$0 = [c_{12} + c_{11}\,e^{i\alpha}A_{(1)}][D_{(1)} + D_{(2)}] \tag{7.16}$$

where, as throughout, only the real part of complex expressions are taken. Equations (9.7) and (9.8) are four linear equations for the real and imaginary parts of the two complex constants from which the displacements and then the stresses are obtained.

When the slip vector is in the x_1 direction so that $a_2 = 0$, we have

$$D_{(1)} = D_{(2)} = -\frac{a_1\,i}{2\sin 2\alpha}\left\{\frac{e^{2i\alpha}c_{11} - c_{12}}{c_{11}}\right\}. \tag{7.17}$$

The most important quantity to be determined in applications of dislocation theory is the shear stress on the slip plane. In the present case this is

$$\tau_{12} = c_{44}\left\{\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right\}$$
$$= a_1\frac{(c_{11}^2 - c_{12}^2)}{4\pi\,c_{11}\sin 2\alpha}\left[\frac{1}{x_1 + e^{i\alpha}x_2} + \frac{1}{x_1 - e^{i\alpha}x_2}\right]e^{i\alpha}$$

$$(7.18) \qquad = a_1 \frac{(c_{11}+c_{12})}{2\pi}\sqrt{\frac{c_{44}\,c'_{44}}{c_{11}\,c'_{11}}} \cdot \left[\frac{x\,(x_1^2 - x_2^2)}{(x_1^2+x_2^2)^2 - \dfrac{2(c_{11}+c_{12})}{c_{11}}\left\{1 - \dfrac{c'_{44}}{c_{44}}\right\} x_1^2\, x_2^2} \right]$$

where c'_{11}, c'_{12}, c'_{44} are the elastic constants referred to axes rotated counter-clockwise through 45° about the x_3-axis and are given by

$$(7.20) \qquad c'_{44} = \frac{c_{11} - c_{12}}{2}, \quad c'_{11} = \frac{c_{11} + c_{12} + 2c_{44}}{2}, \quad c'_{11} + c'_{12} = c_{11} + c_{12}.$$

APPENDIX

(i) *The General Solution: Wedge Dislocations*

The most general type of multiple-valued displacement consistent with continuous and twice-differentiable strains is known from the classical work of Weingarten and Volterra (see, for example, the review article by Nabarro [7]). From their results it appears that by assuming in section 5 that $df_{(l)}/dz_{(l)}$ is analytic and single valued we have excluded Volterra's dislocation of order VI. (The first three orders are included in the analysis of the text, whilst for orders IV and V the elastic state would not be independent of x_3.) Weingarten's and Volterra's results are very general, being essentially geometrical, and depending neither on Hooke's law nor the equations of equilibrium. Nevertheless it is interesting to see how the most general dislocation state arises in our analysis. The stress is assumed to be analytic and single valued; this is equivalent to assuming that the strain is single valued and analytic. Since the strain is somewhat more convenient to work with, we use (2.1) to obtain the strain corresponding to the general equilibrium solution (4.7). This gives

$$(A.1) \qquad e_{ij} = \sum_{l=1}^{3} A_{(l)i}\, p_{(l)j} + A_{(l)j}\, p_{(l)i} \frac{df_{(l)}}{dz_{(l)}}[z_{(l)}]$$

where $p_{(l)1} = 1$, $p_{(l)2} = p_{(l)}$, $p_{(l)3} = 0$ as in the text.

Equations (A.1) are a system of only five linear equations ($i = j = 3$ being trivial) for the real and imaginary parts of the three f's. Thus (A.1) can be solved for five of these functions in terms of the sixth function and the strains. For example if we let $df_{(l)}/dz_{(l)} = U_{(l)} + iV_{(l)}$ we can solve (A.1) for $U_{(l)}$ in terms of $V_{(l)}$ and e_{ij}. Differentiating this solution with respect to the real and imaginary parts of $z_{(l)}$ gives two equations for the first derivatives of $U_{(l)}$ and $V_{(l)}$, the real and imaginary parts of $z_{(l)}$ being taken as the independent variables. These two equations added to the Cauchy-Riemann equations make four equations, which can be solved for the four first derivatives in terms of the strains, which are analytic single-valued functions. Thus $d^2f_{(l)}/d^2z_{(l)}$ is an analytic single-valued function in the good region and, by Laurent's theorem can be represented by a series of positive and negative powers of $z_{(l)}$. Therefore the most general form of $f_{(l)}$ is

$$(A.2) \qquad f_{(l)}[z_{(l)}] = \frac{B_{(l)}}{\pm 2\pi i} z_{(l)} \ln z_{(l)} + \frac{D_{(l)}}{\pm 2\pi i} \ln z_{(l)} + \sum_{n=-\infty}^{\infty} C_{(l)n}\, z_{(l)}^n$$

the sign of $2\pi i$ being chosen as in the text.

(A.2) differs from the expression (5.1) only in the addition of the term in $B_{(l)}$. We now consider the physical meaning of the additional term.

Unlike the other constants in (A.2) the real and imaginary parts of the $B_{(l)}$ are not independent but are related by the five equations for the vanishing of the discontinuity in strain $\Delta e_{ij} = 0$ which from (A.1) and (A.2) gives

$$(A.3) \qquad \sum_{l=1}^{3} [A_{(l)i}\, p_{(l)j} + A_{(l)j}\, p_{(l)i}]\, B_{(l)} = 0.$$

Whatever new feature is introduced by admitting the terms in $B_{(l)}$ may thus be described by a single real constant. We shall now find the physical meaning of this constant.

First consider the force $F_i = \Delta\phi_i$ corresponding to the $B_{(l)}$. From (4.9) and the first term of (A.2) we have

$$(A.4) \qquad F_i = -\sum_{l=1}^{3} C_{i2k\alpha}\, p_{(l)\alpha}\, A_{(l)k}\, B_{(l)}\, z_{(l)}.$$

Remembering that $p_{(l)1} = 1$ and $p_{(l)3} = 0$, we can write (A.4) as

$$(A.5) \qquad F_i = -x_1\, C_{i2\beta\alpha} \sum_{l=1}^{3} p_{(l)\alpha}\, A_{(l)\beta}\, B_{(l)} - x_2\, C_{i2\beta\alpha} \sum_{l=1}^{3} p_{(l)\alpha}\, A_{(l)\beta}\, B_{(l)}\, p_{(l)\alpha}.$$

The first term vanishes because $C_{i2\beta\alpha}$ is symmetrical in α and β while by (A.3) the sum over l is unsymmetrical. This fact enables us to write the second term as

$$(A.6) \qquad F_i = -x_2\, C_{i\beta k\alpha} \sum_{l=1}^{3} p_{(l)\alpha}\, p_{(l)\beta}\, A_{(l)k}\, B_{(l)},$$

which vanishes by the equilibrium conditions in the form (4.6). Thus the $B_{(l)}$ give no contribution to the force and equation (5.3) for F_i in terms of the $D_{(l)}$ is still valid.

Let us now consider the discontinuity in displacement corresponding to the $B_{(l)}$ term in (A.2). This is

$$\text{(A.7)} \qquad \Delta u_k = \sum_{l=1}^{3} A_{(l)k} B_{(l)} p_{(l)\alpha} x_\alpha .$$

If we define

$$\text{(A.8)} \qquad \omega = \sum_{l=1}^{3} A_{(l)1} B_{(l)} p_{(l)2}$$

and make use of (A.3), (A.7) can be written in the vector form

$$\text{(A.9)} \qquad \Delta \bar{u} = \bar{\omega} \times \bar{X}$$

where $\bar{X}$ has components x_1 and x_2 and $\bar{\omega}$ is parallel to the x_3-axis and of magnitude ω (A.8). Thus the discontinuity in displacement corresponding to the $B_{(l)}$ term in the general expression (A.2) represents a rigid body rotation of the adjoining surfaces about the x_3-axis. This would occur if a cylinder were cut and sprung open or a wedge-shaped piece were cut out and the adjoining surfaces cemented together. In a crystal there would clearly be a relative rotation ω of the lattices on opposite sides of the cut, so that the wedge solution is inadmissible in applications to a crystal lattice.

(ii) *Proof that the $p_{(l)}$ are Complex*

The condition that the energy density be positive for any state of strain is

$$\text{(A.10)} \qquad C_{ijkm} e_{ij} e_{km} = C_{ijkm} \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_m} > 0$$

for any real set of e_{ij} or $\partial u_i/\partial x_j$ not all of which vanish.

Suppose that in (4.6), $p_1 = 1$ and p_2 is real. Then the ratios of the A_k found by solving the three equations (4.6) will be real. Hence the A_k may be chosen real and not all zero. Multiplying (4.6) by A_i and summing over i we have

$$A_i A_k p_\alpha p_\beta C_{i\beta k\alpha} = 0.$$

Accordingly the choice

$$\frac{\partial u_k}{\partial x_\alpha} = A_k p_\alpha \ (\alpha = 1, 2), \ \frac{\partial u_k}{\partial x_3} = 0$$

will lead to a zero energy density for a non-zero strain. Hence the assumption that p_2 is real is inadmissible.

We can also give a direct proof from the determinantal equation itself in the special cases considered. It is convenient to write (A.10) in the form

$$\text{(A.11)} \qquad \sum_{i=1}^{6} \sum_{j=1}^{6} c_{ij} e_i e_j > 0$$

with $e_{11} = e_1, \ldots, 2e_{23} = e_4, \ldots$. Putting $e_4 = p$, $e_5 = 1$, and the other e_i zero we have $c_{44} p^2 + 2c_{45} p + c_{55} > 0$, showing that the p of equation (7.4) cannot be real.

The quantity α (equation 7.12) can be written in the more expressive form

$$\alpha = \cos^{-1} \sqrt{\left\{ \tfrac{1}{2} \frac{1}{1-\sigma} \left(1 - \frac{1}{A} \right) \right\}}$$

where $\sigma = c_{12}/(c_{11} + c_{12})$ is Poisson's ratio for extension in the $\langle 100 \rangle$ direction and $A = 2\, c_{44}/(c_{11} - c_{12})$ is the "anisotropy factor" for a cubic crystal [8]. (We are indebted to Dr. H. Brooks for pointing this out.) We have to show that α is never purely imaginary. In (A.11) put successively $e_1 = 1$; $e_4 = 1$; $e_1 = \pm e_2$; $e_1 = e_2 = e_3$, with the unspecified e_j zero in each case. We find that c_{11}, c_{44}, $c_{11} \pm c_{12}$, $c_{11} + 2c_{12}$ are all positive. (Note that $c_{11} = c_{22} = c_{33}$ and $c_{12} = c_{23} = c_{31}$ in a cubic crystal.) From these relations we easily show that

$$-1 < \sigma < \tfrac{1}{2} \text{ and } A > 0.$$

It follows that $\cos \alpha$ is purely imaginary if $0 < A < 1$ or purely real and less than unity if $1 < A < \infty$, and so α is complex or purely real. From Table 3 of [8] it is seen that the common cubic metals fall into the class with real α.

The quantity β^2 introduced at the end of section 7a is equal to A and so the associated p is purely imaginary.

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