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NUMERICAL CALCULATION OF ELASTIC PROPERTIES FOR STRAIGHT DISLOCATIONS IN ANISOTROPIC CRYSTALS

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ABSTRACT

A computer program was written for the anisotropic elastic solution of a straight dislocation based on the formulas developed by A. N. Stroh [Phil. Mag. 3, 625 (1958)]. This program is applicable to a straight dislocation of arbitrary character and orientation in all crystal classes except monoclinic and triclinic systems. Direct applications for the analyses of dislocation interactions, the stability of a curved dislocation, and the displacement field with respect to a dislocation axis are discussed.

INTRODUCTION

The anisotropic elasticity theory of straight dislocations developed by Eshelby, Read, and Shockley[1] has been elaborated and applied by several investigators, as given in an extensive review by Hirth and Lothe.[2] In applying the theory to calculate the elastic properties of a straight dislocation, it is not always possible to obtain analytic expressions for the solutions. This difficulty results from a sextic equation, which, except for few simple cases, cannot be solved analytically. The special dislocation orientations for which analytic solutions can be obtained have been reviewed recently by Teutonico.[3]

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[1]J. D. Eshelby, W. T. Read, and W. Shockley, "Anisotropic Elasticity with Applications to Dislocation Theory," Acta Met. 1, 251 (1953).

[2]J. P. Hirth and J. Lothe, Theory of Dislocations, McGraw Hill Book Co., New York, 1968, p. 411.

[3]L. J. Teutonico, "Analytic Solutions for the Stress Fields of Dislocations in Anisotropic Media," Phil. Mag. 18, 881 (1968).

The original theory was modified into an alternate, but equivalent, form by Stroh[4] so that it could give analytic solutions in simplest possible form. Analytic expressions of the elastic solutions for a dislocation lying in a ⟨111⟩ direction in a cubic crystal have been obtained by this modified formulation.[5–7] Even for a more general case, for which analytic solutions are not tractable, the authors found earlier[8] that an efficient numerical calculation was possible by using Stroh's formulation. In the present study, the symmetry condition that the dislocation line lies normal to a reflection plane — the only restriction in the earlier work[8] — is eliminated so that numerical elastic solutions for the most general case are now available.

The purpose of this report is to present an efficient method of numerically calculating the elastic solutions for a straight dislocation of arbitrary orientation in an anisotropic medium. The elastic equations used for calculation are listed in the following section, and the subsidiary equations are presented in Appendices A and B. A computer program is given in Appendix C. As an illustration, the elastic fields of both screw and edge dislocations of $\frac{1}{2}\langle 111 \rangle$ Burgers vector in α-iron are computed and presented in equal-value contour plots. Finally, several applications of the present results are discussed by giving some typical examples.

ELASTIC EQUATIONS

The derivation of elastic equations is based on the formulas developed by Stroh.[4] Stroh's equations referenced in this report are prefixed

[4]A. N. Stroh, "Dislocations and Cracks in Anisotropic Elasticity," Phil. Mag. 3, 625 (1958).

[5]A. K. Head, "The [111] Dislocation in a Cubic Crystal," Phys. Status Solidi 6, 461 (1964).

[6]Y. T. Chou and T. E. Mitchell, "Stress and Dilatation Fields of the ⟨111⟩ Dislocation in Cubic Crystals," J. Appl. Phys. 38, 1535 (1967).

[7]J. P. Hirth and P. C. Gehlen, "Dislocation Displacement Fields in Anisotropic Media," J. Appl. Phys. 40, 2177 (1969).

[8]M. H. Yoo and B.T.M. Loh, "Characteristics of Stress and Dilatation Fields of Straight Dislocations in Anisotropic Crystals," J. Appl. Phys. 41, 2805–2814 (1970).

with an S. The relationships between the tensor notation and the contracted matrix notation (e.g., $ij \longleftrightarrow M$) are based on the convention given by Nye.[9] Both notations are used interchangeably. Three different types of subscripts are used; those of lower case Latin or Greek letters may take on values 1, 2, or 3; and those of capital Latin type may also take on values 4, 5, or 6. The summation convention is employed for repeated Latin indices, whereas summation over Greek indices will always be shown explicitly.

Dislocation Coordinate System

The dislocation line is parallel to the x_3 axis of a right-handed Cartesian coordinate system, and the unit sense vector $\underset{\sim}{\xi}$ points in the positive x_3 direction. The start-to-finish/right-handed convention[10] for Burgers vector $\underset{\sim}{b} = [b_1\ b_2\ b_3]$ is adopted such that $\underset{\sim}{\xi}$ coincides with $[0\ 0\ b_3]$ for a positive or right-handed screw dislocation, and the positive x_1 direction coincides with $[b_1\ 0\ 0]$ for a positive edge dislocation having "an extra half plane" or compressed zone in the positive x_2 direction.

Under the condition that the elastic solutions are independent of x_3, the generalized Hooke's law can be given by Eqs. (S65) and (S66) as

$$\epsilon_M = S_{MN}\sigma_N \ , \tag{1}$$

and

$$S_{MN} = s_{MN} - s_{M3}s_{3N}/s_{33} \ , \tag{2}$$

where S_{MN} are the modified elastic compliances, and s_{MN} are the elastic compliance constants referred to the x_i dislocation coordinate axes. In turn, s_{MN} are related to the elastic compliance constants s°_{MN} referred to the standard crystal axes x°_i by the transformation rule of fourth-rank tensors,

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[9] J. F. Nye, Physical Properties of Crystals, Oxford University Press, London, 1960, p. 131.

[10] The closed Burgers circuit is defined in a perfect crystal.

$$s_{ijkl} = a_{im}a_{jn}a_{ko}a_{lp}s^{\circ}_{mnop} \ , \tag{3}$$

where a_{ij} are the direction cosines of a coordinate transformation

$$x_i = a_{ij}x^{\circ}_j \ . \tag{4}$$

Sextic Equation

The sextic equation, the secular equation of the elasticity theory, is given in terms of S_{MN} by Eq. (S74) as

$$R_1R_2 - R_3^2 = 0 \ , \tag{5}$$

where

$$\begin{aligned} R_1 &= p_\alpha^4 S_{11} - 2p_\alpha^3 S_{16} + p_\alpha^2(2S_{12} + S_{66}) - 2p_\alpha S_{26} + S_{22} \\ R_2 &= p_\alpha^2 S_{55} - 2p_\alpha S_{45} + S_{44} \\ R_3 &= p_\alpha^3 S_{15} - p_\alpha^2(S_{14} + S_{56}) + p_\alpha(S_{25} + S_{46}) - S_{24} \ . \end{aligned} \tag{6}$$

The Eq. (5) has no real roots; its roots occur in complex conjugate pairs. The three roots with positive imaginary parts will be denoted by $p_\alpha = r_\alpha + iq_\alpha$ ($\alpha = 1,2,3$), with complex conjugates $\bar{p}_\alpha$, where r_α and q_α are real.

Stress Components

All the stress components can be given in the form

$$\sigma_{ij} = \frac{Kb}{2\pi}\sum_\alpha \frac{A_{ij\alpha}x_1 + B_{ij\alpha}x_2}{(x_1 + r_\alpha x_2)^2 + (q_\alpha x_2)^2} \ , \tag{7}$$

where b is the magnitude of Burgers vector $\underset{\sim}{b} = [b_1\ b_2\ b_3]$ and K is the energy factor. The coefficients $A_{ij\alpha}$, $B_{ij\alpha}$, and K are related to the roots of the sextic equation and hence to the elastic constants. The relationships between these coefficients as well as others to follow and the coefficients defined by Stroh[4] are given in Appendix A, and some relationships among $A_{ij\alpha}$ and $B_{ij\alpha}$ are given in Appendix B.

The dislocation line energy per unit length, E, is given[11] by

$$E = \frac{Kb^2}{4\pi} \ln\left(\frac{R}{r_o}\right) , \tag{8}$$

where r_o and R are the inner and outer cut-off radii.

Displacements and Strain Components

The three components of the displacement vector, $\underset{\sim}{u}$, may be given as

$$u_i = \frac{b}{2\pi} \left\{ \sum_\alpha \tfrac{1}{2} R_{i\alpha} \ln\left[(x_1 + r_\alpha x_2)^2 + (q_\alpha x_2)^2 \right] + \sum_\alpha T_{i\alpha} \tan^{-1}\left[\frac{q_\alpha x_2}{x_1 + r_\alpha x_2} \right] \right\}, \tag{9}$$

and their gradients, in more familiar form, as

$$\frac{\partial u_i}{\partial x_j} = \frac{b}{2\pi} \sum_\alpha \frac{P_{ij\alpha} x_1 + Q_{ij\alpha} x_2}{(x_1 + r_\alpha x_2)^2 + (q_\alpha x_2)^2} . \tag{10}$$

The coefficients $R_{i\alpha}$, $T_{i\alpha}$, $P_{ij\alpha}$, and $Q_{ij\alpha}$ are given in Appendix A, and some relationships among these coefficients are given in Appendix B. The strain components can be readily obtained from Eq. (10) by the definition

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) , \tag{11}$$

or from Eqs. (1) and (7).

Dilatation and Hydrostatic Pressure

The dilatation field, $\Delta = \nabla \cdot \underset{\sim}{u} = \epsilon_{ii}$, can be given as

$$\Delta = \frac{b}{2\pi} \sum_\alpha \frac{f_\alpha x_1 + g_\alpha x_2}{(x_1 + r_\alpha x_2)^2 + (q_\alpha x_2)^2} , \tag{12}$$

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[11] A.J.E. Foreman, "Dislocation Energies in Anisotropic Crystals," Acta Met. 3, 322 (1955).

where the coefficients f_α and g_α are related to the coefficients defined previously as given in Appendix A.

In a polar coordinate system (r,θ) the dilatation field is

$$\Delta = \frac{b}{2\pi} \cdot \frac{G}{r} , \tag{13}$$

where

$$G = \sum_\alpha \frac{f_\alpha \cos\theta + g_\alpha \sin\theta}{(\cos\theta + r_\alpha \sin\theta)^2 + (q_\alpha \sin\theta)^2} . \tag{14}$$

Similarly the hydrostatic pressure, $p = -\sigma_{ii}/3$, can be given as

$$p = \frac{Kb}{6\pi} \cdot \frac{H}{r} , \tag{15}$$

where

$$H = \sum_\alpha \frac{h_\alpha \cos\theta + k_\alpha \sin\theta}{(\cos\theta + r_\alpha \sin\theta)^2 + (q_\alpha \sin\theta)^2} . \tag{16}$$

The expressions for the coefficients h_α and k_α are given in Appendix A.

NUMERICAL CALCULATION

A FORTRAN computer program has been written based on the elastic equations presented in the previous section, and it is given in Appendix C. The essential steps of the program are depicted by a flow diagram in Fig. 1. This diagram may be divided into two parts, the input and the output, which correspond to the parts before and after the dashed line. Each step of the computation, as marked by an arrow, is carried out either with the equation quoted or with a subroutine program such as Transformation (TRNSFM) or Inversion (INV). It is the step marked by the dashed line that generally requires a numerical solution of the roots of a sixth-order polynomial.

Although the 39 coefficients together with the energy factor will suffice to give the elastic solution (σ_{ij} and u_i) as mentioned in Appendix B, all the coefficients defined in Appendix A are computed. The total computation time with the IBM system/360 model 91 is

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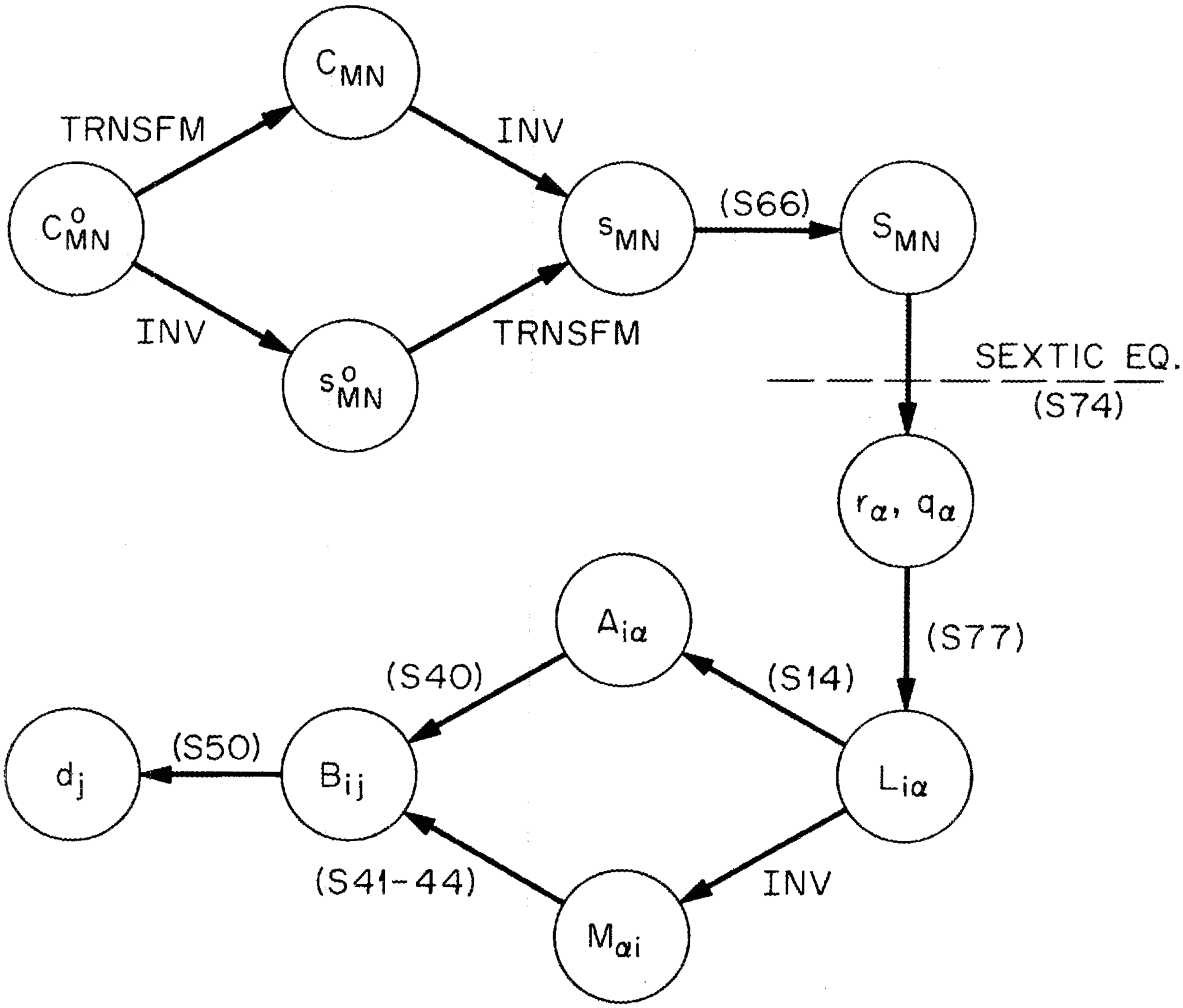

Fig. 1. Flow Diagram of the Essential Steps of Numerical Calculation.

approximately 15 sec and depends on the dislocation orientation with respect to the crystal axes.

RESULTS

The computer print-out of the results for screw and $(1\bar{1}0)$ edge dislocations in α-iron is given in Appendix D. The output gives the two vectors that define the slip plane and the dislocation coordinate system, the Burgers vector, the elastic constants at room temperature,[12] the energy factor, the sextic roots, and the coefficients $A_{m\alpha}$ and $B_{m\alpha}$, where $\alpha = 1,2,3$ and $m = 1,2\ldots23$. The correspondence between these coefficients and those defined in the text may be obtained unambiguously with the aid of Table 1.

Table 1. Correspondence Between the Results $A_{m\alpha}$ and $B_{m\alpha}$ and the Coefficients Defined in the Text

	σ_{ij}	$\frac{\partial u_i}{\partial x_j}$, ϵ_{ij}	Δ	p	u_i
m	1–6	7–16	17,18	19	21,22,23
$A_{m\alpha}$	$A_{ij\alpha}$	$P_{ij\alpha}$	f_α	h_α	$R_{i\alpha}$
$B_{m\alpha}$	$B_{ij\alpha}$	$Q_{ij\alpha}$	g_α	k_α	$T_{i\alpha}$

The results of σ_{ij}, ϵ_{ij}, Δ, and p are plotted in Figs. 2 through 5 as equal-value contour maps for the values of 0, ±2, ±4, ±6, ±8, ±10, ±12, and ±14 in units of $K/400\pi$ for σ_{ij} and p and in units of $1/400\pi$ for ϵ_{ij} and Δ.

For a $\langle 111\rangle$ screw dislocation σ_{23}, σ_{13} and ϵ_{23}, ϵ_{13} are the predominant stress components, whereas σ_{11}, σ_{22}, σ_{33}, σ_{12} and ϵ_{11}, ϵ_{22}, ϵ_{12} are relatively weak components, as shown in Figs. 2 and 3. These weak components are the ones that give rise to the tangential or angular

[12] J. Leese and A. E. Lord, Jr., "Elastic Stiffness Coefficients of Single-Crystal Iron from Room Temperature to 500°C," J. Appl. Phys. **39**, 3986 (1968).

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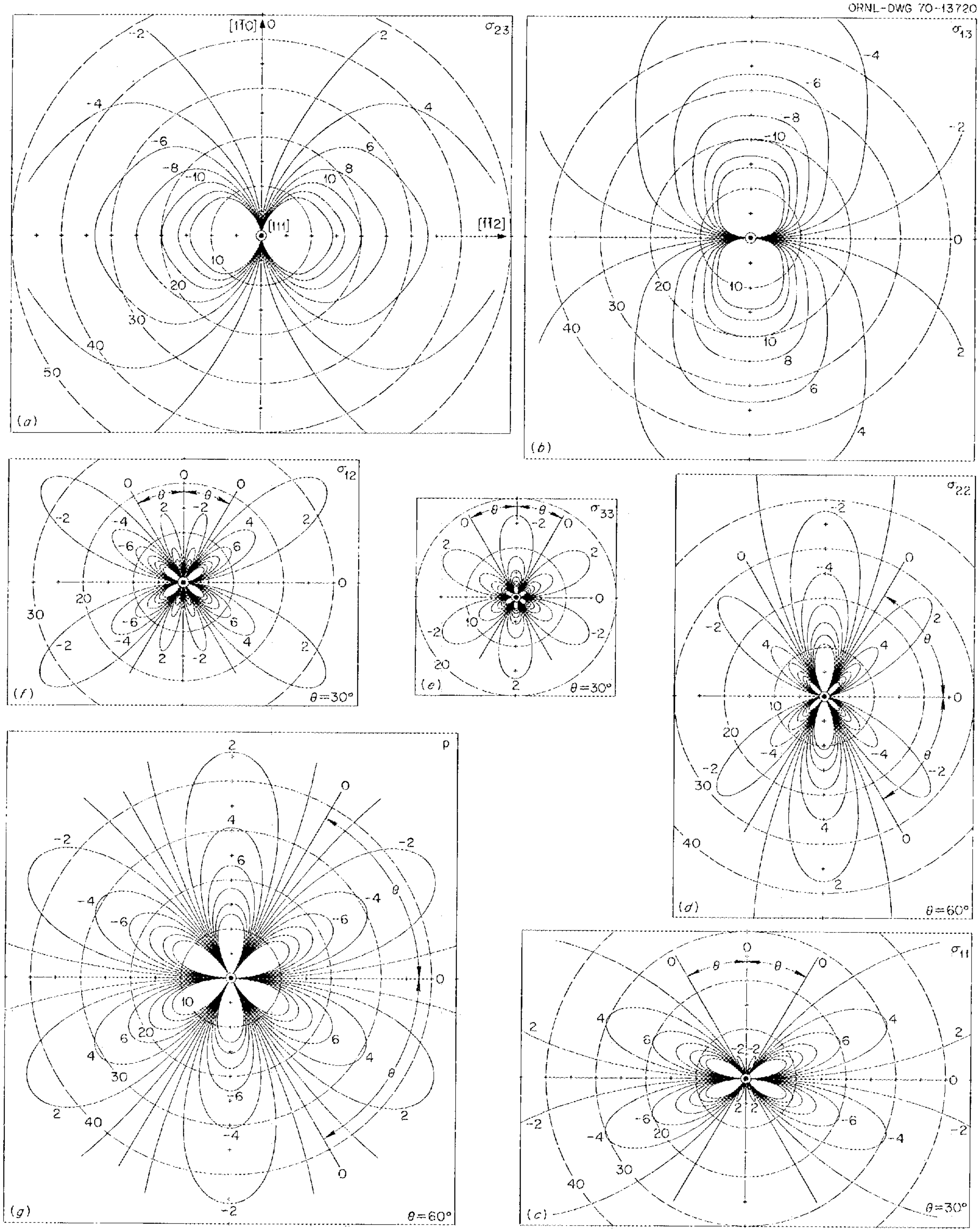

Fig. 2. Stress and Hydrostatic Pressure Fields of a Positive (Right-Handed) ⟨111⟩ Screw Dislocation in Iron. Unit of stress: $K_s/400\pi$. Unit of distance: b.

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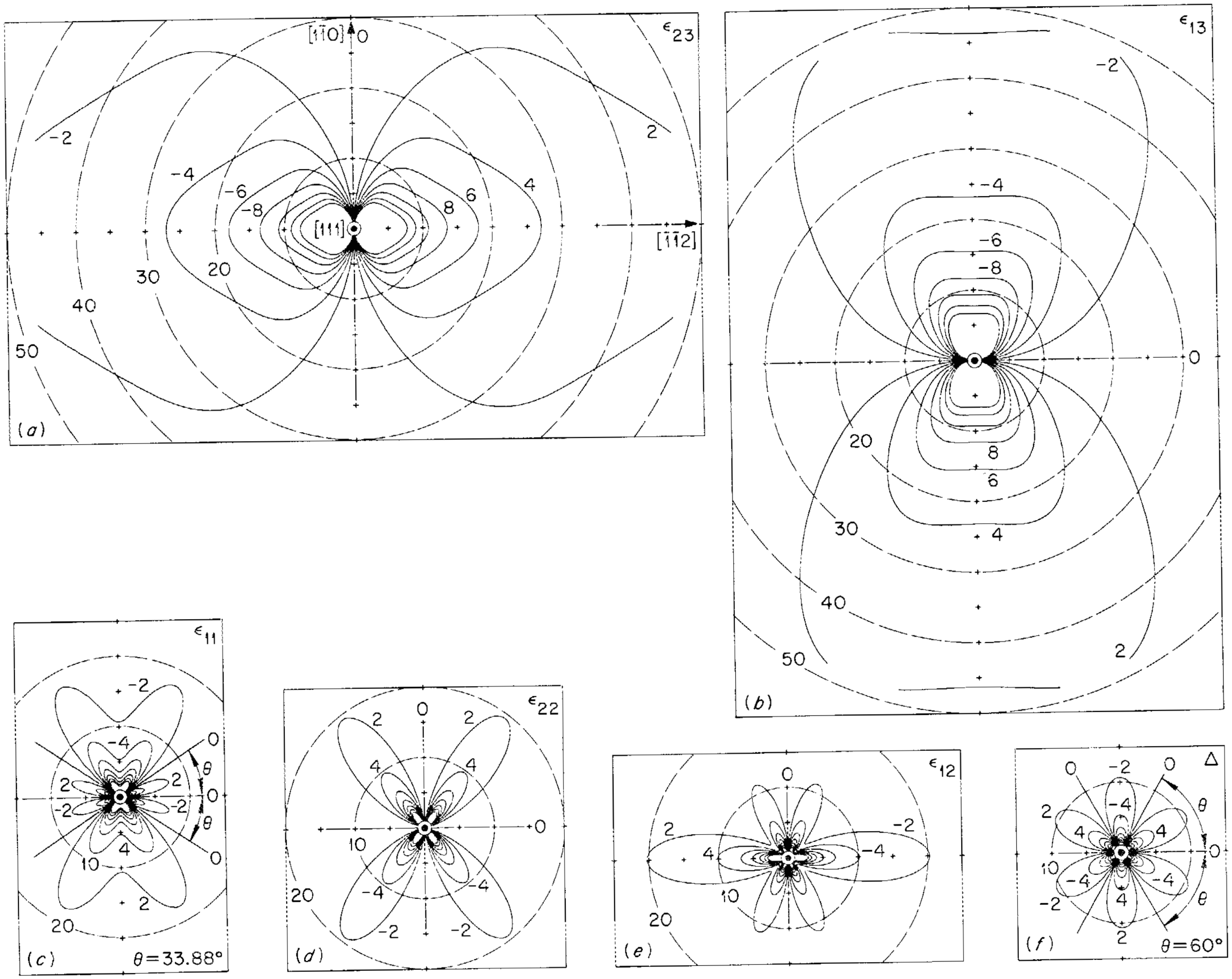

Fig. 3. Strain and Dilatation Fields of a Positive (Right-Handed) ⟨111⟩ Screw Dislocation in Iron. Unit of strain: $1/400\pi$. Unit of distance: b.

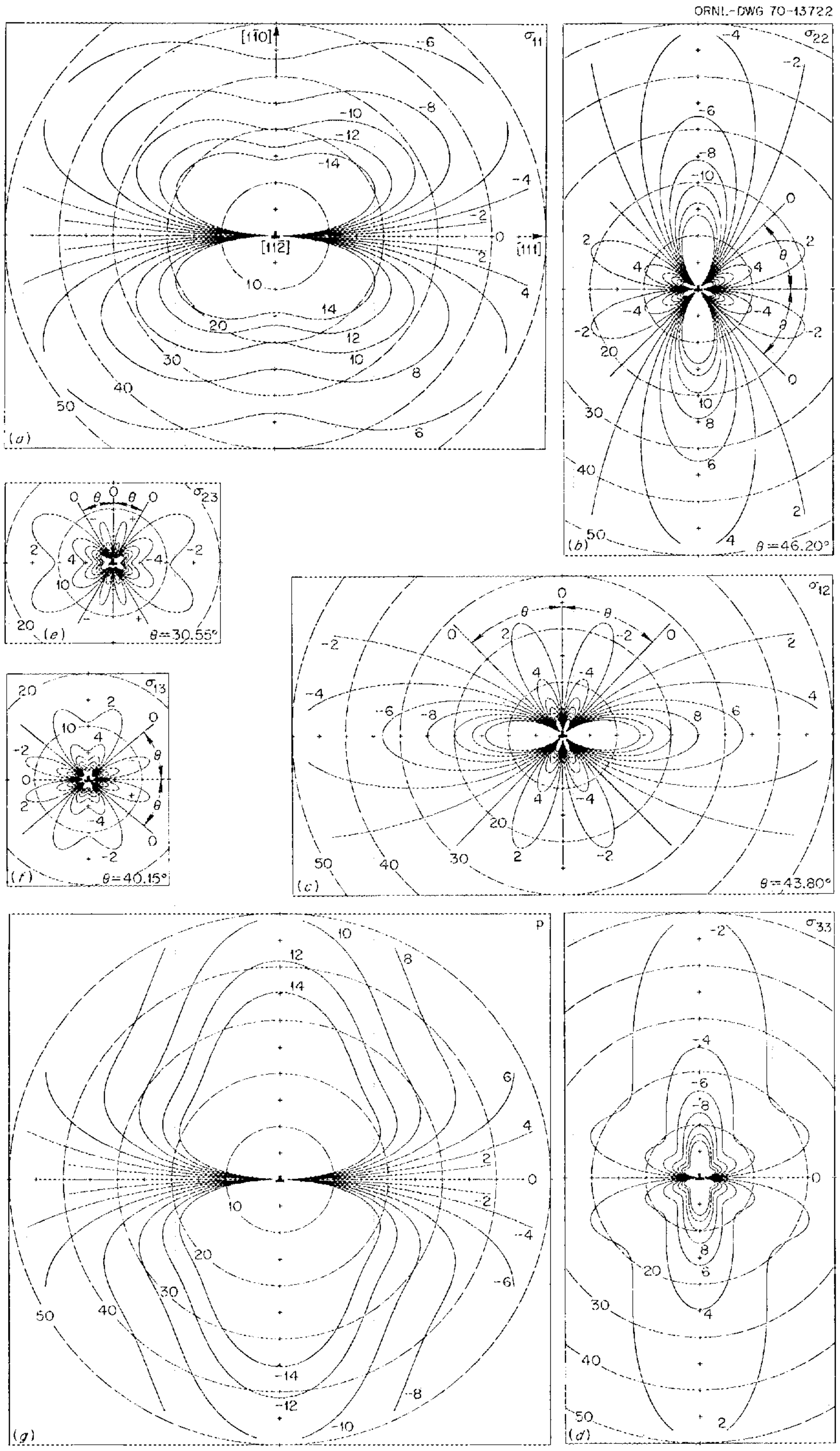

Fig. 4. Stress and Hydrostatic Pressure Fields of a Positive $\{1\bar{1}0\}\langle 111\rangle$ Edge Dislocation in Iron. Unit of stress: $K_e/400\pi$. Unit of distance: b.

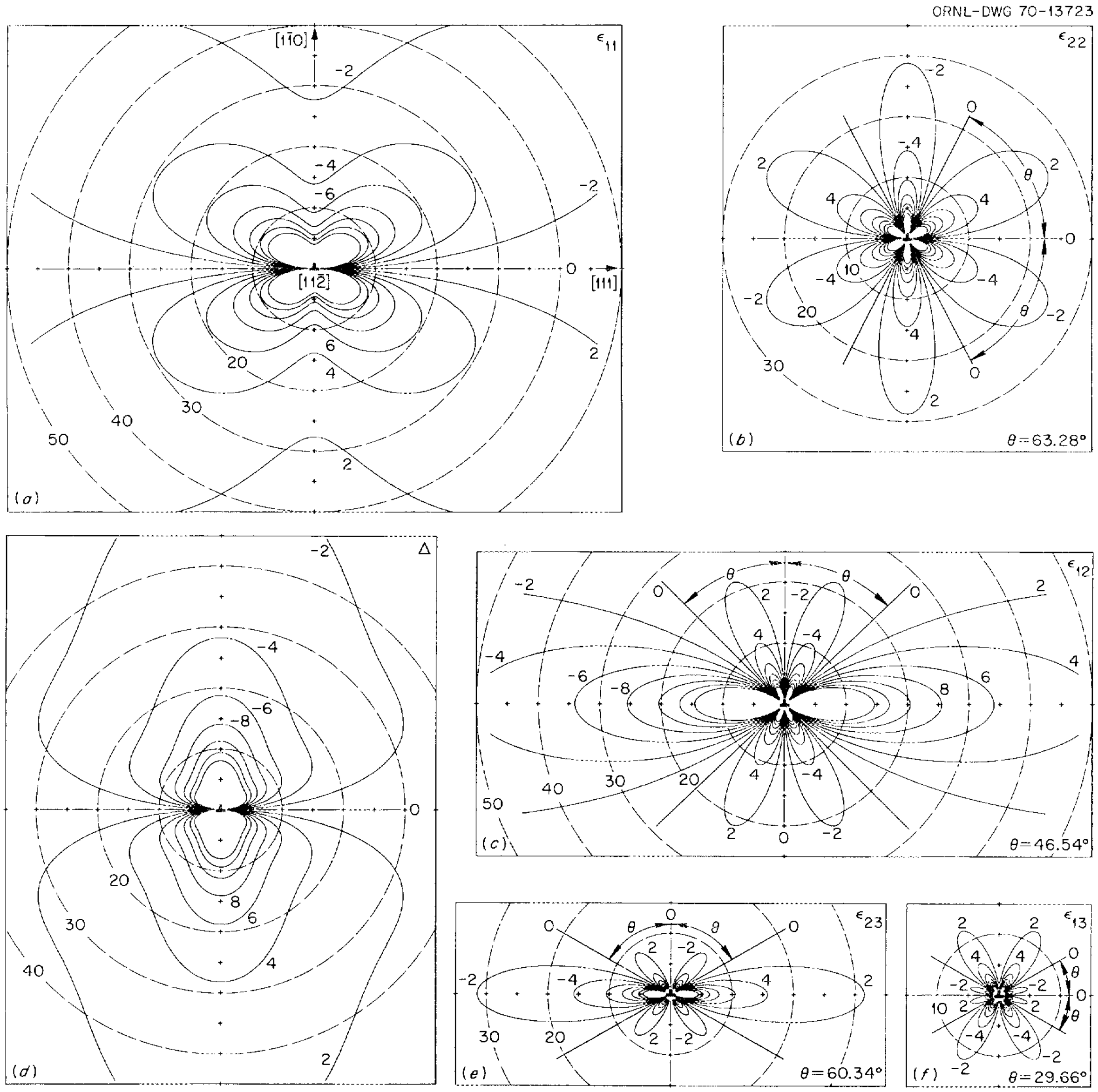

Fig. 5. Strain and Dilatation Fields of a Positive $\{1\bar{1}0\}\langle 111\rangle$ Edge Dislocation in Iron. Unit of strain: $1/400\pi$. Unit of distance: b.

components of interaction force between a pair of screw dislocations. These components are nonexistent under an isotropic condition. This tangential component of interaction force will be discussed further in the following section. The nonzero dilatation, Δ, and the corresponding hydrostatic pressure, p, around a $\langle 111 \rangle$ screw dislocation indicate the existence of the first-order size interaction[13] between a spherical point defect and the screw dislocation. This interaction is absent under an isotropic approximation.

For a $\{1\bar{1}0\}$ edge dislocation, the weaker stress and strain components, which are absent under an isotropic approximation, are σ_{23}, σ_{13} and ϵ_{23}, ϵ_{13}, as shown in Figs. 4 and 5. In the case of a $\{11\bar{2}\}$ edge dislocation, where the dislocation line lies normal to a reflection plane, all the nonzero elastic fields shown in Fig. 6 are asymmetric with respect to the dislocation axis.[14] The effects of asymmetric stress fields on dislocation interaction were discussed previously.[15]

The displacement components are plotted in polar diagrams in Figs. 7, 8, and 9. The amount of displacement based on the isotropic elasticity theory,[16] u_i^i, is subtracted from the corresponding anisotropic displacement components such that all the polar plots in Figs. 7, 8, and 9 are to diminish under an isotropic approximation. Since each displacement component obtained from the elastic solution is referred to an arbitrary origin of the coordinate system, one needs to find the exact location of the origin with respect to the crystal axis of the dislocation. The significance of this problem will be given in the discussion of applications.

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[13] R. Bullough and R. C. Newman, "The Kinetics of Migration of Point Defects to Dislocations," pp. 101–148 in Reports on Progress in Physics, vol 33 (1970).

[14] M. H. Yoo and B.T.M. Loh, "Structural and Elastic Properties of Zonal Twin Dislocations in Anisotropic Crystals," p. 479 in Fundamental Aspects of Dislocation Theory, National Bureau of Standards Spec. Publ. 317, ed. by J. A. Simmons, R. deWit, and R. Bullough, Washington, D.C., 1970.

[15] M. H. Yoo and B.T.M. Loh, "Characteristics of Stress and Dilatation Fields of Straight Dislocations in Anisotropic Crystals," J. Appl. Phys. 41, 2805–2814 (1970).

[16] J. P. Hirth and J. Lothe, Theory of Dislocations, McGraw Hill Book Co., New York, 1968, pp. 59, 75.

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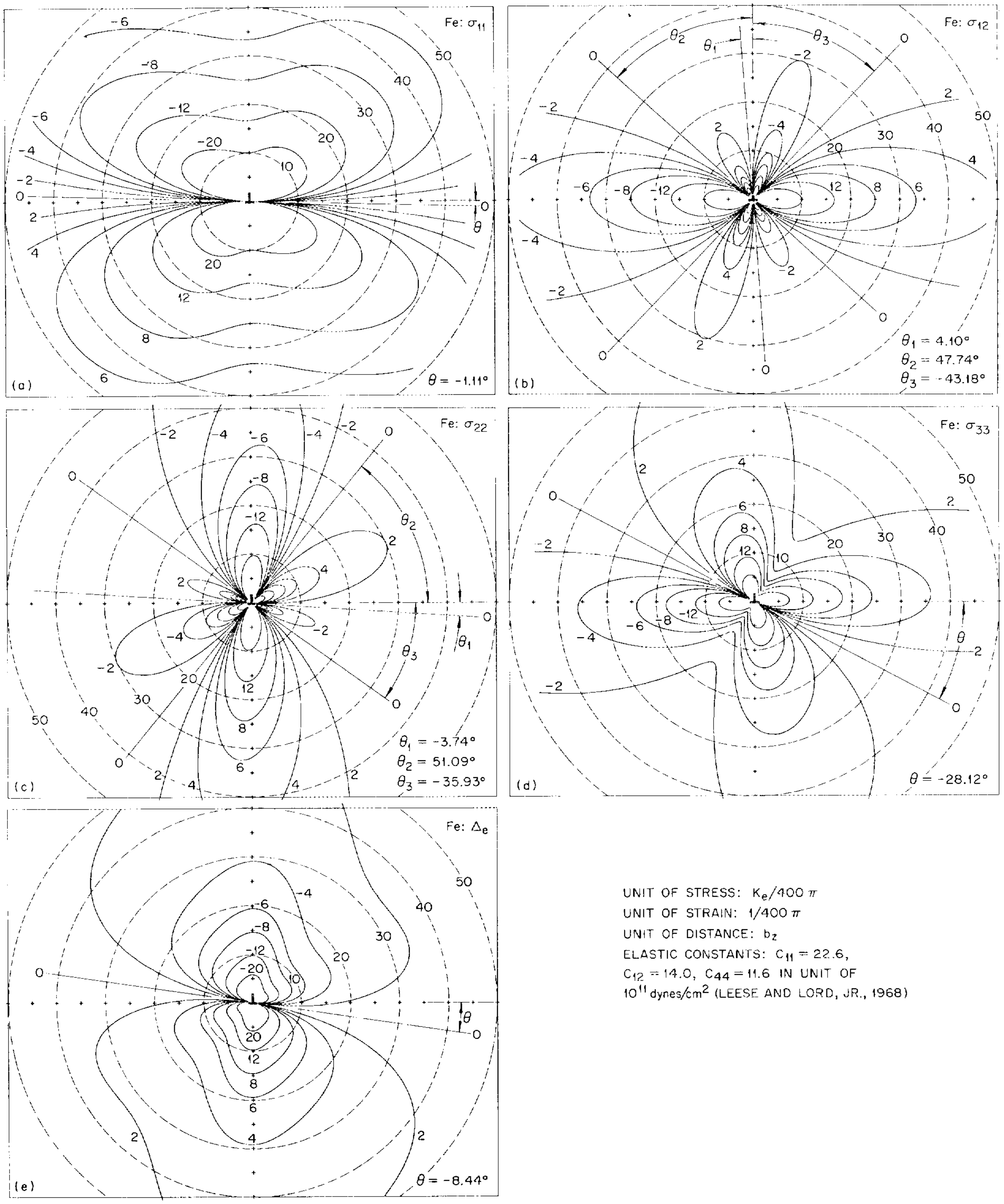

Fig. 6. Stress and Dilatation Fields of a Positive $\{11\overline{2}\}\langle 111\rangle$ Edge Dislocation in Iron.

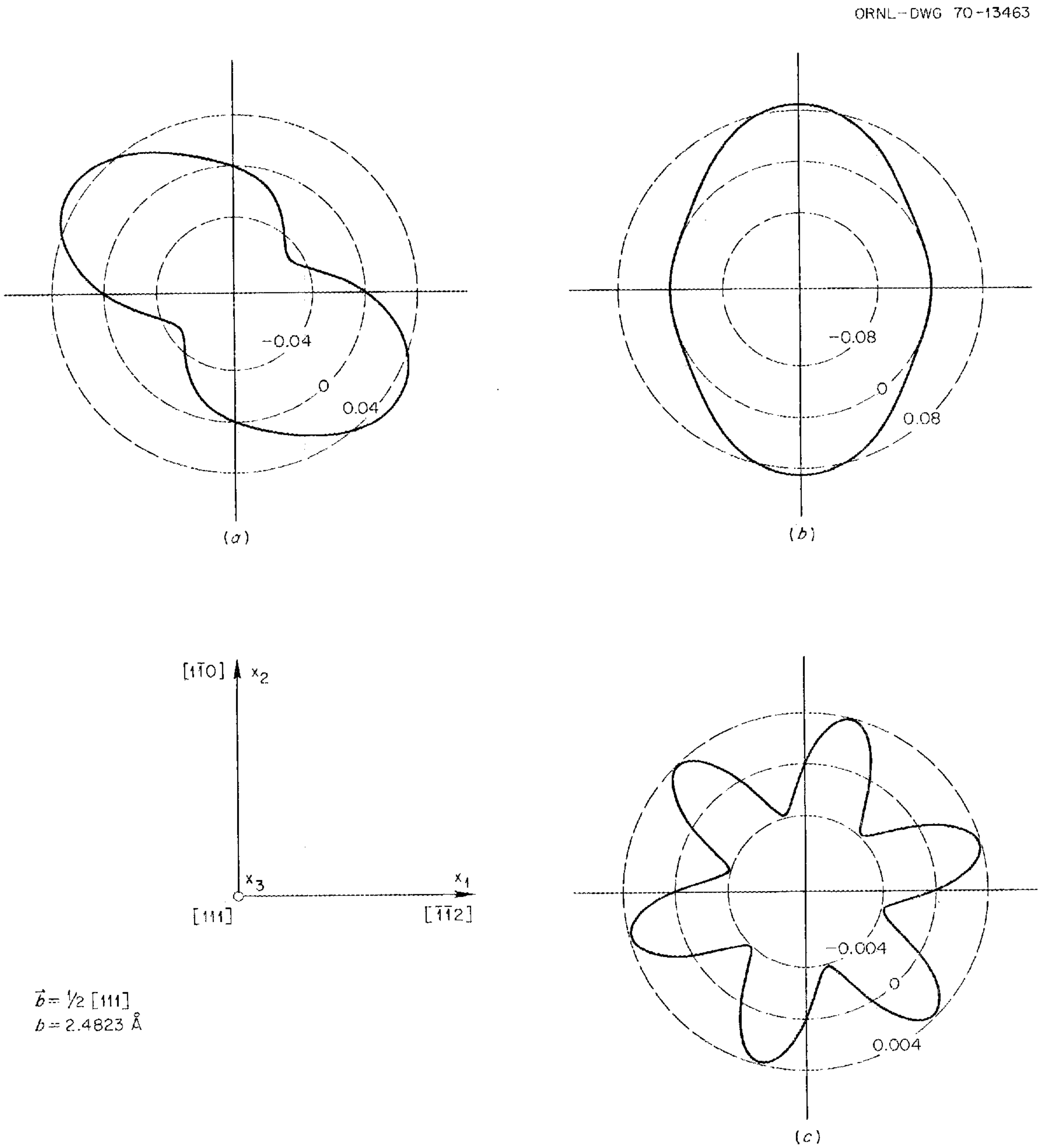

Fig. 7. Displacement Field of a Positive (Right-Handed) ⟨111⟩ Screw Dislocation in Iron. Three displacement components — (a) u_1, (b) u_2, (c) u_3-u_3^{I} — are given in angstroms by polar plots.

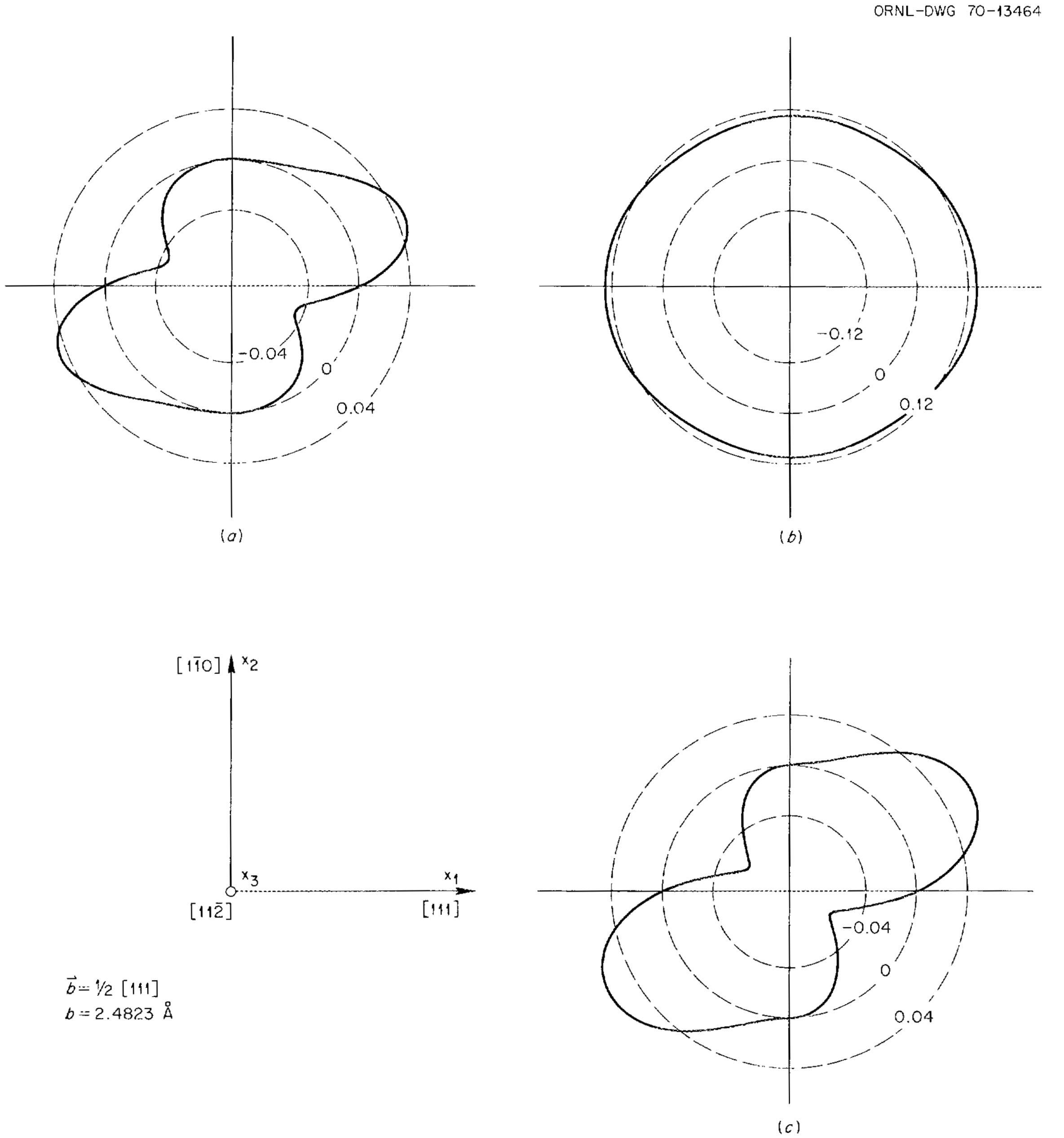

Fig. 8. Displacement Field of a Positive $\{1\bar{1}0\}\langle 111\rangle$ Edge Dislocation in Iron. Three displacement components — (a) u_1-u_1^1, (b) u_2-u_2^1, (c) u_3 — are given in angstroms by polar plots.

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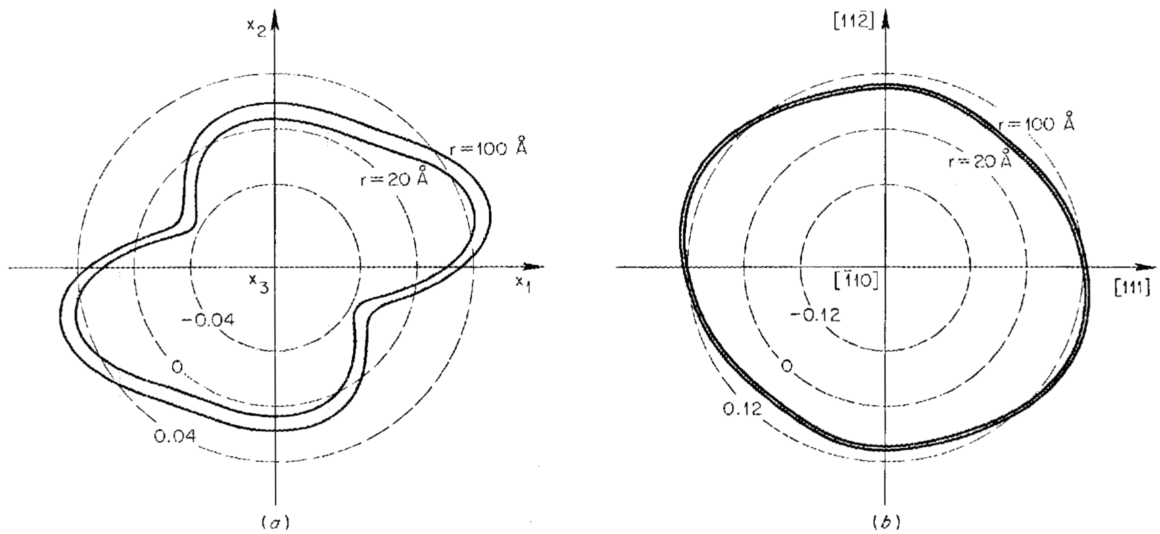

Fig. 9. Displacement Field of a Positive $\{11\bar{2}\}\langle 111\rangle$ Edge Dislocation in Iron. Two displacement components — (a) $u_1 - u_1^1$, (b) $u_2 - u_2^1$ — are given in angstroms by polar plots. $\vec{b} = (1/2)\,[111]$, $b = 2.4823$ Å.

When the coefficients $R_{i\alpha}$ have values such that $\sum_\alpha R_{i\alpha} \neq 0$, the displacement component u_i will be radially dependent. Such is the case for both displacement components of a $\{11\bar{2}\}$ edge dislocation (see Fig. 9). Significances and implications of this radial dependency will be discussed elsewhere.

DISCUSSION OF APPLICATIONS

Dislocation Interactions

The interaction force between two straight dislocation segments with arbitrary orientations may be obtained readily by substituting the appropriate stress components expressed by Eq. (7) into the Peach-Koehler formula [17]

$$F_\ell = \epsilon_{jk\ell} b_i^{(1)} \sigma_{ij}^{(2)} \xi_k^{(1)} , \tag{17}$$

[17] R. deWit, "Some Relations for Straight Dislocations," Phys. Status Solidi 20, 567 (1967).

where $\epsilon_{jk\ell}$ denotes the unit permutation tensor and $\xi_k^{(1)}$ denotes the unit sense vector $\underset{\sim}{\xi}$ for dislocation (1). The glide force F_1 and the total elastic energy U of an edge dislocation dipole consisting of a pair of dislocations (1) and (2) are given schematically in Fig. 10. The well-known isotropic case is depicted by a solid curve (a) that shows two

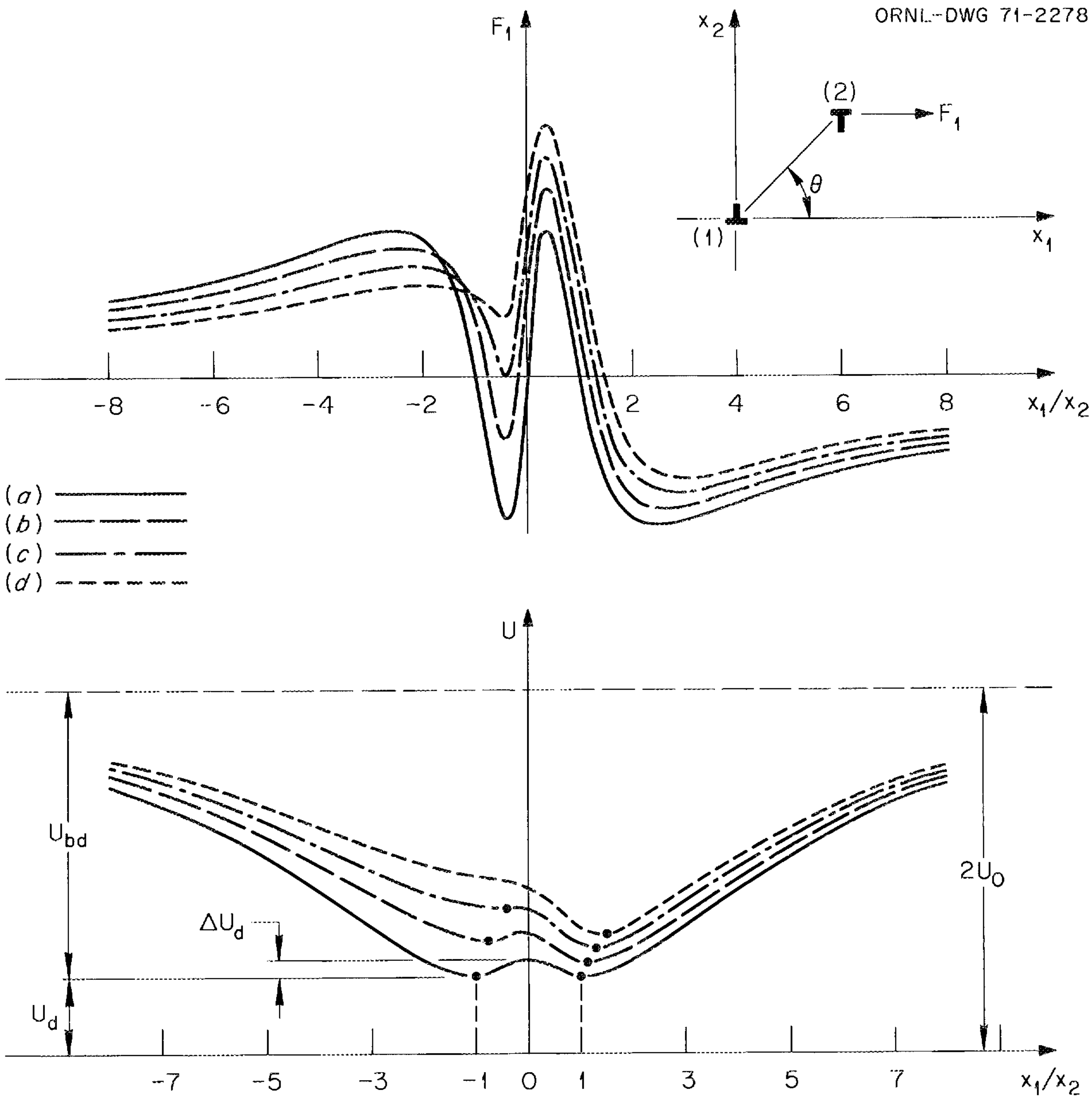

Fig. 10. Glide Force on Dislocation (2) by Dislocation (1) and Total Elastic Energy of an Edge Dislocation Dipole. (a) Elastically isotropic case; (b), (c), (d) three cases of elastic anisotropy.

stable equilibrium positions for $x_1/x_2 = \pm 1$ (i.e., for $\theta = \pm 45°$) and one unstable position for $x_1 = 0$ (i.e., for $\theta = 90°$). According to Kroupa,[18] U_d is the total energy, U_{bd} is the binding energy, and ΔU_d is the flipping energy per unit length of the dipole.

There are three possible anisotropic cases, (b), (c), and (d), when only the dislocation axis, x_3, coincides with a symmetry axis. The asymmetric case (b) in Fig. 10 shows two minima at different angles, neither equal to 45°, and a local maximum between the two minima at an angle $\theta \neq 90°$. There exists of course the absolute minimum to which U_d and U_{bd} must be referred. Along with the possible case (c), which has a minimum and an inflection point, a most interesting case (d), which has only one minimum, may occur. This was called earlier an anomalous case.[19] In such an anomalous case, no flipping energy results from the only stable equilibrium position. Consequently, no contributions to the internal friction by dislocation dipoles, as discussed by Gilman,[20] are possible in this case.

One may discuss the nature of glide force between a pair of like edge dislocations by simply reversing the signs of both F_1 and U in Fig. 10. In the isotropic case (a) as well as an anisotropic case having orthotropic symmetry, the stable equilibrium position is at a right angle ($\theta = 90°$) such that, in the absence of an external stress field, both finite and infinite edge dislocation walls will form normal to the slip plane. In the anisotropic case (b) a finite wall will form at some angle other than a right angle to the slip plane since the stable equilibrium position is at an angle $\theta \neq 90°$. Even for this case, however, Stroh[21]

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[18] F. Kroupa, "Dislocation Dipoles and Dislocation Loops," J. Phys. Radium 27, 23–154 (1966).

[19] M. H. Yoo and B.T.M. Loh, "Characteristics of Stress and Dilatation Fields of Straight Dislocations in Anisotropic Crystals," J. Appl. Phys. 41, 2805–2814 (1970).

[20] J. J. Gilman, "Influence of Dislocation Dipoles on Physical Properties," Dislocations in Solids, the Faraday Society, London, 1964, p. 123.

[21] A. N. Stroh, "Dislocations and Cracks in Anisotropic Elasticity," Phil. Mag. 3, 625 (1958).

verified that a symmetric tilt boundary at right angles to a slip plane in <u>any</u> crystal produces no long-range stress if it is composed of edge dislocations with their Burgers vectors in this slip plane. Thus a paradoxical conclusion may be drawn as given by Nabarro[22] that a tilt boundary in an infinite anisotropic medium is in stable equilibrium when perpendicular to the slip plane, even if the constituent edge dislocations possess an asymmetric σ_{12} stress field.

No paradox exists in the anisotropic case (d). In this case there are no stable equilibrium positions for other like dislocations around an edge dislocation. Therefore, a dislocation wall of any extent cannot be formed by accretion of other like dislocations. This conclusion offers some far-reaching influences on the physical processes of polygonization and on the formation of an incoherent twin boundary by a group of twin dislocations. An anomalous σ_{12} stress field is found in zinc for the $\{11\bar{2}2\}\langle 11\bar{2}\bar{3}\rangle$ slip system below room temperature and also for the $\{10\bar{1}2\}\langle 10\bar{1}\bar{1}\rangle$ twin system at all temperatures. It also occurs in antimony for the $\{110\}\langle 00\bar{1}\rangle$ twin system and in graphite for the $\{11\bar{2}1\}\langle \bar{1}\bar{1}26\rangle$ twin system at room temperature.

The radial and tangential components of interaction force between a pair of parallel dislocations, $F_r = f_r/2\pi r$ and $F_\theta = f_\theta/2\pi r$, respectively, may be calculated directly from the following formulas given by Stroh:[21]

$$f_r = B_{ij} d_i^{(1)} d_j^{(2)} \ , \tag{18}$$

$$f_\theta = -b_i^{(2)} \mathrm{Re} \sum_\alpha L_{i\alpha} M_{\alpha j} d_j \left(\frac{p_\alpha \cos\theta - \sin\theta}{\cos\theta + p_\alpha \sin\theta} \right) . \tag{19}$$

Minor modifications to the program given in Appendix C enable one to write a computer program for the above two equations. Figures 11 and 12 show the results of f_θ and f_r between a pair of $\langle \vec{c} + \vec{a} \rangle$ screw dislocations in zinc and titanium, respectively. The isotropic values for f_r

[22]F.R.N. Nabarro, <u>Theory of Crystal Dislocations</u>, Oxford University Press, London, 1967, p. 98.

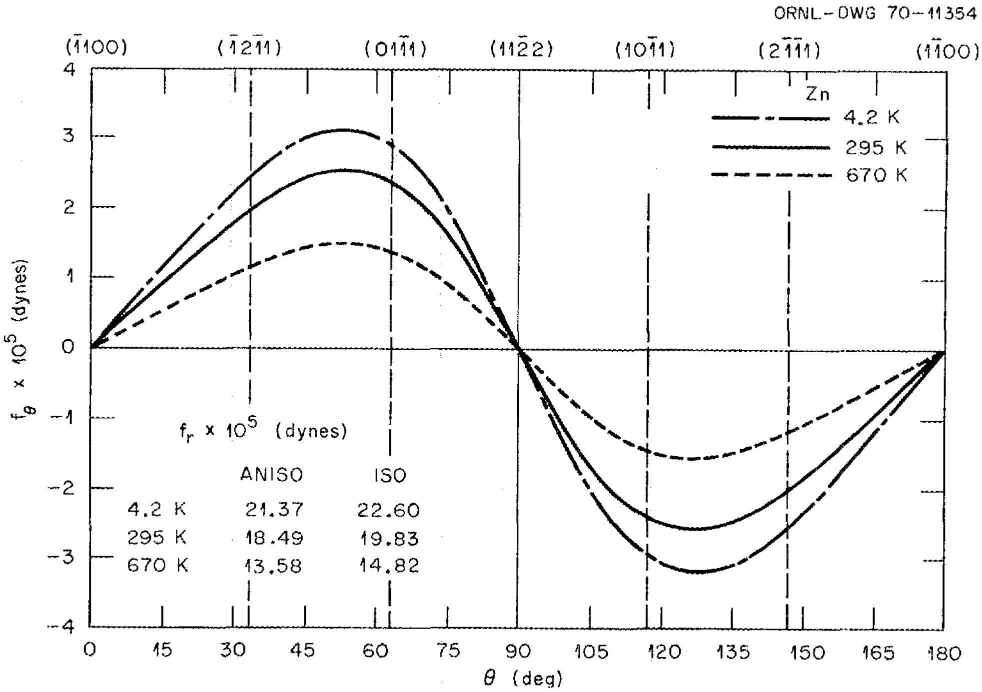

Fig. 11. Interaction Force Between a Pair of $\langle \vec{c} + \vec{a} \rangle$ Screw Dislocations in Zinc.

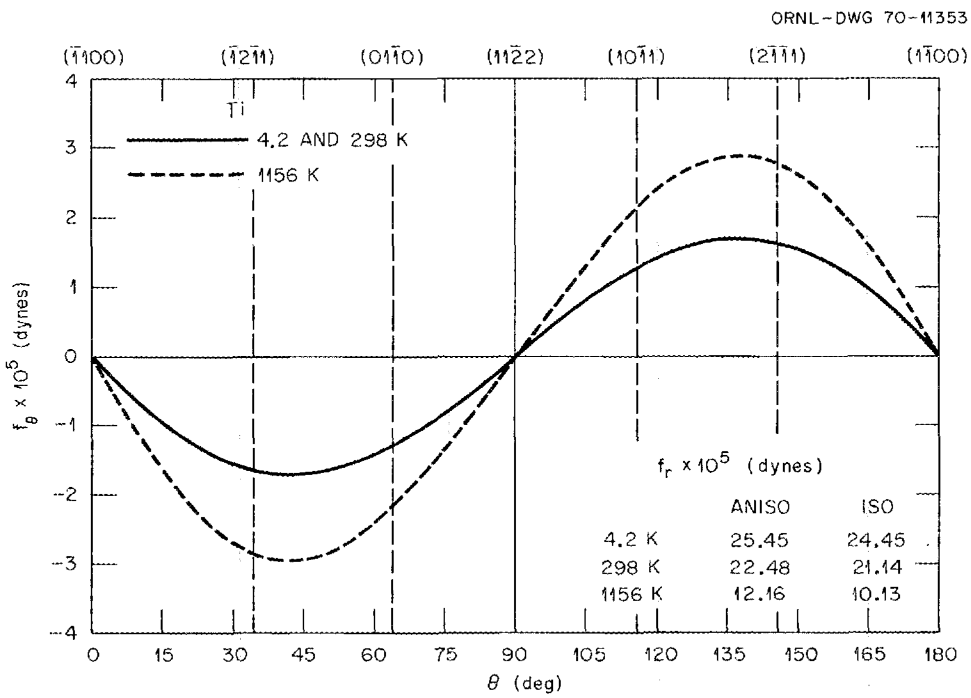

Fig. 12. Interaction Force Between a Pair of $\langle \vec{c} + \vec{a} \rangle$ Screw Dislocations in Titanium.

are obtained from Hill's average of elastic moduli (i.e., the arithmetic means of Voigt's and Reuss' averages). The maximum of f_θ reaches a value as much as 14% of f_r. For zinc and other metals f_r and f_θ both decrease as temperature rises. It is interesting to note, however, that in titanium f_r decreases but f_θ increases with increasing temperature.

The processes of cross-slip and double cross-slip of screw dislocations in an isotropic medium as induced by a locked parallel screw dislocation were analyzed by Li.[23] Such processes for the cases of $\langle 111\rangle$ screw dislocations in bcc crystals and $\langle \vec{c} + \vec{a}\rangle$ screw dislocations in hcp crystals will be strongly influenced by the magnitude of f_θ.

Various cases of dislocation interaction are summarized in Table 2, which compares notable features between the isotropic and anisotropic cases.

Self-Energy and Line Tension

The elastic strain energy per unit length of a straight dislocation is calculated by Eq. (B4) in Appendix B with the results expressed by Eq. (8). Defining, for a given slip plane, α to be the angle between the unit sense vector $\underset{\sim}{\xi}$ and the Burgers vector $\underset{\sim}{b}$, one can calculate $E(\alpha)$ numerically for any α. Since the condition that $E(\alpha) = E(\alpha + \pi)$ must be met because the elastic strain energy of a dislocation cannot depend on the sense of its Burgers vector, a computation over a 180° range of α will suffice to give a complete description of the angular dependence. A knowledge of $E(\alpha)$ enables one to calculate the self-stress of an angular dislocation by use of the formulas given by Lothe.[24] Furthermore, the elastic fields of a dislocation loop of any configuration may be solved,[25] in principle, from such a knowledge of $E(\alpha)$.

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[23] J.C.M. Li, "Cross Slip and Cross Climb of Dislocations Induced by a Locked Dislocation," J. Appl. Phys. 32, 593 (1961).

[24] J. Lothe, "Dislocation Bends in Anisotropic Media," Phil. Mag. 15, 353 (1967).

[25] K. Malén, "Numerical Analysis of Properties of Dislocations in Anisotropic Media within the Range of Linear Elasticity," Phys. Status Solidi 38, 259 (1970).

Table 2. Some Examples of Dislocation Interaction

Arrangement of Dislocations	Isotropic	Anisotropic
A screw parallel to an edge	No interaction	Interaction exists
A screw perpendicular to an edge not in the same plane	No resultant force on each other; the screw exerts a couple on the edge	No resultant force on each other; the screw exerts a couple on the edge and vice versa
Two parallel edges of same sign in a slip plane	No climb force	Climb force exists
Two parallel screws of same sign	No tangential force	Tangential force exists
Two parallel edges of same sign in different slip planes	Equilibrium positions lie along slip plane normal	Equilibrium positions lie along a direction making an angle with the slip plane normal; in some cases, no equilibrium position exists at all
Edge dipole	Equilibrium positions lie symmetrically 45° from the slip plane normal	Equilibrium positions lie asymmetrically about the slip plane normal; in some cases, only one equilibrium position exists

An explicit expression of the line tension, $T(\alpha)$, of the curved portion of a dislocation line is given by deWit and Koehler:[26]

$$T(\alpha) = E + \frac{d^2E}{d\alpha^2} = \frac{b^2}{4\pi}\,\ell n\left(\frac{R}{r_o}\right)\left(K + \frac{d^2K}{d\alpha^2}\right) . \tag{20}$$

The interaction between the bowed and straight portions of a dislocation was neglected in the derivation of Eq. (20).

The line tension is important in the analysis of the stability of a dislocation.[27] If $T(\alpha) < 0$, the dislocation is unstable and it assumes a polygonal shape along such directions as to satisfy the stable condition, $T(\alpha) > 0$. In Fig. 13 inverse Wulff plots of $K(\alpha)$ normalized to $K(\alpha = 0)$ of screw orientation are given for $\langle\vec{c} + \vec{a}\rangle$ dislocations in the

[26] G. deWit and J. S. Koehler, "Interaction of Dislocations with an Applied Stress in Anisotropic Crystals," Phys. Rev. 116, 1113 (1959).

[27] A. K. Head, "Unstable Dislocations in Anisotropic Crystals," Phys. Status Solidi 19, 185 (1967).

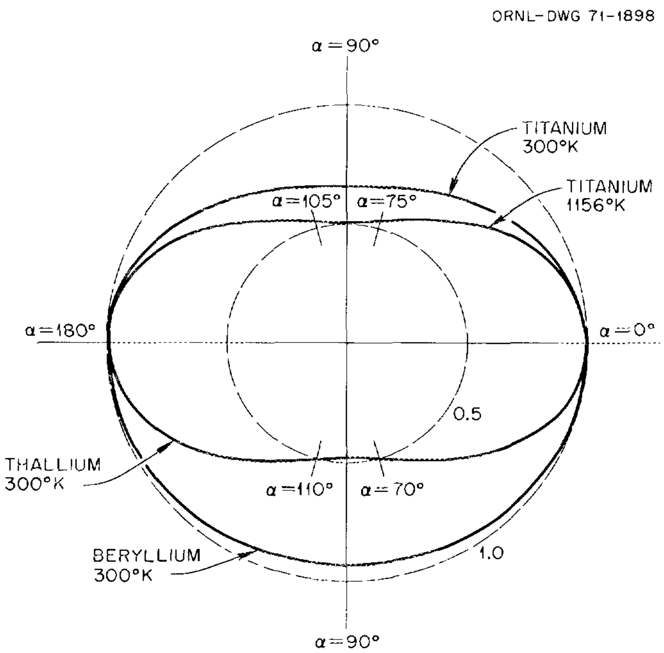

Fig. 13. Inverse Wulff Plot of Energy Factor Normalized to that of Screw Orientation for $\langle\vec{c} + \vec{a}\rangle$ Dislocations in $\{11\bar{2}2\}$ Planes of Some Hexagonal Metals.

second-order pyramidal $\{11\bar{2}2\}$ plane of several hexagonal metals. A region of negative $T(\alpha)$ corresponds to a concave region bounded by two inflection points. While the dislocation in titanium is stable for all orientation at room temperature, it is found unstable for $75 < \alpha < 105°$ at 1156°K. The inverse Wulff plot for the dislocation in beryllium appears much closer to a circle, indicating that the line energy of an edge orientation is not too much greater than that of a screw orientation. This is indicative of the peculiarly small value of Poisson's ratio in beryllium. The same dislocation in thallium is found to be unstable near the edge orientation at a range of $70 < \alpha < 110°$.

Displacement Fields

Two notable areas of application requiring the exact solution of the displacement field are dislocation contrast analysis in transmission electron microscopy and the atomistic calculation of dislocation core structures. In the former case one need not know the origin of the coordinate system or the integration constants, since the differential equations of the dynamical theory of electron diffraction[28] involve only the gradient of displacement vector in the electron beam direction along the column under consideration. When referred to an appropriate coordinate system, therefore, Eq. (10) can be used to compute the images from dislocations in anisotropic materials, as demonstrated by Head et al.[29]

In the latter application, however, one needs to find the integration constants, since the exact magnitude of the displacement is to be

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[28] P. B. Hirsch et al., Electron Microscopy of Thin Crystals, Plenum Press, New York, 1965, p. 247.

[29] A. K. Head, M. H. Loretto, and P. Humble, "The Influence of Large Elastic Anisotropy on the Determination of Burgers Vectors of Dislocations in β-Brass by Electron Microscopy," Phys. Status Solidi **20**, 205 (1967).

used as a boundary condition.[30–32] In other words, the origin of the coordinate system used to describe the long-range elastic displacement field of a dislocation must coincide with that of the discrete structure of the dislocation.

For ⟨111⟩ screw dislocations in α-iron, for example, imposing a threefold symmetry about the dislocation axis, x_3-axis, shows that the only integration constant necessary is $c_2 = 0.0327$ Å. The component of the displacement vector directed normal to the dislocation axis may be obtained from u_1 and $u_2 + c_2$ in Fig. 7. This is shown in Fig. 14. The solid closed curve describes the displaced positions of a medium with respect to the unstrained medium, the dashed reference circle, and the

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[30]V. Vitek, R. C. Perrin, and D. K. Bowen, "The Core Structure of $\frac{1}{2}$⟨111⟩ Screw Dislocations in B.C.C. Crystals," Phil. Mag. 21, 1049 (1970).

[31]Z. S. Basinski, M. S. Duesbery, and Roger Taylor, "Screw Dislocations in a Model Sodium Lattice," Phil. Mag. 21, 1201 (1970).

[32]P. C. Gehlen, "The Structure of the $\frac{a}{2}$⟨111⟩ Screw Dislocation in α-Iron," J. Appl. Phys. 41, 5165 (1970).

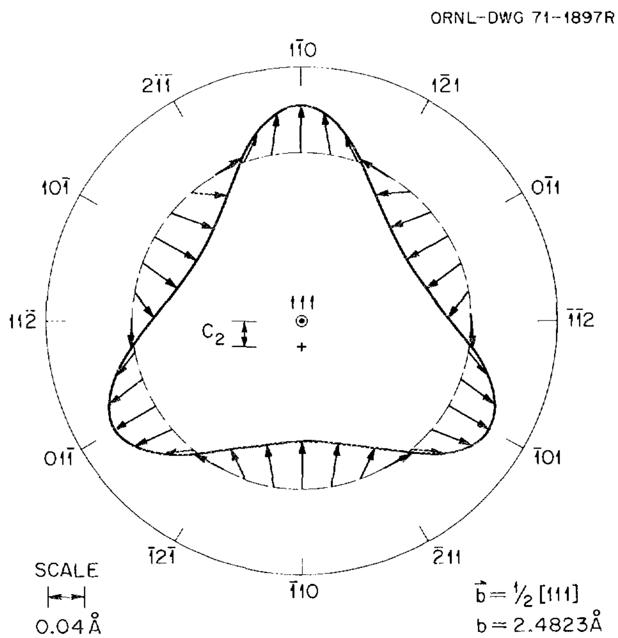

Fig. 14. Displacement Field Normal to the Dislocation Line of α-Iron at Room Temperature. $C_2 = 0.0327$ Å.

arrows indicate the directions of displacement vectors. It is interesting to note that the displacements are radially either inward or outward along the two sets of three $\langle 110 \rangle$ directions, whereas they are purely tangential to the reference circle along the two sets of three $\langle 112 \rangle$ directions.

A general method of determining the integration constants in accordance with the crystal symmetry with respect to the dislocation axes will be described elsewhere.

ACKNOWLEDGMENTS

The authors are indebted to W. A. Coghlan and R. O. Williams for valuable comments on the manuscript.

APPENDIX A

APPENDIX A

Definition of Coefficients Used to Calculate Elastic Fields of a Straight Dislocation

The coefficients introduced in the text are related to the following set of matrices and vector introduced by Stroh:[33] $[L_{i\alpha}]$, $[M_{\alpha i}] = [L_{i\alpha}]^{-1}$, $[A_{i\alpha}]$, $[B_{ij}]$, and $[d_j]$. Once $[L_{i\alpha}]$ is defined by Eq. (S77),[34] $[A_{i\alpha}]$ can be obtained from $[L_{i\alpha}]$ by use of Eq. (S14) or (S15). One determines $[B_{ij}]$ directly from Eq. (S40), where $[B_{ij}]$ is related to $[d_j]$ and Burgers vector $[b_i]$ by Eq. (S50). Then the energy factor is obtained from Eqs. (S56) and (S50) as follows

$$Kb^2 = B_{ij} d_i d_j \tag{A1}$$

or

$$K = B_{ij}^{-1} \beta_i \beta_j \ , \tag{A2}$$

where β_i are the direction cosines of the Burgers vector. The coefficients for the stress components are determined from Eq. (S51):

$$A_{i1\alpha} = -\mathrm{Re}[L_{i\alpha} p_\alpha M_{\alpha j} d_j]/Kb \ , \tag{A3}$$

$$B_{i1\alpha} = -\mathrm{Re}[L_{i\alpha} p_\alpha \bar{p}_\alpha M_{\alpha j} d_j]/Kb \ ; \tag{A4}$$

and from Eq. (S52):

$$A_{i2\alpha} = \mathrm{Re}[L_{i\alpha} M_{\alpha j} d_j]/Kb \ , \tag{A5}$$

$$B_{i2\alpha} = \mathrm{Re}[L_{i\alpha} \bar{p}_\alpha M_{\alpha j} d_j]/Kb \ . \tag{A6}$$

Re and Im denote the real and imaginary parts, respectively, of the complex functions that follow.

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[33]A. N. Stroh, "Dislocations and Cracks in Anisotropic Elasticity," Phil. Mag. 3, 625 (1958).

[34]As was mentioned in the body of this report, the prefix S denotes Stroh's[33] equation numbers.

By setting $\epsilon_3 = 0$ in Eq. (S64) the coefficients for the σ_{33} component are found as

$$A_{33\alpha} = -(s_{3M}/s_{33})A_{M\alpha} \tag{A7}$$

$$B_{33\alpha} = -(s_{3M}/s_{33})B_{M\alpha} \ . \tag{A8}$$

The coefficients for the displacements are obtained from Eq. (S45)

$$R_{i\alpha} = \mathrm{Re}[A_{i\alpha}M_{\alpha j}d_j]/b \tag{A9}$$

$$T_{i\alpha} = -\mathrm{Im}[A_{i\alpha}M_{\alpha j}d_j]/b \ , \tag{A10}$$

and those for the strain components are

$$P_{i1\alpha} = R_{i\alpha} \tag{A11}$$

$$Q_{i1\alpha} = \mathrm{Re}[A_{i\alpha}\bar{p}_\alpha M_{\alpha j}d_j]/b \tag{A12}$$

$$P_{i2\alpha} = \mathrm{Re}[A_{i\alpha}p_\alpha M_{\alpha j}d_j]/b \tag{A13}$$

$$Q_{i2\alpha} = \mathrm{Re}[A_{i\alpha}p_\alpha\bar{p}_\alpha M_{\alpha j}d_j]/b \ . \tag{A14}$$

For the dilatation, then, the coefficients are

$$f_\alpha = P_{ii\alpha} \tag{A15}$$

$$g_\alpha = Q_{ii\alpha} \tag{A16}$$

or

$$f_\alpha = K(S_{1M} + S_{2M})A_{M\alpha} \tag{A17}$$

$$g_\alpha = K(S_{1M} + S_{2M})B_{M\alpha} \ , \tag{A18}$$

and for the hydrostatic pressure they are

$$h_\alpha = -A_{ii\alpha} \tag{A19}$$

$$k_\alpha = -B_{ii\alpha} \ . \tag{A20}$$

All the coefficients defined here, $A_{ij\alpha}$, $B_{ij\alpha}$, $R_{i\alpha}$, $T_{i\alpha}$, $P_{ij\alpha}$, $Q_{ij\alpha}$, f_{α}, g_{α}, h_{α}, and k_{α}, are dimensionless real numbers. The energy factor K has dimensions of dynes per square centimeter, and the Burgers vector $\underset{\sim}{b}$ is in centimeters.

Thirty coefficients (15 for each of $A_{ij\alpha}$ and $B_{ij\alpha}$) for stress tensor and 18 coefficients (nine for each of $R_{i\alpha}$ and $T_{i\alpha}$) for displacement vector will suffice to give a complete description of the elastic properties of a dislocation.

APPENDIX B

APPENDIX B

Some Useful Relationships Between the Coefficients Defined in Appendix A

Since $[M_{\alpha i}]$ is the matrix reciprocal to $[L_{i\alpha}]$, Eq. (S38) must hold:

$$\sum_{\alpha} L_{i\alpha} M_{\alpha j} = \delta_{ij} \ , \tag{B1}$$

where δ_{ij} is the Kronecker delta (1 if $i = j$; 0 if $i \neq j$). The above relationship yields a number of relationships among certain $A_{ij\alpha}$ and $B_{ij\alpha}$ coefficients for a pure edge or screw dislocation with Burgers vector components b_i. Namely for a given value of i

$$\sum_{\alpha} A_{i2\alpha} = 1 \tag{B2}$$

$$\sum_{\alpha} B_{i1\alpha}/(r_{\alpha}^2 + q_{\alpha}^2) = -1 \ . \tag{B3}$$

With the relationships given above, the dislocation line energy,

$$E = \frac{1}{2} \int_{r_o}^{R} b_i \sigma_{i2}(x_1,0)\, dx_1 = -\frac{1}{2} \int_{r_o}^{R} b_i \sigma_{i1}(0,x_2)\, dx_2 \ , \tag{B4}$$

can be simplified to the form given in Eq. (8) with the corresponding energy factor and the magnitude of the Burgers vector.

According to Stroh,[33] the matrix $[\sum_{\alpha} A_{i\alpha} M_{\alpha j}]$ is skew-Hermitian and satisfies Eq. (S39)

$$\sum_{\alpha} \bar{A}_{j\alpha} \bar{M}_{\alpha i} = -\sum_{\alpha} A_{i\alpha} M_{\alpha j} \ . \tag{B5}$$

The following relationship results from Eq. (B5):

$$\sum_{\alpha} T_{i\alpha} = \beta_i \ , \tag{B6}$$

where β_i is the direction cosine of the Burgers vector, such that the residue of a displacement component upon going around the dislocation line, along a closed path c, is

$$\oint \left(\frac{\partial u_i}{\partial c}\right) dc = b_i \ , \qquad \text{(B7)}$$

the corresponding Burgers vector component.

Thus, using the relationships given by Eqs. (B2), (B3), and (B6), one can reduce the number of independent coefficients by nine — three from each equation — to the total of 39, 24 for stress and 15 for displacement.

APPENDIX C

APPENDIX C

Program to Calculate Elastic Fields of a Straight Dislocation

```
**FTN,L,E,G,M.

C   A PROGAM TO CALCULATE THE ELASTIC FIELDS OF A STRAIGHT DISLOCATION
C   OF ANY ARBITRARY ORIENTATICN IN AN ANISOTROPIC HCMCGENEOUS CONTINUUM

      IMPLICIT REAL*8 (A-H,O-Z)
      COMPLEX*16 XCP,XCL,XCCL,XCM,XCA,XCB,XXX
      COMMON IA(21),IB(21),IC(21),ID(21),MM(3,3)
      COMMCN/T/R(3),Q(3)
      DIMENSION ARRAY(4),C(6,6),S(6,6),CT(6,6),ST(6,6),CS(6,6),AA(3,3)
     1NJ(3),NK(3),NB(3),X1(3),X2(3),X3(3),X4(3),A(3,3),BD(3),BV(3)
     2XCP(3),XCL(3),XCCL(3,3),XCM(3,3),XXX(3,3),XCA(3,3),XCB(3,3),SD(3)
     3CB(3,3),CBI(3,3),VER(3,3),A1(23,3),B1(23,3)

C   THE ARRAY OF MM FCR INTERRELATING TENSOR AND MATRIX NOTATIONS

      READ 1, MM(1,1),MM(2,2),MM(3,3),MM(2,3),MM(1,3),MM(1,2)
    1 FORMAT(6I1)
      DO 11 I=1,3 $ DO 11 J=1,3
   11 MM(J,I)=MM(I,J)

C   THE ARRAYS OF IA,IB,IC, AND ID ARE THE 21 COMBINATICNS OF IJKL USED
C   IN THE SUMMING PROCESS OF THE TRANSFOMATION SUBROUTINE

      READ 2, ((IA(I),IB(I),IC(I),ID(I)), I=1,21)
    2 FORMAT(80I1)

C   THE ALPHANUMERIC VARIABLE, ARRAY, IS FOR IDENTIFICATION OF MATERIALS

  102 READ 3, ARRAY
    3 FORMAT(4A8)

C   C(I,J)= ELASTIC STIFFNESSES REFERRED TO CRYSTAL AXES
C   S(I,J)= ELASTIC COMPLIANCES REFERRED TO CRYSTAL AXES
C   CT(I,J)=TRANSFORMED C(I,J) TC DISLOCATION COORDINATE SYSTEM
C   ST(I,J)=TRANSFORMED S(I,J) TO DISLOCATION COORDINATE SYSTEM
C   CS(I,J)=MODIFIED COMPLIANCES

      DO 12 I=1,6 $ DO 12 J=1,6
   12 C(I,J)=S(I,J)=CT(I,J)=ST(I,J)=CS(I,J)=0.0

C   INPUT  NO=STOP(WHEN NONZERC) SIGNAL OF THE PROGRAM
C          N1=IDENTIFICATION OF CRYSTAL CLASSES
C             1=CUBIC, 2=HEXAGONAL, 3=TETRAGONAL,
C             4=ORTHORHOMBIC, 5=TRIGONAL
C          GAMMA=C/A RATIO, BETA=B/A RATIO, ALPHA=RHCMBCHEDRAL ANGLE
C          PLAT=LATTICE PARAMETER

      READ 4, NO,N1,GAMMA,BETA,ALPHA,PLAT,C(1,1),C(2,2),C(3,3),C(4,4),
     1C(5,5),C(6,6),C(1,2),C(1,3),C(2,3),C(1,4)
    4 FORMAT(I1,X,I1,7X, 7F10.0/8F10.0)
      C(2,4)=-C(1,4) $ C(5,6)=C(1,4)
      DO 13 I=1,6 $ DO 13 J=1,6
   13 C(J,I)=C(I,J)

C   SUBROUTINE INV INVERTS STIFFNESSES INTO COMPLIANCES OR THE REVERSE
```

```
      CALL INV(C,S)

C   SUBROUTINE CRYS ESTABLISHES THE MATRIX, AA, WHICH RELATES THE
C   COMPONENTS OF A VECTOR IN CRYSTAL AXES TO THOSE IN THE REFERENCE
C   CARTESIAN COORDINATE SYSTEM

      CALL CRYS(N1,GAMMA,BETA,ALPHA,AA,PLAT)

C   INPUT  N2=STOP(WHEN NONZERO) SIGNAL OF SLIP SYSTEMS FOR A GIVEN MAT'L
C          NK=CRYSTALLOGRAPHIC DIRECTION OF THE DISLOCATION LINE
C          NJ=A VECTOR LYING IN THE SLIP PLANE SUCH THAT A CROSS PRODUCT
C             OF NJ AND NK GIVES A VECTOR, X2, NORMAL TO THE SLIP PLANE
C          NB=DIRECTION OF BURGERS VECTOR IN MILLER INDICES
C          NM=MODULUS SUCH THAT BURGERS VECTOR IS EQUAL TO (NB)/NM

  100 READ 5, N2,NJ,NK,NB,NM
    5 FORMAT(I1,X,3I2,X,3I2,2X,4I2)

C   SUBROUTINE DCOM CONVERTS THE COMPONENTS OF A LATTICE VECTOR TO THOSE
C   IN THE CARTESIAN COORDINATE SYSTEM(E.G. NJ TO X4,SGH=STREGNTH OF X4)

      CALL DCOM(NJ,AA,X4,SGH) $ CALL DCOM(NK,AA,X3,SGH)

C   SUBROUTINE XPDT YIELDS THE CROSS PRODUCT OF TWO VECTORS(E.G. X4 CROSS
C   X3=X2)

      CALL XPDT(X4,X3,X2,SGH) $ CALL XPDT(X2,X3,X1,SGH)
      DO 14 I=1,3 $ A(1,I)=X1(I) $ A(2,I)=X2(I)
   14 A(3,I)=X3(I)

C   SUBROUTINE DCD TRANSFORMS A VECTOR FROM THE REFERENCE CARTESIAN
C   COORDINATE SYSTEM TO THE DISLOCATION COORDINATE SYSTEM

      CALL DCOM(NB,AA,BD,DSGH) $ CALL DCD(BD,A,BV)

C   THE BURGERS VECTOR, BV, IS REFERRED TO THE DISLOCATION COORDINATE AND
C   ITS MAGNITUDE IS BM

      BM=DSGH/NM*PLAT

C   SUBROUTINE TRNSFM TRANSFOMS C(I,J) TO CT(I,J) IN DISLOCATION COORD.

      CALL TRNSFM(C,A,CT)
      CALL INV(CT,ST)
      DO 15 I=1,6 $ DO 15 J=1,6
      IF(J-I)15,16,16
   16 CS(I,J)=ST(I,J)-ST(I,3)*ST(3,J)/ST(3,3)
   15 CS(J,I)=CS(I,J)

C   SUBROUTINE SEXTIC SOLVES THE SEXTIC EQUATION TO GIVE THE COMPLEX
C   ROOTS, XCP, AND A VECTOR, XCL.

      CALL SEXTIC(CS,XCP,XCL,IK)

C   THE MATRICES, XCCL AND XCM, ARE DEFINED IN TERMS OF XCP AND XCL
C   THE STEP 31 IS FOR THE SPECIAL CASE WHEN THE DISLOCATION LINE IS
C   NORMAL TO A REFLECTION PLANE OF THE CRYSTAL
```

```
      DO 21 I=1,3
      XCCL(1,I)=-XCP(I) $ XCCL(2,I)=(1.0,0.0)
   21 XCCL(3,I)=XCL(I)
      IF(IK)31,32
   31 XCCL(1,3)=(0.0,0.0) $ XCCL(2,3)=(0.0,0.0)
   32 DO 22 J=1,3 $ DO 22 I=1,3 $ XXX(I,J)=XCCL(I,J)
      IF(I.EQ.J)33,34
   34 XCM(I,J)=(0.0,0.0) $ GO TO 22
   33 XCM(I,J)=(1.0,0.0)
   22 CONTINUE

C  SUBROUTINE CMATEQ AVAILABLE AT ORNL SUBROUTINE LIBRARY(F04011) GIVES
C  INVERSION OF A COMPLEX MATRIX(E.G. XXX(3,3) INVERTED TO XCM(3,3))

      CALL CMATEQ(XXX,XCM,3,3,3)

C  SUBROUTINE SAKA CALCULATES A COMPLEX MATRIX, XCA, FROM XCCP, XCP, CT

      CALL SAKA(XCCL,XCP,XCA,CT)

C  SUBROUTINE SBIJ CALCULATES A SYMMETRIC REAL MATRIX,CB, FROM XCA, XCM

      CALL SBIJ(XCA,XCM,XCB,CB)

C  CALCULATION OF A VECTOR, SD, FROM THE INVERSE OF CB, CBI, WHICH IS
C  OBTAINED BY A SUBROUTINE DMATEQ AVAILABLE AT ORNL SUBROUTINE LIBRARY
C  (F04013).

      DO 41 J=1,3 $ DO 41 I=1,3 $ VER(I,J)=CB(I,J)
      IF(I.EQ.J)51,52
   51 CBI(I,J)=1.0 $ GO TO 41
   52 CBI(I,J)=0.0
   41 CONTINUE
      CALL DMATEQ(VER,CBI,3,3,3)
      DO 42 J=1,3 $ SD(J)=0.0 $ DO 42 I=1,3
   42 SD(J)=SD(J)+CBI(J,I)*BV(I)

C  CALCULATION OF THE ENERGY FACTOR, EF, FROM CB AND SD

      EF=0.0 $ DO 43 J=1,3 $ DO 43 I=1,3
   43 EF=EF+CB(I,J)*SD(I)*SD(J)

C  THE COEFFICIENTS OF THE ELASTIC SOLUTIONS, A1(M,N) AND B1(M,N), ARE
C  CALCULATED IN SUBROUTINE  COEFF, WHERE N TAKES ON 1,2,3 AND M TAKES
C  ON 1 TO 23 SUCH THAT
C    M=1,2,3,4,5,6  FOR STRESS COMPONENTS(IJ=11,22,33,23,13,12)
C    M=7,8,9,10     FOR DU(I)/DX(J)(IJ=12,21,31,32)
C    M=11,12,13,14,15,16  FOR STRAIN COMPONENTS(IJ=11,22,33,23,13,12)
C    M=17 AND M=18  FOR DILATATION FIELD
C    M=19           FOR HYDROSTATIC PRESSURE FIELD
C    M=21,22,23     FOR DISPLACEMENT COMPONENTS(I=1,2,3)

      CALL COEFF(XCCL,XCM,XCA,XCP,SD,EF,ST,CS,A1,B1)

C  OUTPUT   PRINT OUT THE FOLLOWING RESULTS- MATERIAL, TEMPERATURE,
C           ELASTIC CONSTANTS C(I,J), SLIP SYSTEM NJ AND NK, BURGERS
```

```
C           VECTOR BV AND BM, ENERGY FACTOR EF, SEXTIC ROOTS, AND
C           COEFFICIENTS A1(M,N) AND B1(M,N)
      PRINT 91, ARRAY,NJ,NK,BV,BM
   91 FORMAT(1H1,4A8///10X,3I2,5X,3I2,10X,3F10.5,5X,F10.5//)
      PRINT 92, (J, J=1,6)
   92 FORMAT(1H0,24X,6(I1,9X))
      PRINT 93, ((I,(C(I,J),J=1,6)),I=1,6)
   93 FORMAT(1H0,/6(14X,I1,5X,6F10.5/))
      PRINT 94, EF
   94 FORMAT(1H0,F18.8)
      PRINT 95, (N, N=1,3)
   95 FORMAT(1H0,/27X,I1,2(39X,I1))
      PRINT 96,(R(I),Q(I),I=1,3)
   96 FORMAT(1H0,/6X,3(2F18.8,4X))
      PRINT 97, ((M,(A1(M,N),B1(M,N),N=1,3)),M=1,23)
   97 FORMAT(1H0,/6(4X,I2,3(2F18.8,4X)/)/,4(4X,I2,3(2F18.8,4X)/)/,6(4X,
     1I2,3(2F18.8,4X)/)/,4(4X,I2,3(2F18.8,4X)/)/,3(4X,I2,3(2F18.8,4X)/))
      IF(N2)101,100,101
  101 IF(NO)103,102,103
  103 STOP
      END
```

```
      SUBROUTINE INV (C,S)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION C(6,6),S(6,6),A(21)
      N=0 $ DO 1 J=1,6 $ DO 1 I=J,6 $ N=N+1
    1 A(N)=C(J,I)

C  SUBROUTINE DCHOLY AVAILABLE FROM ORNL SUBROUTINE LIBRARY(F04024)
C  GIVES MATRIX INVERSION

      CALL DCHOLY(A,6,NF)
      N=0 $ DO 2 J=1,6 $ DO 2 I=J,6 $ N=N+1
    2 S(I,J)=S(J,I)=A(N)
      RETURN
      END


      SUBROUTINE CRYS(N,G,B,AL,A,P)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(3,3)
      DO 11 I=1,3 $ DO 11 J=1,3
   11 A(I,J)=0.0
      PI=3.1415926536 $ AN=PI/3. $ AR=PI*AL/90.
      GO TO(1,2,3,4,5),N
    1 A(1,1)=A(2,2)=A(3,3)=1.0 $ GC TO 10
    2 A(1,1)=1.0 $ A(1,2)=-DCOS(AN) $ A(2,2)=DSIN(AN) $ A(3,3)=G
      GO TO 10
    3 A(1,1)=A(2,2)=1.0 $ A(3,3)=G $ GC TO 10
    4 A(1,1)=1.0 $ A(2,2)=B $ A(3,3)=G $ GO TO 10
    5 A(1,1)=1.0 $ A(1,2)=-DCOS(AN) $ A(2,2)=DSIN(AN) $ A(3,3)=DSQRT(9./
     1(4.*DSIN(AR)*DSIN(AR))-3.) $ P=DSQRT(9.*P*P/A(3,3)*A(3,3)+3.)
   10 RETURN
      END

      SUBROUTINE DCOM(N,A,X,SS)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION N(3),A(3,3),X(3)
      S=0.0 $ DO 13 J=1,3 $ X(J)=0.0 $ DO 12 I=1,3
   12 X(J)=X(J)+A(J,I)*N(I)
   13 S=S+X(J)*X(J) $ SS=DSQRT(S)
      DO 14 J=1,3
   14 X(J)=X(J)/SS
      RETURN
      END


      SUBROUTINE XPDT(X,Y,Z,SS)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION X(3),Y(3),Z(3)
      Z(1)=X(2)*Y(3)-X(3)*Y(2) $ Z(2)=X(3)*Y(1)-X(1)*Y(3)
      Z(3)=X(1)*Y(2)-X(2)*Y(1) $ SS=DSQRT(Z(1)*Z(1)+Z(2)*Z(2)+Z(3)*Z(3))
      DO 1 I=1,3
    1 Z(I)=Z(I)/SS
      RETURN
      END
```

```
      SUBROUTINE DCD(X,A,B)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION X(3),A(3,3),B(3)
      DO 1 J=1,3 $ B(J)=0.0 $ DO 1 I=1,3
    1 B(J)=B(J)+X(I)*A(J,I)
      RETURN
      END

      SUBROUTINE TRNSFM(C,A,CT)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON IA(21),IB(21),IC(21),ID(21),MM(3,3)
      DIMENSION C(6,6),A(3,3),CT(6,6),S(21)
      DO 10 M=1,21 $ II=IA(M) $ JJ=IB(M) $ KK=IC(M) $ LL=ID(M)
      S(M)=0.0 $ DO 9 I=1,3 $ DO 9 J=1,3 $ NI=MM(I,J)
      DO 9 K=1,3 $ DO 9 L=1,3 $ NK=MM(K,L)
      R=C(NI,NK)*A(II,I)*A(JJ,J)*A(KK,K)*A(LL,L)
    9 S(M)=S(M)+R
      LIL=MM(II,JJ) $ LJL=MM(KK,LL) $ CT(LIL,LJL)=CT(LJL,LIL)=S(M)
   10 CONTINUE
      RETURN
      END

      SUBROUTINE SAKA(XCCL,XCP,XCA,C)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMPLEX*16 XCCL,XCP,XCA,XCT,XCTI,XCAT,XC,XLL,XAB,XCDL
      COMMON IA(21),IB(21),IC(21),ID(21),MM(3,3)
      DIMENSION XCCL(3,3),XCP(3),XCA(3,3),XCT(3,3),XCTI(3,3),XCAT(3)
     1XC(4),XLL(3,3),XAB(3,3),XCDL(3),C(6,6)
      DO 9 J=1,3 $ DO 1 K=1,3 $ XCDL(K)=XCCL(K,J)
      DO 1 I=1,3 $ II=MM(I,2) $ JJ=MM(K,1) $ KK=MM(K,2)
      XC(1)=DCMPLX(C(II,JJ),0.0) $ XC(2)=DCMPLX(C(II,KK),0.0)
    1 XCT(I,K)=XC(1)+XCP(J)*XC(2)
      DO 2 K=1,3 $ DO 2 I=1,3 $ IF(I.EQ.K)11,12
   12 XCTI(I,K)=(0.0,0.0) $ GO TO 2
   11 XCTI(I,K)=(1.0,0.0)
    2 XAB(I,K)=XCT(I,K)
      CALL CMATEQ(XAB,XCTI,3,3,3) $ DO 3 I=1,3 $ XC(3)=(0.0,0.0)
      DO 4 K=1,3 $ XC(4)=XCTI(I,K)*XCDL(K) $ XC(3)=XC(3)+XC(4)
    4 CONTINUE
    3 XCAT(I)=XC(3)
      DO 5 I=1,3
    5 XCA(I,J)=XCAT(I)
    9 CONTINUE
      RETURN
      END

      SUBROUTINE SBIJ(XCA,XCM,XCB,CB)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMPLEX*16 XCA,XCM,XCB,XC,XCN
      EQUIVALENCE (G(1,1),XCN(1,1))
      DIMENSION XCA(3,3),XCM(3,3),XCB(3,3),CB(3,3),XC(3),XCN(3,3),G(6,3)
      XC(2)=(0.0,0.5)
      DO 1 J=1,3 $ DO 1 I=1,3 $ XC(3)=(0.0,0.0) $ DO 2 L=1,3
    2 XC(3)=XC(3)+XCA(I,L)*XCM(L,J)-DCONJG(XCA(I,L))*DCONJG(XCM(L,J))
      XCN(I,J)=XC(2)*XC(3) $ IW=2*I-1 $ XCB(I,J)=XCN(I,J)
    1 CB(I,J)=G(IW,J)
      RETURN
      END
```

```
      SUBROUTINE SEXTIC(C,XCP,XCL,IK)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMPLEX*16 XCP,XCL,XC,XCN
      COMMON/T/R(3),Q(3)
      EQUIVALENCE (XCPD(1),XCN(1))
      DIMENSION C(6,6),G(7),G1(7),RR(6),RI(6),XCP(3),XCL(3),XC(11)
     1XCPD(6),XCN(3)

C  CALCULATION OF THE 7 COEFFICIENTS, G(I), OF A SEXTIC EQUATION

      A1=C(1,5) $ A2=C(1,4)+C(5,6) $ A3=C(2,5)+C(4,6) $ A4=C(2,4)
      B1=C(1,1) $ B2=2.*C(1,6) $ B3=2.*C(1,2)+C(6,6) $ B4=2.*C(2,6)
      B5=C(2,2) $ C1=C(5,5) $ C2=2.*C(4,5) $ C3=C(4,4)
      G(1)=C3*B5-A4*A4 $ G(2)=-(C2*B5+C3*B4-2.*A3*A4)
      G(3)=C1*B5+C2*B4+B3*C3-A3*A3-2.*A2*A4
      G(4)=-(C1*B4+C2*B3+B2*C3-2.*(A1*A4+A2*A3))
      G(5)=C1*B3+B2*C2+B1*C3-A2*A2-2.*A1*A3
      G(6)=-(B1*C2+B2*C1-2.*A1*A2) $ G(7)=B1*C1-A1*A1

C  SUBROUTINE POLRT AVAILABLE FROM ORNL SUBROUTINE LIBRARY(C02007)
C  SOLVES FOR THE ROOTS(REAL PARTS, RR, AND IMAGINARY PARTS, RI) OF
C  A SIXTH ORDER POLYNOMIAL EQUATION

      CALL POLRT(G,G1,6,RR,RI,IER)

C  CALCULATION OF THE VECTOR XCL FROM THE ROOTS AND C(I,J)

      XC(2)=DCMPLX(A1,0.0) $ XC(3)=DCMPLX(A2,0.0) $ XC(4)=DCMPLX(A3,0.0)
      XC(5)=DCMPLX(A4,0.0) $ XC(6)=DCMPLX(C1,0.0) $ XC(7)=DCMPLX(C2,0.0)
      XC(8)=DCMPLX(C3,0.0)

C  SELECT THE THREE ROOTS WITH POSITIVE IMAGINARY PARTS

      II=0 $ IK=0 $ DO 10 L=2,6,2 $ II=II+1
      IF(RI(L))20,21,21
   20 I=L-1 $ GO TO 22
   21 I=L

C  TEST EACH ROOT WITH THE QUADRATIC EQUATION FOR THE SPECIAL CASE

   22 XC(10)=DCMPLX(RR(I),RI(I)) $ XC(11)=XC(10)*XC(10)
      XC(9)=XC(6)*XC(11)-XC(7)*XC(10)+XC(8) $ AX=CDABS(XC(9))
      IF(AX.LT.1.D-6)11,12
   11 XCN(3)=XC(10) $ II=II-1 $ IK=IK+1 $ GO TO 10
   12 XCN(II)=XC(10)
   10 CONTINUE
      DO 30 I=1,3 $ IW=2*I-1 $ IV=2*I $ R(I)=XCPD(IW) $ XCP(I)=XCN(I)
   30 Q(I)=XCPD(IV)
      IF(IK)13,14,13
   13 XCL(3)=(1.0,0.0) $ K=2 $ GO TO 15
   14 K=3
   15 DO 40 I=1,K $ XC(1)=XCN(I)*XCN(I)
   40 XCL(I)=(XC(1)*XCN(I)*XC(2)-XC(1)*XC(3)+XCN(I)*XC(4)-XC(5))/
     1(XC(1)*XC(6)-XCN(I)*XC(7)+XC(8))
      RETURN
      END
```

```
      SUBROUTINE COEFF(XCCL,XCM,XCA,XCP,SD,EF,ST,CS,A,B)
      IMPLICIT REAL*8 (A-H,O-Z)
      COMPLEX*16 XCCL,XCM,XCA,XMD,XMY,XX,XC,XCP
      COMMON/T/R(3),Q(3)
      EQUIVALENCE (PP(1),XC(1))
      DIMENSION XCCL(3,3),XCM(3,3),XCA(3,3),XCP(3),SD(3),XC(23),PP(46)
     1ST(6,6),CS(6,6),A(23,3),B(23,3),XMD(3)
      DO 11 I=1,3 $ XMY=(0.0,0.0)
      DO 12 J=1,3 $ XX=DCMPLX(SD(J),0.0)
   12 XMY=XMY+XCM(I,J)*XX
   11 XMD(I)=XMY
      F=1./EF
      DO 3 I=1,3

C   CALCULATION OF THE COEFFICIENTS FOR STRESS COMPONENTS 1,2,6

      XC(1)=XCCL(1,I)*XMD(I) $ XC(2)=XC(1)*XCP(I)
      XC(3)=XCCL(2,I)*XMD(I) $ XC(4)=DCONJG(XCP(I))
      XC(5)=XC(2)*XC(4) $ XC(6)=XC(3)*XC(4) $ XC(7)=XC(1)*XC(4)
      A(1,I)=-PP(3)*F $ A(2,I)=PP(5)*F $ A(6,I)=PP(1)*F
      B(1,I)=-PP(9)*F $ B(2,I)=PP(11)*F $ B(6,I)=PP(13)*F

C   FOR STRESS COMPONENTS 4,5

      XC(8)=XCCL(3,I)*XMD(I) $ XC(9)=XC(8)*XCP(I)
      XC(10)=XC(8)*XC(4) $ XC(11)=XC(9)*XC(4)
      A(4,I)=PP(15)*F $ B(4,I)=PP(19)*F
      A(5,I)=-PP(17)*F $ B(5,I)=-PP(21)*F

C   FOR STRESS COMPCNENTS 3 AND CILATATION FIELD 17 CALCULATED FROM THE
C   NORMAL STRESS COMPONENTS

      A(3,I)=B(3,I)=A(17,I)=B(17,I)=0.0
      DO 9 IQ=1,6
      IF(IQ.EQ.3)9,10
   10 GW=ST(3,IQ)/ST(3,3) $ GU=EF*(CS(1,IQ)+CS(2,IQ))
      A(3,I)=A(3,I)-GW*A(IQ,I) $ B(3,I)=B(3,I)-GW*B(IQ,I)
      A(17,I)=A(17,I)+GU*A(IQ,I) $ B(17,I)=B(17,I)+GU*B(IQ,I)
    9 CONTINUE

C   FOR DISPLACEMENT COMPONENTS 21,22,23

      XC(12)=XCA(1,I)*XMD(I) $ XC(13)=XCA(2,I)*XMD(I)
      XC(14)=XCA(3,I)*XMD(I) $ XC(15)=XC(12)*XC(4)
      XC(16)=XC(12)*XCP(I) $ XC(17)=XC(15)*XCP(I)
      XC(18)=XC(13)*XC(4) $ XC(19)=XC(13)*XCP(I) $ XC(20)=XC(18)*XCP(I)
      A(21,I)=PP(23) $ B(21,I)=-PP(24)
      A(22,I)=PP(25) $ B(22,I)=-PP(26)
      A(23,I)=PP(27) $ B(23,I)=-PP(28)

C   FOR DISPLACEMENT GRADIENTS 7,8,9,10 AND STRAIN CCMPCNENTS 11,12,13,
C   14,15,16

      XC(21)=XC(14)*XC(4) $ XC(22)=XC(14)*XCP(I) $ XC(23)=XC(21)*XCP(I)
      A(7,I)=PP(31)  $  B(7,I)=PP(33)
      A(8,I)=A(22,I) $  B(8,I)=PP(35)
```

```
      A(9,I)=PP(27)   $  B(9,I)=PP(41)
      A(10,I)=PP(43) $  B(10,I)=PP(45)
      A(11,I)=A(21,I) $ B(11,I)=PP(29)
      A(12,I)=PP(37) $  B(12,I)=PP(39) $ A(13,I)=B(13,I)=0.0
      A(14,I)=0.5*PP(43) $ B(14,I)=0.5*PP(45)
      A(15,I)=0.5*PP(27) $ B(15,I)=0.5*PP(41)
      A(16,I)=0.5*(PP(31)+A(8,I)) $ B(16,I)=0.5*(PP(33)+PP(35))
C  FOR DILATATION FIELD, 18, CALCULATED DIRECTLY FROM THE NORMAL STRAIN
C  COMPONENTS AND FOR HYDROSTATIC PRESSURE FIELD 19
      A(18,I)=A(11,I)+A(12,I) $ B(18,I)=B(11,I)+B(12,I)
      A(19,I)=-(A(1,I)+A(2,I)+A(3,I)) $ B(19,I)=-(B(1,I)+B(2,I)+B(3,I))
    3 A(20,I)=B(20,I)=0.0
      RETURN
      END
```

APPENDIX D

APPENDIX D

Results for a Screw and an Edge Dislocation in α-Iron

The results for a screw and an edge dislocation in α-iron are given as computer print-outs. The diagram preceding the print-outs identifies the numerical values.

Crystal, Temp.

NJ	NK	β_i	b

Elastic Stiffness Constants

C°_{ij} in 10^{11} dynes/cm^2

K

NJ,NK: Vectors in Miller indices defining dislocation coordinate

β_i: Burgers vector components

b: Magnitude of Burgers vector in Å

K: Energy factor in 10^{11} dynes/cm^2

α / m	1		2		3	
	r_1	q_1	r_2	q_2	r_3	q_3
1 ↓ 23	A_{m1}	B_{m1}	A_{m2}	B_{m2}	A_{m3}	B_{m3}

ALPHA IRON 298 K

1 1-2	1 1 1	0.0	0.0	1.00000	2.48229

	1	2	3	4	5	6
1	22.60000	14.00000	14.00000	0.0	0.0	0.0
2	14.00000	22.60000	14.00000	0.0	0.0	0.0
3	14.00000	14.00000	22.60000	0.0	0.0	0.0
4	0.0	0.0	0.0	11.60000	0.0	0.0
5	0.0	0.0	0.0	0.0	11.60000	0.0
6	0.0	0.0	0.0	0.0	0.0	11.60000

5.87230616

	1		2		3	
	0.40198522	0.61174777	-0.40198522	0.61174777	-0.00000000	2.01404295
1	0.04773145	-0.20607392	-0.04773145	-0.20607392	0.00000000	3.12007859
2	-0.66612957	-0.15095840	0.66612957	-0.15095840	-0.00000000	-0.76918017
3	-0.13620666	-0.07863895	0.13620666	-0.07863895	0.00000000	0.51780238
4	0.33333333	0.13399507	0.33333333	-0.13399507	0.33333333	-0.00000000
5	-0.13399507	-0.17860915	0.13399507	-0.17860915	-0.00000000	-1.35212300
6	0.38459008	0.35693051	0.38459008	-0.35693051	-0.76918017	0.00000000
7	0.12909584	0.03779743	0.12909584	-0.03779743	-0.66332583	0.00000000
8	0.04072646	0.19085768	0.04072646	-0.19085768	-0.08145292	0.00000000
9	0.00000000	-0.20391592	-0.00000000	-0.20391592	-0.00000000	-0.67134765
10	0.20391592	0.00000000	0.20391592	-0.00000000	0.67134765	-0.00000000
11	0.07054030	-0.07238352	-0.07054030	-0.07238352	0.00000000	0.66332583
12	-0.15811481	0.02182236	0.15811481	0.02182236	-0.00000000	-0.33040311
13	0.0	0.0	0.0	0.0	0.0	0.0
14	0.10195796	0.00000000	0.10195796	-0.00000000	0.33567382	-0.00000000
15	0.00000000	-0.10195796	-0.00000000	-0.10195796	-0.00000000	-0.33567382
16	0.08491115	0.11432756	0.08491115	-0.11432756	-0.37238938	0.00000000
17	-0.08757451	-0.05056117	0.08757451	-0.05056117	0.00000000	0.33292272
18	-0.08757451	-0.05056117	0.08757451	-0.05056117	0.00000000	0.33292272
19	0.75460478	0.43567127	-0.75460478	0.43567127	-0.00000000	-2.86870080
20	0.0	0.0	0.0	0.0	0.0	0.0
21	0.07054030	0.16467519	-0.07054030	0.16467519	0.00000000	-0.32935039
22	0.04072646	-0.28522580	0.04072646	0.28522580	-0.08145292	-0.00000000
23	0.00000000	0.33333333	-0.00000000	0.33333333	-0.00000000	0.33333333

ALPHA IRON 298 K

-1-1-1 1 1-2 1.00000 0.0 -0.00000 2.48229

	1	2	3	4	5	6
1	22.60000	14.00000	14.00000	0.0	0.0	0.0
2	14.00000	22.60000	14.00000	0.0	0.0	0.0
3	14.00000	14.00000	22.60000	0.0	0.0	0.0
4	0.0	0.0	0.0	11.60000	0.0	0.0
5	0.0	0.0	0.0	0.0	11.60000	0.0
6	0.0	0.0	0.0	0.0	0.0	11.60000

11.58106358

	1		2		3	
	0.21377568	0.62625499	-0.21377568	0.62625499	0.00000000	2.26405100
1	0.24237626	0.01699853	-0.24237626	0.01699853	0.00000000	-5.52389061
2	-0.51560097	-0.25926460	0.51560097	-0.25926460	-0.00000000	1.07763741
3	-0.31207535	-0.05932666	0.31207535	-0.05932666	0.00000000	-1.14822102
4	-0.14747759	-0.24903850	-0.14747759	0.24903850	0.18726666	-0.00000000
5	-0.18598425	0.06457975	0.18598425	0.06457975	-0.00000000	-0.95991521
6	-0.03881870	0.22577927	-0.03881870	-0.22577927	1.07763741	0.00000000
7	0.03861767	0.07607450	0.03861767	-0.07607450	2.25335766	0.00000000
8	-0.23906800	0.20547416	-0.23906800	-0.20547416	0.18980443	0.00000000
9	-0.47713778	0.05757157	0.47713778	0.05757157	0.00000000	-1.15377665
10	-0.26157247	-0.20893642	-0.26157247	0.20893642	1.15377665	0.00000000
11	0.17372759	0.03565980	-0.17372759	0.03565980	0.00000000	-2.25335766
12	-0.30768801	-0.10468677	0.30768801	-0.10468677	-0.00000000	0.97292363
13	0.0	0.0	0.0	0.0	0.0	0.0
14	-0.13078624	-0.10446821	-0.13078624	0.10446821	0.57688832	0.00000000
15	-0.23856889	0.02878578	0.23856889	0.02878578	0.00000000	-0.57688832
16	-0.10022517	0.14077433	-0.10022517	-0.14077433	1.22158104	0.00000000
17	-0.13396042	-0.06902697	0.13396042	-0.06902697	0.00000000	-1.28043402
18	-0.13396042	-0.06902697	0.13396042	-0.06902697	0.00000000	-1.28043402
19	0.58530007	0.30159272	-0.58530007	0.30159272	-0.00000000	5.59447422
20	0.0	0.0	0.0	0.0	0.0	0.0
21	0.17372759	0.00236155	-0.17372759	0.00236155	0.00000000	0.99527690
22	-0.23906800	-0.40970705	-0.23906800	0.40970705	0.18980443	-0.00000000
23	-0.47713778	-0.25480359	0.47713778	-0.25480359	0.00000000	0.50960718

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