WORK HARDENING DURING PYRAMIDAL SLIP IN ZINC

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ABSTRACT

The elastic stress field and energy associated with an infinite straight edge dislocation in a hexagonal crystal parallel to the line of intersection of the (0001) and the $(11\bar{2}2)$ planes with its Burger's Vector in the $(11\bar{2}2)$ plane and the $[\bar{1}\bar{1}23]$ direction is determined taking into account the anisotropy of the crystal. The nature of the solution is found to depend on the relative numerical values of the five independent elastic constants. All possible solutions are investigated and the solution for an isotropic crystal determined as a limiting case.

The interaction force between two edge dislocations of opposite sign gliding on consecutive glide planes is studied. Expressions for the total energy of such a dislocation dipole are developed. Numerical results are given at three temperatures, -77°C, 31° C, and 139° C.

These results are used to develop a quantitative theory of strain hardening in a single zinc crystal subjected to uniaxial tension or compression in the direction of its crystallographic axis. It is proposed that such strain hardening is produced by the dislocation dipoles that are formed on dislocations which are moving on any one of the six $(11\bar{2}2)$ pyramidal planes when they intersect similar dislocations which are moving on other planes of the same type. The density of such dislocation dipoles as a function of the uniaxial strain along the crystallographic axis is determined and possible future avenues of research that could utilize these results indicated.

TABLE OF CONTENTS

CHAPTER I. INTRODUCTION

Zinc single crystals fracture readily along the basal plane at low temperatures. Stoffel and Wood [1] * in an investigation undertaken to determine the dependence of basal cleavage fracture in zinc on basal slip and tensile stress normal to the basal plane found that such cleavage fracture is preceded by plastic elongation in the direction of the hexagonal crystallographic axis. Such plastic deformation occurred by slip on two different types of slip systems. One was the usual basal slip produced by shear or torsion in that plane. The other was nonbasal slip on $\{\bar{2}112\}$ pyramidal planes in $\langle 2\bar{1}\bar{1}3\rangle$ directions. The latter type of slip was produced by tension normal to the basal plane and resulted in permanent deformation along the hexagonal crystallographic axis.

Figure 1.1 indicates typical uniaxial stress vs strain curves at two different temperatures 25° C and -77° C for a single zinc crystal loaded parallel to the hexagonal crystallographic axis. It is seen that the rate of strain hardening during this c-axis plastic deformation is very large. This is because slip occurs simultaneously on six intersecting slip planes. Stoffel and Wood have suggested that when two $\frac{1}{3}\langle 2\bar{1}\bar{1}3\rangle$ dislocations of a screw orientation moving on $\{\bar{2}112\}$ planes cut across each other they leave a trail of interstitial atoms behind them. This requires a large amount of energy. A lesser amount of energy is required if the

*Numbers in brackets indicate references at the end of this thesis.

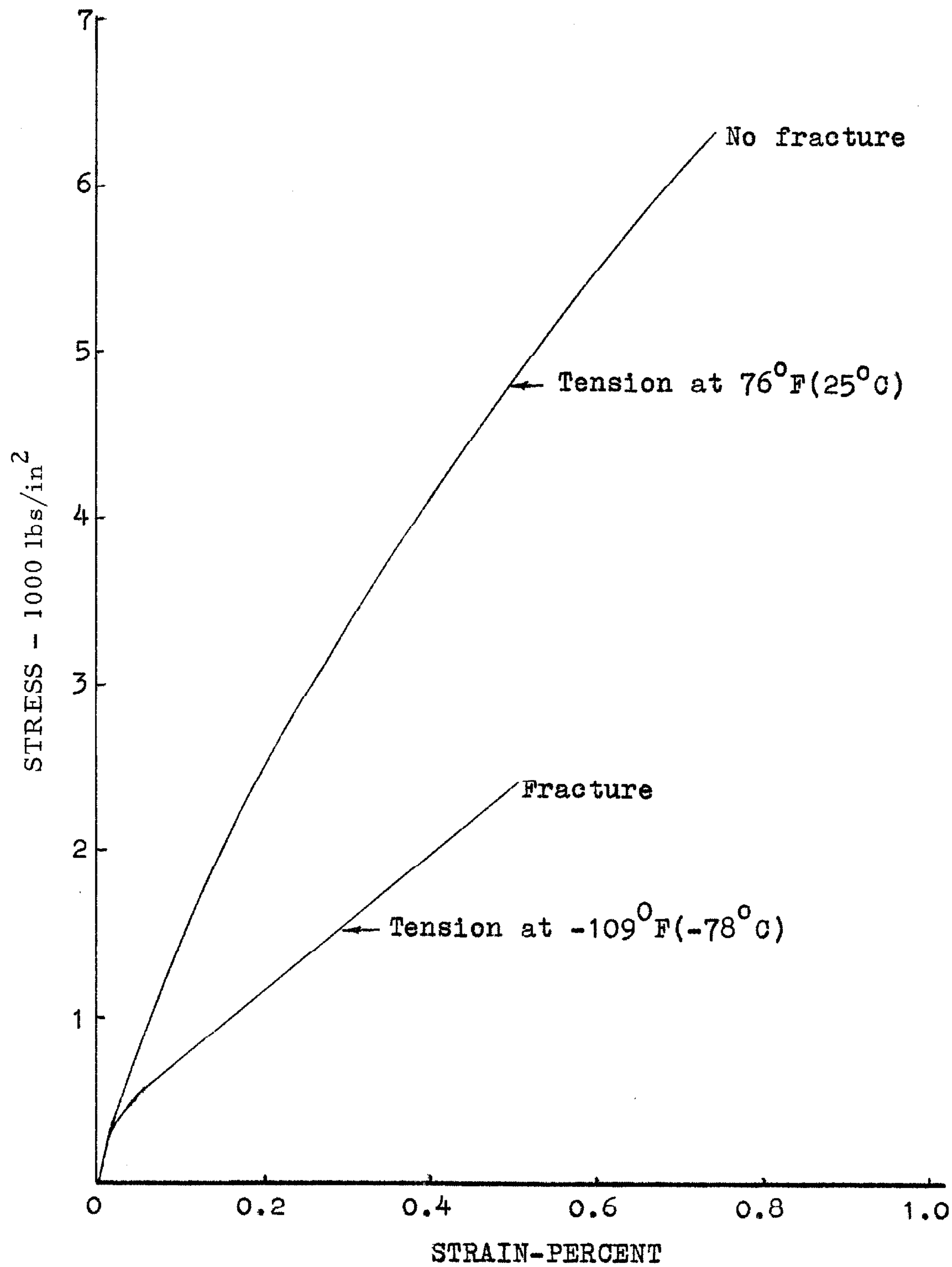


FIGURE 1.1. Typical uniaxial stress vs strain curves at 25°C and -77°C for a single zinc crystal loaded parallel to the hexagonal crystallographic axis.

dislocations cut so as to form a pair of edge dislocation dipoles. Such dipoles act as a drag on the moving dislocations. The energy of their formation has to be supplied by the work done by the applied force on the moving dislocations. As plastic flow proceeds more and more dislocations cut across each other, the density of the edge dislocation dipoles increases. This increased density of dipoles increases the drag on the moving dislocations proportionately. Thus the crystal strain hardens.

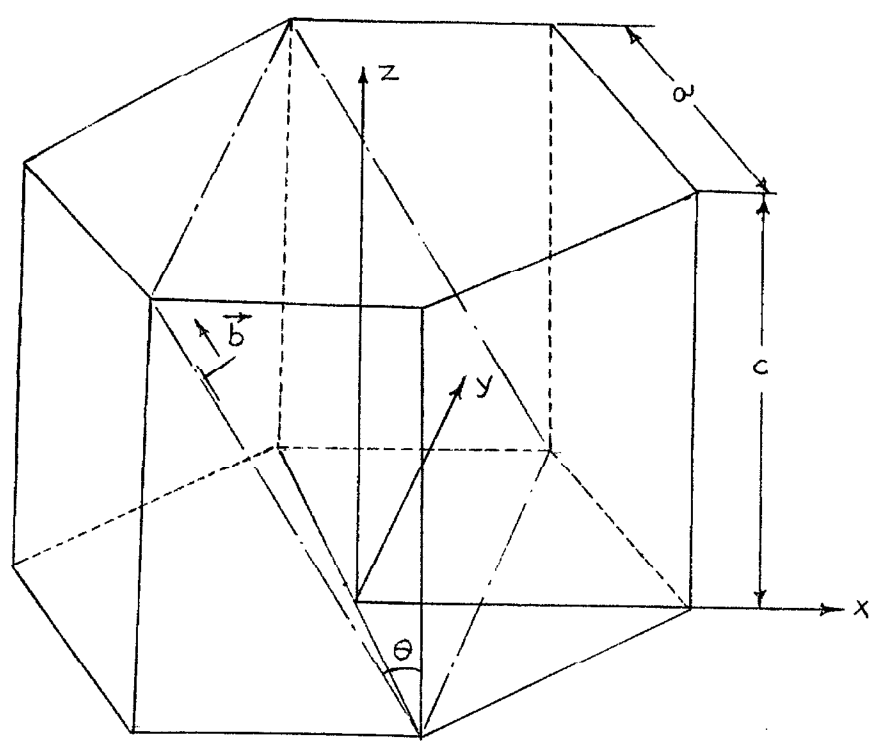
To formulate a quantitative theory of this mechanism of strain hardening, it is necessary to know the stress field and energy associated with, first, an edge dislocation and, second, of an edge dislocation dipole on a pyramidal plane. The elastic stress field in the region outside the core of a general dislocation line in a general anisotropic crystal is very complex and has been expressed in terms of certain line and surface integrals by Burgers [2] and by Peach and Koehler [3] . The theory of the elastic stress field of an infinitely long straight dislocation was given by Eshelby, Read, and Shockley [4] and was extended by Foreman [5] and Stroh [6] . While this general method gives results in the form of sum of complex functions and their conjugates, the rationalisation of these formulae is rather laborious. Spence [7] has carried out this rationalisation for dislocations in the basal plane of graphite, for dislocations in the basal plane and a plane perpendicular to the basal plane in a hexagonal crystal and for dislocations in certain directions in other crystal systems. The stress field and elastic energy of an edge dislocation dipole, with dislocation lines parallel to the line of intersection of the (0001) basal plane and the $(11\bar{2}2)$ pyramidal plane, formed by the intersection of dislocations of at least partially screw orientation, Burger's Vector $\frac{1}{3}\langle 2\bar{1}\bar{1}3\rangle$ moving on $\{\bar{2}112\}$ planes, is determined in this thesis.

CHAPTER II. ELASTIC STRESS FIELD ASSOCIATED WITH AN INFINITE STRAIGHT EDGE DISLOCATION ON A $\{11\bar{2}2\}$ PYRAMIDAL PLANE WITH ITS BURGER'S VECTOR IN THE $[\bar{1}\bar{1}23]$ DIRECTION

2.1. Formulation of the problem

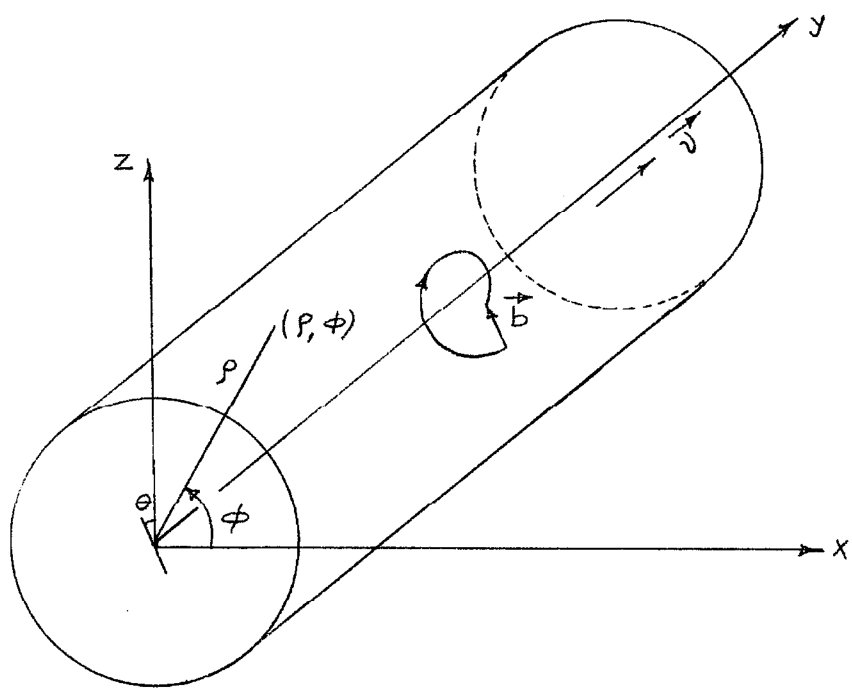
Figure 2.1 shows an infinitely long straight edge dislocation located on a $\{11\bar{2}2\}$ pyramidal plane in a hexagonal crystal. The dislocation line lies parallel to a line defined by the intersection of (0001) basal plane and the $(11\bar{2}2)$ pyramidal plane. The Burger's Vector is in the $(2\bar{1}\bar{1}2)$ plane and in the $\langle\bar{2}113\rangle$ direction. Rectangular cartesian coordinates are chosen so that the y-axis coincides with the dislocation line; the x-y plane then defines the basal plane of the crystal. The z-axis

FIG. 2.1



is the crystallographic c-axis. In figure 2.2 the same dislocation is assumed to coincide with the axis of an infinitely long cylinder of a homogeneous hexagonal crystal of outer radius R. Such an assumption while reducing the mathematical complexity considerably is found to give results consistent with the elasticity theory of dislocations developed so far. The positive direction $\vec{\nu}$ along the dislocation is chosen along the positive y-axis and the

FIG. 2.2



Burger's Vector $\vec{b}$ is the closure failure of a right handed Burger's circuit about the positive y-axis. Cylindrical polar coordinates (ρ, ϕ) will also be used where ϕ is the angle between the radius ρ and the positive x-axis. The inclination of the glide plane θ to the c-axis is fixed by the crystal structure. If 'a' and 'c' are the lattice dimensions as in Figure 2.1

$$\sin\theta = \frac{a}{\sqrt{a^2+c^2}}, \quad \cos\theta = \frac{c}{\sqrt{a^2+c^2}}$$

For such a state one can assume a plane strain situation in which the y-displacement 'v' vanishes and the x and z displacements are independent of y. In an aelotropic elastic medium the strains are related to the stresses by

$$\begin{aligned}
\epsilon_x &= S_{11}\sigma_x + S_{12}\sigma_y + S_{13}\sigma_z + S_{14}\tau_{yz} + S_{15}\tau_{xz} + S_{16}\tau_{xy} \\
\epsilon_y &= S_{21}\sigma_x + S_{22}\sigma_y + S_{23}\sigma_z + S_{24}\tau_{yz} + S_{25}\tau_{xz} + S_{26}\tau_{xy} \\
\epsilon_z &= S_{31}\sigma_x + S_{32}\sigma_y + S_{33}\sigma_z + S_{34}\tau_{yz} + S_{35}\tau_{xz} + S_{36}\tau_{zx} \\
&\quad \ldots\ldots\ldots\ldots\ldots\ldots \\
\gamma_{xy} &= S_{61}\sigma_x + S_{62}\sigma_y + S_{63}\sigma_z + S_{64}\tau_{yz} + S_{65}\tau_{xz} + S_{66}\tau_{zx}
\end{aligned} \qquad (2.1)$$

The matrix of elastic constants for a hexagonal crystal is

$$\begin{array}{cccccc}
S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\
 & S_{11} & S_{13} & 0 & 0 & 0 \\
 & & S_{33} & 0 & 0 & 0 \\
 & & & S_{44} & 0 & 0 \\
 & & & & S_{44} & 0 \\
 & & & & & 2(S_{11} - S_{12})
\end{array} \qquad (2.2)$$

For plane strain in the x-z plane the components of strain in the y-direction vanish

$$\epsilon_y = S_{21}\sigma_x + S_{22}\sigma_y + S_{23}\sigma_z + S_{24}\tau_{yz} + S_{25}\tau_{xz} + S_{26}\tau_{xy} = 0$$

$$\gamma_{xy} = S_{61}\sigma_x + S_{62}\sigma_y + S_{63}\sigma_z + S_{64}\tau_{yz} + S_{65}\tau_{xz} + S_{66}\tau_{xy} = 0 \qquad (2.3)$$

$$\gamma_{yz} = S_{41}\sigma_x + S_{42}\sigma_y + S_{43}\sigma_z + S_{44}\tau_{yz} + S_{45}\tau_{xz} + S_{46}\tau_{xy} = 0$$

Equations (2.3) are used to eliminate σ_y, τ_{xy} , τ_{yz} from expressions for ϵ_x , ϵ_z , ϵ_{zx} which are now written

$$\epsilon_x = \bar{S}_{11}\sigma_x + \bar{S}_{13}\sigma_z + \bar{S}_{15}\tau_{zx}$$

$$\epsilon_z = \bar{S}_{31}\sigma_x + \bar{S}_{33}\sigma_z + \bar{S}_{35}\tau_{zx} \qquad (2.4)$$

$$\epsilon_{zx} = \bar{S}_{51}\sigma_x + \bar{S}_{53}\sigma_z + \bar{S}_{55}\tau_{zx}$$

where making use of (2.3) for a hexagonal crystal

$$\bar{S}_{11} = \frac{S_{11}^2 - S_{12}^2}{S_{11}}$$

$$\bar{S}_{33} = \frac{S_{11}S_{33} - S_{13}^2}{S_{11}} \qquad (2.5)$$

$$\bar{S}_{13} = \bar{S}_{31} = \frac{S_{12}(S_{11} - S_{12})}{S_{11}}$$

$$\bar{S}_{55} = S_{44}$$

$$\bar{S}_{15} = \bar{S}_{51} = \bar{S}_{35} = \bar{S}_{53} = 0$$

Thus the stress strain relationships (2.1) become

$$\epsilon_x = \bar{S}_{11}\,\sigma_x + \bar{S}_{13}\,\sigma_z$$

$$\epsilon_z = \bar{S}_{13}\,\sigma_x + \bar{S}_{33}\,\sigma_z \qquad (2.6)$$

$$\epsilon_{zx} = \bar{S}_{55}\,\tau_{zx}$$

The equations of equilibrium in tensor notation are

$$\sigma_{ij,j} = 0 \qquad i,j = x,y,z \qquad (2.7)$$

For plane strain in the x-z plane these are satisfied if the stresses are chosen in terms of a stress function χ such that

$$\sigma_x = \chi_{zz}$$

$$\sigma_z = \chi_{xx} \qquad (2.8)$$

$$\tau_{zx} = -\chi_{xz}$$

where the subscripts denote differentiation with respect to the indicated independent variable χ.

The compatibility conditions are

$$\frac{\partial^2 \epsilon_x}{\partial z^2} + \frac{\partial^2 \epsilon_z}{\partial x^2} = \frac{\partial^2 \epsilon_{xz}}{\partial x\,\partial z} \qquad (2.9)$$

Substituting for the strains in terms of stresses and for stresses in terms of the stress function χ from equations (2.6) and (2.8) the governing field equation becomes

$$\bar{S}_{33}\frac{\partial^4\chi}{\partial x^4} + (2\bar{S}_{13} + \bar{S}_{55})\frac{\partial^4\chi}{\partial x^2\partial z^2} + \bar{S}_{11}\frac{\partial^4\chi}{\partial z^4} = 0 \qquad (2.10)$$

This can be put in the form

$$\left(\frac{\partial^2}{\partial x^2} + K_1\frac{\partial^2}{\partial x\,\partial y} + \alpha_1\frac{\partial^2}{\partial y^2}\right)\left(\frac{\partial^2\chi}{\partial x^2} + K_2\frac{\partial^2\chi}{\partial x\,\partial y} + \alpha_2\frac{\partial^2\chi}{\partial y^2}\right) = 0 \qquad (2.11)$$

where

$$\alpha_1 + \alpha_2 + K_1 K_2 = \frac{2\bar{S}_{13} + \bar{S}_{55}}{\bar{S}_{33}}$$

$$\alpha_1 \alpha_2 = \frac{\bar{S}_{11}}{\bar{S}_{33}}$$

$$K_1 + K_2 = 0$$

$$K_1\alpha_2 + K_2\alpha_1 = 0$$

To perform this factorisation α_1 and α_2 are confined to real and positive values and K_1 and K_2 to real values. The restriction that is implied by this means that the roots of the quartic equation

$$\bar{S}_{33}\, p^4 + (2\bar{S}_{13} + \bar{S}_{55})\, p^2 + \bar{S}_{11} = 0$$

for p are all complex. This condition is necessary in order that physically realisable results may be obtained. That all the roots for p are in fact complex follows from certain inequalities satisfied by the elastic constants as a result of the condition that the strain energy function

$$\tfrac{1}{2}\bar{S}_{11}\sigma_x^2 + \tfrac{1}{2}\bar{S}_{33}\sigma_z^2 + \tfrac{1}{2}\bar{S}_{55}\tau_{xz}^2 + \bar{S}_{13}\sigma_x\sigma_z$$

is positive definite [8]. Thus equation (2.10) can always be put in the form of equation (2.11)

2.2 Boundary conditions

To represent an edge dislocation a solution is needed which gives a closure failure of $\vec{b}$, the Burger's Vector, for a Burger's circuit around the dislocation. Further, if a closed circuit in the material containing the dislocation is considered, the total force and couple on the surface of any such closed circuit must be zero, for equilibrium. Hence the boundary conditions are

On the surface of a closed circuit around the dislocation

(a) The resultant couple M vanishes

(b) The resultant force Y vanishes

(c) The resultant force X vanishes

and, (d) The closure failure is the Burger's Vector $\vec{b}$ for a Burger's circuit around the dislocation.

Further, on the outer surface of the cylinder $\rho = R$ the stresses $\sigma_{\rho\rho}$, $\sigma_{\rho\phi}$ must vanish.

2.3 Solution

Equations of the kind represented by (2.10) were studied by Green [9]. Eshelby [10] adopted this solution to obtain the stress field of a straight edge dislocation in an anisotropic medium for certain configurations of the dislocation. The solution to the problem at hand follows after these works.

Let
$$z_1 = x + i\lambda_1 y$$
$$z_2 = x + i\lambda_2 y$$

be two complex variables where λ_1, λ_2 are related to the elastic constants S_{ij} by

$$\lambda_n = \frac{1-\gamma_n - i\delta_n}{1+\gamma_n + i\delta_n} \qquad n=1,2$$

$$\gamma_n = \frac{\alpha_n - 1}{\alpha_n + 1 + 2(\alpha_n - \frac{1}{4}K_n^2)^{\frac{1}{2}}} \tag{2.12}$$

$$\delta_n = \frac{-K_n}{\alpha_n + 1 + 2(\alpha_n - \frac{1}{4}K_n^2)^{\frac{1}{2}}}$$

α_n and $\alpha_n - \frac{1}{4}K_n^2$ are real and positive and K_n, γ_n, δ_n are real.

Then a general solution of equation (2.10) is

$$\chi = 2\,\mathrm{Re}\left\{\Sigma f_n(z_n)\right\} \qquad n=1,2 \tag{2.13}$$

To this correspond the displacements

$$u = -2\mathrm{Re}\left[\Sigma C_n f_n'(z_n)\right]$$
$$v = -2\mathrm{Re}\left[i\,\Sigma D_n f_n'(z_n)\right]$$

where

$$C_n = \bar{s}_{11}\lambda_n^2 - \bar{s}_{13}$$

$$D_n = \frac{1}{\lambda_n}\left(\bar{s}_{13}\lambda_n^2 - \bar{s}_{33}\right)$$

and the stresses

$$\sigma_x = -2\mathrm{Re}\left[\Sigma\lambda_n^2\, f_n''(z_n)\right]$$

$$\sigma_z = +2\mathrm{Re}\left[\; f_n''(z_n)\right]$$

$$\sigma_{zx} = -2\mathrm{Re}\left[\, i\Sigma\lambda_n\, f_n''(z_n)\right]$$

The primes denote differentiation with respect to z_n.

The force components (X,Y) and the couple M on any complete circuit in the material are the changes in the values of the expressions

$$X = 2\mathrm{Re}\left\{-i\,\Sigma\lambda_n\, f_n'(z_n)\right\}$$

$$Y = 2\mathrm{Re}\left\{\Sigma\, f_n'\,(z_n)\right\} \qquad (2.14)$$

$$M = 2\mathrm{Re}\left\{z_n f_n'(z_n) - f_n(z_n)\right\}$$

on going round it.

Having obtained the general solution (2.13) one proceeds to adopt it to the boundary conditions. A solution of the form

$$f_n'(z_n) = \tfrac{1}{2} A_n \log z_n \qquad (2.15)$$

provides the necessary multivalued displacement that increases by $\vec{b}$ the Burger's Vector when ϕ increases by 2π provided the complex constants A_n are suitably chosen to satisfy the boundary conditions. Let the suffixes r and i denote the real and imaginary parts of a complex function.

Condition (a) is satisfied for any choice of A_1 , A_2

Condition (b) yields $A_{2i} = -A_{1i}$

Condition (c) gives

$$\lambda_{1r} A_{1r} + \lambda_{2r} A_{2r} - (\lambda_{1i} - \lambda_{2i}) A_{1i} = 0 \qquad (2.16)$$

If $\vec{b}_x$ and $\vec{b}_z$ are the components of the Burger's Vector $\vec{b}$ for a straight edge dislocation on a $\{\bar{2}112\}$ plane, condition (d) yields

$$C_{1i} A_{1r} + C_{2i} A_{2r} + (C_{1r} - C_{2r}) A_{1i} = \frac{b_x}{2\pi} \qquad (2.17)$$

and

$$D_{1r} A_{1r} + D_{2r} A_{2r} - (D_{1i} - D_{2i}) A_{1i} = \frac{b_z}{2\pi} \qquad (2.18)$$

When the A_i's are so chosen the stress function χ is given by

$$\chi = \mathrm{Re}\,(A_1 z_1 \log z_1 + A_2 z_2 \log z_2 - A_1 z_1 - A_2 z_2)$$

The nature of the solution depends on the relative magnitudes of $(2\bar{S}_{13}+\bar{S}_{55})^2$ and $4\bar{S}_{33}\bar{S}_{11}$. For the present investigation on zinc the adiabatic elastic constants as given by G.A. Alers and J.R. Neighbors [11] are used. These experimental values show that at high temperatures of the magnitude of 100° C

$$(2\bar{S}_{13}+\bar{S}_{55})^2 > 4\bar{S}_{33}\bar{S}_{11}$$

This inequality gets smaller as the temperature is reduced until at 31°C

$$(2\bar{S}_{13}+\bar{S}_{55})^2 = 4\bar{S}_{33}\bar{S}_{11}$$

For temperatures lower than 31°C

$$(2\bar{S}_{13}+\bar{S}_{55})^2 < 4\bar{S}_{33}\bar{S}_{11}$$

These elastic constants from Alers et al are plotted in figure 2.3. Numerical values for $(2\bar{S}_{13}+\bar{S}_{55})^2-4\bar{S}_{33}\bar{S}_{11}$ are given in table 2.1 at a few selected temperatures.

TABLE 2.1

Temperature °K	$(2\bar{S}_{13}+\bar{S}_{55})^2-4\bar{S}_{33}\bar{S}_{11}$ in $(10^{-13}\ cm^2/\ dyne)^2$
500	10,483
350	1,756
308	427
304	0
302	-102
295	-352

Accordingly one has to distinguish three cases

Case (1): $(2\bar{S}_{13}+\bar{S}_{55})^2 > 4\bar{S}_{11}\bar{S}_{33}$

Case (2): $(2\bar{S}_{13}+\bar{S}_{55})^2 = 4\bar{S}_{11}\bar{S}_{33}$

Case (3): $(2\bar{S}_{13}+\bar{S}_{55})^2 < 4S_{11}S_{33}$

Case (1): $(2\bar{S}_{13} +\bar{S}_{55})^2 > 4\bar{S}_{11}\bar{S}_{33}$

λ_1 and λ_2 are real

$$\lambda_1 = \lambda_{1r} = \alpha_1^{-\frac{1}{2}}$$

$$\lambda_1 = \lambda_{2r} = \alpha_2^{-\frac{1}{2}}$$

where α_1 and α_2 are the roots of

$$\bar{S}_{33}\alpha^2 -(2\bar{S}_{13}+\bar{S}_{55})\alpha +\bar{S}_{11}=0$$

Solving for A_1, A_2 from (16) to (19)

$$A_{1r} = \frac{-b_z \lambda_{2r}}{2\pi\bar{S}_{33}(\alpha_1^{\frac{1}{2}}\alpha_2^{-\frac{1}{2}} - \alpha_1^{-\frac{1}{2}}\alpha_2^{\frac{1}{2}})}$$

$$A_{2r} = \frac{b_z \lambda_{1r}}{2\pi\bar{S}_{33}(\alpha_1^{\frac{1}{2}}\alpha_2^{-\frac{1}{2}} - \alpha_1^{-\frac{1}{2}}\alpha_2^{\frac{1}{2}})}$$

$$A_{1i} = -A_{2i} = \frac{b_x}{2\pi\bar{S}_{11}(\alpha_1^{-1} - \alpha_2^{-1})}$$

Thus

$$A_1 = \frac{b_z \lambda_1 \lambda_2^2}{2\pi \bar{S}_{33}(\lambda_1^2 - \lambda_2^2)} + \frac{i b_x}{2\pi \bar{S}_{11}(\lambda_1^2 - \lambda_2^2)} \qquad (2.19)$$

$$A_2 = \frac{-b_z \lambda_1^2 \lambda_2}{2\pi \bar{S}_{33}(\lambda_1^2 - \lambda_2^2)} - \frac{i b_x}{2\pi \bar{S}_{11}(\lambda_1^2 - \lambda_2^2)} \qquad (2.20)$$

The radial stress $\sigma_{\rho\rho}$ at any point is given by

$$\sigma_{\rho\rho} = \frac{1}{\rho} \frac{\partial \chi}{\partial \rho} + \frac{1}{\rho 2} \frac{\partial^2 \chi}{\partial \phi^2}$$

Substituting for χ and differentiating

$$\sigma_{\rho\rho} = \frac{1}{\rho} \text{Re} \frac{A_1(-\text{Sin}\phi + i\lambda_1 \text{Cos}\phi)^2}{\text{Cos}\,\phi + i\,\lambda_1 \text{Sin}\,\phi} + \text{Re} \frac{A_2(-\text{Sin}\phi + i\lambda_2 \text{Cos}\phi)^2}{\text{Cos}\,\phi + i\,\lambda_2\,\text{Sin}\,\phi} \qquad (2.21)$$

Similarly

$$\sigma_{\phi\phi} = \frac{\partial^2 \chi}{\partial \rho^2}$$

$$= \frac{1}{\rho} \text{Re} \left\{ A_1 (\text{Cos}\,\phi + i\lambda_1 \text{Sin}\,\phi) + A_2 (\text{Cos}\,\phi + i\lambda_2 \text{Sin}\,\phi) \right\} \qquad (2.22)$$

and

$$\sigma_{\rho\phi} = -\frac{\partial}{\partial \rho}\left(\frac{1}{\rho} \frac{\partial \chi}{\partial \phi}\right)$$

$$= \frac{1}{\rho} \text{Re} \left[A_1 (\text{Sin}\,\phi - i\lambda_1 \text{Cos}\,\phi) + A_2 (\text{Sin}\,\phi - i\lambda_2 \text{Cos}\,\phi) \right] \qquad (2.23)$$

Equations (2.21) to (2.23) show that the external surface of the cylinder r=R is stress free only if R is infinitely large.

For a finite radius R additional terms must be added that cancel the stresses given by equations (2.21) to (2.23). These terms must in addition satisfy the equations of equilibrium and yield stresses that are single valued and continuous everywhere within the body and finite everywhere else including the origin. These additional terms are

$$\sigma_{\rho\rho} = -\frac{\rho}{R^2} \quad \mathrm{Re}\left[\frac{A_1(-\mathrm{Sin}\,\phi + i\lambda_1 \mathrm{Cos}\,\phi)^2}{\mathrm{Cos}\,\phi + i\,\lambda_1 \mathrm{Sin}\,\phi} + \frac{A_2(-\mathrm{Sin}\,\phi + i\lambda_2 \mathrm{Cos}\,\phi)^2}{\mathrm{Cos}\,\phi + i\lambda_2 \mathrm{Sin}\,\phi}\right]$$

$$\sigma_{\phi\phi} = -\frac{3\rho}{R^2} \,\mathrm{Re}\left[A_1(\mathrm{Cos}\,\phi + i\,\lambda_1 \mathrm{Sin}\,\phi) + A_2(\mathrm{Cos}\,\phi + i\lambda_2 \mathrm{Sin}\,\phi)\right] \qquad (2.24)$$

$$\sigma_{\rho\phi} = -\frac{\rho}{R^2} \,\mathrm{Re}\left[A_1(\mathrm{Sin}\,\phi - i\,\lambda_1 \mathrm{Cos}\,\phi) + A_2(\mathrm{Sin}\,\phi - i\lambda_2 \mathrm{Cos}\,\phi)\right]$$

Thus the expressions for the total stress components of the stress field of the dislocation in the cylinder of finite radius R are given by

$$\sigma_{\rho\rho} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\mathrm{Re}\left[\frac{A_1(-\mathrm{Sin}\,\phi + i\,\lambda_1 \mathrm{Cos}\,\phi)^2}{\mathrm{Cos}\,\phi + i\lambda_1 \mathrm{Sin}\,\phi} + \frac{A_2(-\mathrm{Sin}\,\phi + i\,\lambda_2 \mathrm{Cos}\,\phi)^2}{\mathrm{Cos}\,\phi + i\lambda_2 \mathrm{Sin}\,\phi}\right]$$

$$\sigma_{\phi\phi} = \left(\frac{1}{\rho} - \frac{3\rho}{R^2}\right)\mathrm{Re}\left[A_1(\mathrm{Cos}\,\phi + i\lambda_1 \mathrm{Sin}\,\phi) + A_2(\mathrm{Cos}\,\phi + i\lambda_2 \mathrm{Sin}\,\phi)\right] \qquad (2.25)$$

$$\sigma_{\rho\phi} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\mathrm{Re}\left[A_1(\mathrm{Sin}\,\phi - i\lambda_1 \mathrm{Cos}\,\phi) + A_2(\mathrm{Sin}\,\phi - i\lambda_2 \mathrm{Cos}\,\phi)\right]$$

$$\sigma_{\rho z} = \sigma_{z\phi} = 0$$

Usually the correction terms are neglected because they are very small when the outer dimensions of a body are large compared to the position vector magnitude of the point at which the stresses are being computed. However, these terms are retained in the work that follows because in the stress field of an edge dislocation dipole the terms of order $\frac{1}{\rho}$ cancel so that the correction terms may be of more relative significance in the field of a dipole than in the field of an individual dislocation.

Substituting for A_1 and A_2 from (2.19) and (2.20) and rationalising, the complete stress field for case (1) is given by

$$\sigma_{\phi\phi}=\left(\frac{1}{\rho}-\frac{3\rho}{R^2}\right)\left[\frac{-\lambda_1\lambda_2 b_z \operatorname{Cos}\phi}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)}-\frac{b_x \operatorname{Sin}\phi}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right] \qquad (2.26)$$

$$\sigma_{\rho\phi}=\left(\frac{1}{\rho}-\frac{\rho}{R^2}\right)\left[\frac{-\lambda_1\lambda_2 b_z \operatorname{Sin}\phi}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)}+\frac{b_x \operatorname{Cos}\phi}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right] \qquad (2.27)$$

$$\sigma_{\rho\rho}=\left(\frac{1}{\rho}-\frac{\rho}{R^2}\right)\frac{1}{(\operatorname{Cos}^2\phi+\lambda_1^2\operatorname{Sin}^2\phi)(\operatorname{Cos}^2\phi+\lambda_2^2\operatorname{Sin}^2\phi)} \times \left[\frac{b_z\lambda_1\lambda_2 \operatorname{Cos}\phi}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)}A_1+\frac{b_x \operatorname{Sin}\phi}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}A_2\right]$$

where

$$A_1=-\operatorname{Sin}^2\phi\left\{\operatorname{Cos}^2\phi+(\lambda_1^2+\lambda_1\lambda_2+\lambda_2^2)\operatorname{Sin}^2\phi\right\}-\lambda_1\lambda_2(\operatorname{Cos}^2\phi-\lambda_1\lambda_2\operatorname{Sin}^2\phi)$$
$$-\lambda_1\lambda_2\operatorname{Sin}^2\phi\,(\operatorname{Cos}^2\phi-\lambda_1\lambda_2\operatorname{Sin}^2\phi)$$

$$A_2=(\cos^2\phi-\lambda_1\lambda_2\sin^2\phi)(1+\cos^2\phi)\ -\cos^2\phi\ \cos^2\phi(\lambda_1^2+\lambda_1\lambda_2+\lambda_2^2)$$
$$+\lambda_1^2\ \lambda_2^2\sin^2\phi \qquad (2.28)$$

$$\sigma_{\rho y}=\sigma_{y\phi}=0 \qquad (2.29)$$

It is seen that the stresses relax as $\frac{1}{\rho}$ as in an isotropic elastic medium.

The stresses in rectangular cartesian coordinates when the outer radius $R\to\infty$ are

$$\sigma_{xx}=\frac{-xb_z\lambda_1\lambda_2}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)}\left[\frac{\lambda_1\lambda_2\cdot x^2-\lambda_1^2\lambda_2^2\ z^2}{(x^2+\lambda_1^2z^2)\ (x^2+\lambda_2^2z^2)}\right]$$
$$\frac{zb_x}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\left[\frac{x^2(\lambda_1^2+\lambda_1\lambda_2+\lambda_2^2)+\lambda_1^2\lambda_2^2z^2}{(x^2+\lambda_1^2z^2)(x^2+\lambda_2^2z^2\ )}\right] \qquad (2.30)$$

$$\sigma_{zz}=\frac{xb_z\ \lambda_1\ \lambda_2}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)}\left[-x^2-z^2(\lambda_1^2+\lambda_1\lambda_2+\lambda_2^2)\right]$$
$$+\frac{b_xz}{2\pi\bar{S}_{11}\ (\lambda_1+\lambda_2)}\left[x^2-\lambda_1\lambda_2z^2\right] \qquad (2.31)$$

$$\sigma_{xz}=\frac{-b_z\lambda_1^2\lambda_2^2\ z}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)}\left[\frac{x^2-\lambda_1\lambda_2\ z^2}{(x^2+\lambda_1^2z^2\ )\ (x^2+\lambda_2^2z^2\ )}\right]$$
$$+\frac{b_x\ x}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\left[\frac{x^2\ -\lambda_1\lambda_2\ z^2}{(x^2+\lambda_1^2z^2)(x^2+\lambda_2^2z^2)}\right] \qquad (2.32)$$

$$\sigma_{yz}=\sigma_{yx}\ =0 \qquad (2.33)$$

$$\sigma_{yy}=-\frac{1}{S_{22}}(S_{21}\sigma_x+S_{13}\sigma_z) \qquad (2.34)$$

Case (2): $(2\bar{S}_{13}+\bar{S}_{55})^2 = 4\ \bar{S}_{11}\bar{S}_{33}$

One of the chief merits of this method is the ease with which the stress field for this limiting case could be determined.

Here $\lambda_1 = \lambda_2 = 1$

Taking the limit as $\lambda_1 \rightarrow 1$, the expressions for stresses in polar coordinates become from (2.26) to (2.29)

$$\sigma_{\rho\rho} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left(\frac{-b_z \operatorname{Cos}\phi}{4\pi\bar{S}_{33}} - \frac{b_x \operatorname{Sin}\phi}{4\pi\bar{S}_{11}}\right) \quad (2.35)$$

$$\sigma_{\phi\phi} = \left(\frac{1}{\rho} - \frac{3\rho}{R^2}\right)\left(\frac{-b_z \operatorname{Cos}\phi}{4\pi\bar{S}_{33}} - \frac{b_x \operatorname{Sin}\phi}{4\pi\bar{S}_{11}}\right) \quad (2.36)$$

$$\sigma_{\rho\phi} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left(\frac{-b_z \operatorname{Sin}\phi}{4\pi\bar{S}_{33}} + \frac{b_x \operatorname{Cos}\phi}{4\pi\bar{S}_{11}}\right) \quad (2.37)$$

Similarly the expressions for the stresses in rectangular cartesian coordinates become from (2.30) to (2.34)

$$\sigma_{xx} = \frac{-x b_z}{4\pi\bar{S}_{33}}\left[\frac{x^2-z^2}{(x^2+z^2)^2}\right] - \frac{z b_x}{4\pi\bar{S}_{11}}\left[\frac{3x^2+z^2}{(x^2+z^2)^2}\right] \quad (2.38)$$

$$\sigma_{zz} = \frac{x b_z}{4\pi\bar{S}_{33}}\left(-x^2-3z^2\right) + \frac{b_x z}{4\pi\bar{S}_{11}}\left(x^2-z^2\right) \quad (2.39)$$

$$\sigma_{xz} = \frac{1}{4\pi}\left[\frac{x^2-z^2}{(x^2+y^2)^2}\right]\left(\frac{b_x x}{\bar{S}_{33}} - \frac{b_z z}{\bar{S}_{11}}\right) \quad (2.40)$$

$$\sigma_{yy} = -\frac{1}{S_{22}}\left(S_{12}\sigma_{xx}+S_{13}\sigma_{zz}\right) \quad (2.41)$$

It is instructive to carry this limiting case to that for an isotropic elastic body. In engineering notation the elastic constants S_{ij} are

$$S_{11} = \frac{1}{E_{xx}}$$

$$S_{12} = -\frac{\nu_{yx}}{E_{xx}}$$

$$S_{13} = -\frac{\nu_{zx}}{E_{xx}}$$

$$S_{33} = \frac{1}{E_{zz}}$$

$$S_{22} = \frac{1}{E_{yy}}$$

$$S_{44} = \frac{1}{G_{yz}}$$

where E_{xx} , E_{yy} , E_{zz} are the Young's moduli for tension-compression with respect to the directions x,y,z; G_{yz} is the shear modulus for a plane that is parallel to yoz; ν_{yx} is the coefficient which charecterises the decrease in the x-direction for tension in the y-direction.

For an isotropic elastic medium

$$\bar{S}_{11} = \bar{S}_{33} = \frac{1}{E}\,(1 - \nu^2)$$

$$\frac{E}{2(1+\nu)} = G$$

and equations (2.35) to (2.41) become

$$\sigma_{\rho\rho} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left[\frac{-Gb_z \operatorname{Cos}\phi}{2\pi(1-\nu)} - \frac{Gb_x \operatorname{Sin}\phi}{2\pi(1-\nu)}\right]$$

$$\sigma_{\phi\phi} = \left(\frac{1}{\rho} - \frac{3\rho}{R^2}\right)\left\{\frac{-Gb_z \cos\phi}{2\pi(1-\nu)} - \frac{Gb_x \sin\phi}{2\pi(1-\nu)}\right\}$$

$$\sigma_{\rho\phi} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left\{\frac{-Gb_z \sin\phi}{2\pi(1-\nu)} + \frac{Gb_x \cos\phi}{2\pi(1-\nu)}\right\}$$

$$\sigma_{yy} = \frac{-\nu G}{\pi(1-\nu)}\left(\frac{1}{\rho} - \frac{2\rho}{R^2}\right)\left\{(b_z \cos\phi + b_x \sin\phi)\right\}$$

$$\sigma_{\rho y} = \sigma_{y\phi} = 0 \tag{2.43}$$

$$\sigma_{xx} = \frac{-Gb_z x}{2\pi(1-\nu)}\left\{\frac{x^2-z^2}{(x^2+z^2)^2}\right\} - \frac{Gb_x z}{2\pi(1-\nu)}\left\{\frac{3x^2+z^2}{(x^2+z^2)^2}\right\}$$

$$\sigma_{zz} = \frac{Gb_z x}{2\pi(1-\nu)}\left\{\frac{-x^2-3z^2}{(x^2+z^2)^2}\right\} + \frac{Gb_x z}{2\pi(1-\nu)}\left\{\frac{x^2-z^2}{(x^2+z^2)^2}\right\}$$

$$\sigma_{xz} = \frac{G}{2\pi(1-\nu)}\left\{\frac{x^2-z^2}{(x^2+z^2)^2}\right\}(b_x x - b_z z)$$

$$\sigma_{xy} = \sigma_{zy} = 0$$

For $b_z=0$, $b_x= b$, equations (2.43) become

$$\sigma_{\rho\rho} = \frac{-Gb}{2\pi(1-\nu)}\left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\sin\phi$$

$$\sigma_{\phi\phi} = \frac{-Gb}{2\pi(1-\nu)}\left(\frac{1}{\rho} - \frac{3\rho}{R^2}\right)\sin\phi$$

$$\sigma_{yy} = \frac{-\nu Gb}{\pi(1-\nu)}\left(\frac{1}{\rho} - \frac{2\rho}{R^2}\right)\sin\phi$$

$$\sigma_{\rho\phi} = \frac{Gb}{2\pi(1-\nu)}\left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\operatorname{Cos}\phi$$

$$\sigma_{y\phi} = \sigma_{y\rho} = 0$$

$$\sigma_{xx} = \frac{-Gzb}{2\pi(1-\nu)}\left\{\frac{3x^2+z^2}{(x^2+z^2)^2}\right\} \tag{2.44}$$

$$\sigma_{yy} = \frac{Gzb}{2\pi(1-\nu)}\left\{\frac{x^2-y^2}{(x^2+z^2)^2}\right\}$$

$$\sigma_{xz} = \frac{Gbx}{2\pi(1-\nu)}\left\{\frac{x^2-z^2}{(x^2+z^2)^2}\right\}$$

Equations (2.44) are recognized as those obtained from isotropic elasticity theory.

Case (3): $(2S_{13}+S_{55})^2 < 4S_{11}S_{33}$

Here λ_1 and λ_2 are complex conjugates

$$\alpha_1 = \alpha_2 = \sqrt{\frac{\bar{S}_{11}}{\bar{S}_{33}}}$$

and

$$K_1^2 = K_2^2 = 2\left(\frac{\bar{S}_{11}}{\bar{S}_{33}}\right) - \frac{(2\bar{S}_{13}+\bar{S}_{55})}{\bar{S}_{33}} \tag{2.45}$$

This solution for the α_n and K_n keeps α_n and $\alpha_n - \frac{1}{4}K_n^2$ real and positive and K_n, γ_n, δ_n positive.

Hence the eigenvalues λ_n are defined through γ_n

δ_n, as in equation (2.12)

From equations (2.16) to (2.18) the solution for the real and imaginary parts of the complex constants A_i is

$$A_{1i} = -A_{2i} = \frac{b_z \lambda_{1r}}{4\pi(\lambda_{1i} D_{1r} - \lambda_{1r} D_{1i})}$$

$$A_{2r} = \frac{b_z \lambda_{1i}}{4\pi(\lambda_{1i} D_{1r} - \lambda_{1r} D_{1i})} + \frac{b_x}{4\pi C_{1i}} \tag{2.46}$$

$$A_{1r} = \frac{b_z \lambda_{1i}}{4\pi(\lambda_{1i} D_{1r} - \lambda_{1r} D_{1i})} - \frac{b_x}{4\pi C_{1i}}$$

Hence the stresses are

$$\sigma_{\rho\rho} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left\{\frac{A_1}{(\operatorname{Cos}\phi - \lambda_{1i}\operatorname{Sin}\phi)^2 + \lambda_{1r}^2 \operatorname{Sin}^2\phi} + \frac{A_2}{(\operatorname{Cos}\phi + \lambda_{1i}\operatorname{Sin}\phi)^2 + \lambda_{1r}^2\operatorname{Sin}^2\phi}\right\}$$

where

$$\begin{aligned} A_1 = {} & \left\{A_{1r}(\operatorname{Cos}\phi - \lambda_{1i}\operatorname{Sin}\phi) + A_{1i}\lambda_{1r}\operatorname{Sin}\phi\right\}\left\{\operatorname{Sin}^2\phi - \lambda_{1r}^2\operatorname{Cos}^2\phi + \lambda_{1i}^2\operatorname{Cos}^2\phi + 2\lambda_{1i}\operatorname{Sin}\phi\operatorname{Cos}\phi\right\} \\ & + 2\left\{A_{1i}(\operatorname{Cos}\phi - \lambda_{1i}\operatorname{Sin}\phi) - \lambda_{1r}\operatorname{Sin}\phi\, A_{1r}\right\}\left\{\lambda_{1r}\lambda_{1i}\operatorname{Cos}^2\phi + \lambda_{1r}\operatorname{Sin}\phi\operatorname{Cos}\phi\right\} \end{aligned} \tag{2.47}$$

$$\begin{aligned} A_2 = {} & \left\{A_{2r}(\operatorname{Cos}\phi + \lambda_{1i}\operatorname{Sin}\phi) - A_{1i}\lambda_{1r}\operatorname{Sin}\phi\right\}\left\{\operatorname{Sin}^2\phi - \lambda_{1r}^2\operatorname{Cos}^2\phi + \lambda_{1i}^2\operatorname{Cos}^2\phi - 2\lambda_{1i}\operatorname{Sin}\phi\operatorname{Cos}\phi\right\} \\ & + 2\left\{-A_{1i}(\operatorname{Cos}\phi + \lambda_{1i}\operatorname{Sin}\phi) - \lambda_{1r}A_{1r}\operatorname{Sin}\phi\right\}\left\{-\lambda_{1r}\lambda_{1i}\operatorname{Cos}^2\phi + \lambda_{1r}\operatorname{Sin}\phi\operatorname{Cos}\phi\right\} \end{aligned}$$

$$\sigma_{\phi\phi} = \left(\frac{1}{\rho} - \frac{3\rho}{R^2}\right)\left[\frac{b_x\lambda_{1i}\operatorname{Sin}\phi}{2\pi C_{1i}} + \frac{b_z\lambda_{1i}\operatorname{Cos}\phi}{2\pi(\lambda_{1i}D_{1r} - \lambda_{1r}D_{1i})}\right] \tag{2.48}$$

$$\sigma_{\rho\phi} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left\{\frac{b_z\lambda_{1i}\sin\phi}{2\pi(\lambda_{1i}D_{1r} - \lambda_{1r}D_{1i})} - \frac{b_x\lambda_{1i}\cos\phi}{2\pi C_{1i}}\right\} \qquad (2.49)$$

$$\sigma_{\rho y} = \sigma_{y\phi} = 0 \qquad (2.50)$$

$$\sigma_{xx} = -\frac{\{A_{1r}(\lambda_{1r}^2 - \lambda_{1i}^2) - 2\lambda_{1r}\lambda_{1i}A_{1i}\}(x - \lambda_{1i}z) + \lambda_{1r}z\{2\lambda_{1r}\lambda_{1i}A_{1i} + A_{1i}(\lambda_{1r}^2 - \lambda_{1i}^2)\}}{(x - \lambda_{1i}z)^2 + \lambda_{1r}^2 z^2}$$

$$-\frac{\{A_{2r}(\lambda_{1r}^2 - \lambda_{1i}^2) - 2\lambda_{1r}\lambda_{1i}A_{1i}\}(x + \lambda_{1i}z) - \lambda_{1r}z\{2\lambda_{1r}\lambda_{1i}A_{2r} + A_{1i}(\lambda_{1r}^2 - \lambda_{1i}^2)\}}{(x + \lambda_{1i}z)^2 + \lambda_{1r}^2 z^2}$$

$$(2.51)$$

$$\sigma_{zz} = -\frac{A_{1r}(x - \lambda_{1i}z) + A_{1i}\lambda_{1r}z}{(x - \lambda_{1i}z)^2 + \lambda_{1r}^2 z^2} - \frac{A_{2r}(x + \lambda_{1i}z) - A_{1i}\lambda_{1r}z}{(x + \lambda_{1i})^2 + \lambda_{1r}^2 z^2} \qquad (2.52)$$

$$\sigma_{xz} = \frac{\lambda_{1i}\{A_{1r}(x - \lambda_{1i}z) + A_{1i}\lambda_{1r}z\} + \lambda_{1r}\{A_{1i}(x - \lambda_{1i}z) - \lambda_{1r}zA_{1r}\}}{(x - \lambda_{1i}z)^2 + \lambda_{1r}^2 z^2}$$

$$+\frac{\lambda_{1i}\{A_{2r}(x + \lambda_{1i}z) - A_{1i}\lambda_{1r}z\} + \lambda_{1r}\{A_{1i}(x + \lambda_{1i}z)\lambda_{1r}zA_{2r}\}}{(x + \lambda_{1i}z)^2 + \lambda_{1r}^2 z^2} \qquad (2.53)$$

$$\sigma_{yy} = -\frac{1}{S_{22}}(S_{12}\sigma_{xx} + S_{13}\sigma_{zz}) \qquad (2.54)$$

$$\sigma_{xy} = \sigma_{zy} = 0 \qquad (2.55)$$

It can be shown that these equations collapse to those for case (2) as $\lambda_{1r} = \lambda_{2r} \rightarrow 1$ and $\lambda_{1i} = -\lambda_{2i} \rightarrow 0$.

These expressions are valid only beyond a certain minimum radius r_o where the strains are small enough so that the linear theory of elasticity holds. The problem now is to estimate this radius r_o. Substitution of the expressions for the stresses into equations (6) shows that the maximum strain component at a radius r_o is the shear strain ϵ_{zx} evaluated at $\phi = 90^o$. For zinc at 31^oC, assuming the elastic constants given by Alers et al [11] this shear strain is found to be

$$\epsilon_{zx}(r_o, \phi = 90^o) = 0.2166 \frac{b}{r_o}$$

Thus the maximum shear strain is proportional to the Burger's Vector b which is of atomic dimensions. For such small dimensions it is reasonable to assume that the linear theory of elasticity breaks down at a maximum strain of 0.1. Then the core radius r_o is given by

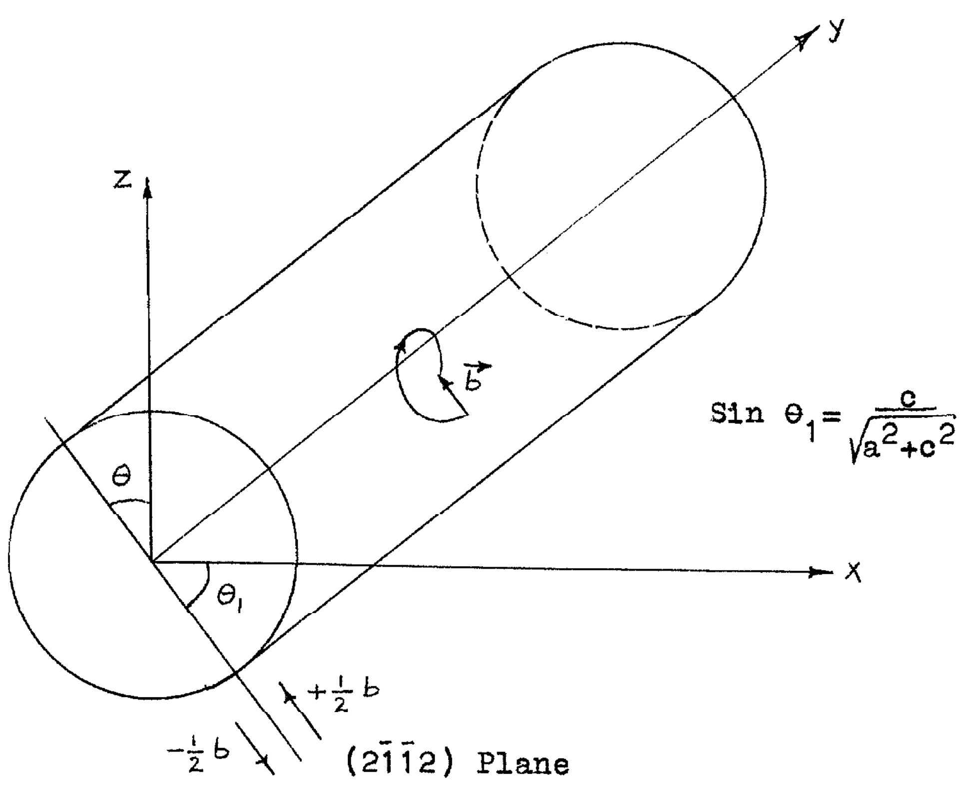
$$r_o = 2.166 \text{ b}$$

This compares with $r_o \doteq 2\frac{1}{2}$ b in an isotropic linear elastic medium.

CHAPTER III: STRAIN ENERGY OF A STRAIGHT EDGE DISLOCATION CONSIDERED IN CHAPTER II.

The elastic strain energy per unit length of the dislocation may be determined from the known elastic stress field. This is the strain energy contained in an annular disc of material of unit thickness with inner radius r_o and outer radius R. It could be conceived of as either the volume integral of strain energy density or as the work done by the forces that have to be applied to the surfaces of a cut made to form the dislocation.

FIG. 3.1



Referring to figure 3.1 a cut is formed along a line defined by $\phi = 360^{\circ} - \theta_1$ where $\theta_1 = \mathrm{Sin}^{-1}\frac{c}{\sqrt{a^2+c^2}}$

The dislocation is formed by displacing the upper half of the cut a distance $+\frac{1}{2}$ b and the bottom half a distance $-\frac{1}{2}$ b.

Let + and - denote the upper and lower surfaces of the cut.

$\bar{n}_+$, $\bar{n}_-$ their outward normal vectors.

$\pm$ b' their respective displacements at an intermediate stage of making the cut.

$\bar{e}_\rho$ unit vector in the direction of the cut.

When the cut surfaces are moved by $\pm \frac{1}{2}$ db' their respective displacements increase by

$$d\bar{u}_{\pm} = \pm \bar{e}_\rho \frac{1}{2} db'$$

At this stage the stresses in the material are those corresponding to a pure edge dislocation of Burger's Vector b' and hence are given by equations (2.26) to (2.55) with b replaced by b' ($0 \leqslant b' \leqslant b$)

The traction on the upper surface of the cut with the outward normal $\bar{n}$ is

$$\bar{T}_+ = \bar{\bar{\sigma}} . \bar{n}_+$$

where $\bar{\bar{\sigma}}$ is the stress tensor.

Similarly that on the lower surface of the cut is

$$\bar{T}_{-} = \bar{\bar{\sigma}}.\bar{n}_{-} = -\bar{\bar{\sigma}}.\bar{n}_{+}$$

Three cases are to be distinguished as before.

Case (I): $(2\bar{S}_{13}+\bar{S}_{55})^2 > 4\bar{S}_{11}\bar{S}_{33}$

$$\bar{T}_{-} = -\bar{T}_{+} = \bar{\bar{\sigma}}.\bar{n}_{-} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left[\frac{-\lambda_1\lambda_2 b_z' \operatorname{Sin}\phi_o}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)} + \frac{b_x' \operatorname{Cos}\phi_o}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right]\bar{e}_\rho$$

Increase in elastic energy per unit length along the dislocation due to the increase in displacements $\pm d\bar{u}$

$$dU = \int_{\rho=r_o}^{R} (\bar{T}_{-}.d\bar{u}_{-} + \bar{T}_{+}.d\bar{u}_{+})d\rho$$

Substituting for $\bar{T}$ the increase in elastic energy is

$$dU = \left[\frac{-\lambda_1\lambda_2 b_z' db_z' \operatorname{Sin}\phi_o}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)} + \frac{b_x' db_x' \operatorname{Cos}\phi_o}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right]\int_{\rho=r_o}^{R}\left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)d\rho$$

or

$$dU = \left[\frac{-\lambda_1\lambda_2 b_z' db_z' \operatorname{Sin}\phi_o}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)} \quad \frac{b_x' db_x' \operatorname{Cos}\phi_o}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right]\left(\ln\frac{R}{r_o} - \frac{1}{2} + \frac{1}{2}\frac{r_o^2}{R^2}\right)$$

The strain energy associated with a dislocation of Burger's Vector $\vec{b}$ is then given by

$$U = \int_{b=0}^{b} dU$$

Hence

$$U=\left[\frac{-\lambda_1\lambda_2 b_z^2\ \mathrm{Sin}\,\phi_o}{4\pi\bar{S}_{33}(\lambda_1+\lambda_2)}+\frac{b_x^2\ \mathrm{Cos}\,\phi_o}{4\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right]\left(\ln\frac{R}{r_o}-\tfrac{1}{2}+\tfrac{1}{2}\frac{r_o^2}{R^2}\right) \quad (3.1)$$

In performing this integration it is assumed that the core surface is traction free. The contribution due to this source is small and can be neglected in a first order linear theory. In equation (3.1) the second and third terms in the second bracket are small compared to the first term except for a body whose external dimensions are small. Hence for most practical purposes the elastic strain energy could be written

$$U=\left[\frac{-\lambda_1\lambda_2 b_z^2\ \mathrm{Sin}\,\phi_o}{4\pi\bar{S}_{33}(\lambda_1+\lambda_2)}+\frac{b_x^2\ \mathrm{Cos}\,\phi_o}{4\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right]\left(\ln\frac{R}{r_o}\right) \quad (3.2)$$

Case (2): $(2\bar{S}_{13}+\bar{S}_{55})^2=4\bar{S}_{33}\bar{S}_{11}$

The expression for the strain energy is obtained by carrying equations (3.1) and (3.2) to the limiting case $\lambda_i \rightarrow 1$.

$$U=\left\{\frac{-b_z^2\,\mathrm{Sin}\,\phi_o}{8\pi\bar{S}_{33}}+\frac{b_x^2\,\mathrm{Cos}\,\phi_o}{8\pi\bar{S}_{11}}\right\}\left(\ln\frac{R}{r_o}-\tfrac{1}{2}+\tfrac{1}{2}\frac{r_o^2}{R^2}\right) \quad (3.3)$$

and for $R \gg r_o$

$$U=\left\{\frac{-b_z^2\,\mathrm{Sin}\,\phi_o}{8\pi\bar{S}_{33}}+\frac{b_x^2\,\mathrm{Cos}\,\phi_o}{8\pi\bar{S}_{11}}\right\}\left(\ln\frac{R}{r_o}\right) \quad (3.4)$$

For an isotropic elastic medium, equation (3.3) becomes

$$U=\left[\frac{-Gb_z^2 \sin\phi_o}{4\pi(1-\nu)}+\frac{Gb_x^2 \cos\phi_o}{4\pi(1-\nu)}\right]\left(\ln\frac{R}{r_o}-\tfrac{1}{2}+\tfrac{1}{2}\frac{r_o^2}{R^2}\right) \quad (3.5)$$

In particular when $b_z=o$, $b_x=b$, and the dislocation glide plane is along $\phi_o=0$

$$U=\frac{Gb^2}{4\pi(1-\nu)}\left(\ln\frac{R}{r_o}-\tfrac{1}{2}+\tfrac{1}{2}\frac{r_o^2}{R^2}\right) \quad (3.6)$$

These results are recognized as those obtained from isotropic elasticity theory.

The elastic strain energyper unit length of a single dislocation in an infinite body is thus infinite as in isotropic elasticity theory. As shown above, for zinc at 31°C, $r_o=2.166$ b. Varying R from 10^{-3} cms to 10 cms

$$7.48 \times 10^{10} b^2 < U < 14.52 \times 10^{10} b^2 \text{ ergs/cm}$$

or

$$3.89 < U < 7.565 \text{ eV/atom length "a"}$$

For practical purposes the elastic energy of a single edge dislocation could be given as

$$U \doteq 10 \times 10^{10} b^2 \text{ergs/cm}$$

where b is expressed in cms.

Case (3): $(2\bar{S}_{13}+\bar{S}_{55})^2 < 4\bar{S}_{11}\bar{S}_{33}$

λ_1 and λ_2 are complex conjugates

Following the same reasoning as before

$$U=\left[\frac{\lambda_{1i} b_z^2 \ \mathrm{Sin}\,\phi_0}{4\pi(\lambda_{1i}D_{1r}-\lambda_{1r}D_{1i})} - \frac{b_x^2\lambda_{1i}\mathrm{Cos}\,\phi_0}{4\pi C_{1i}}\right]\left(\ln\frac{R}{r_o} - \frac{1}{2} + \frac{1}{2}\frac{r_o^2}{R^2}\right) \quad (3.7)$$

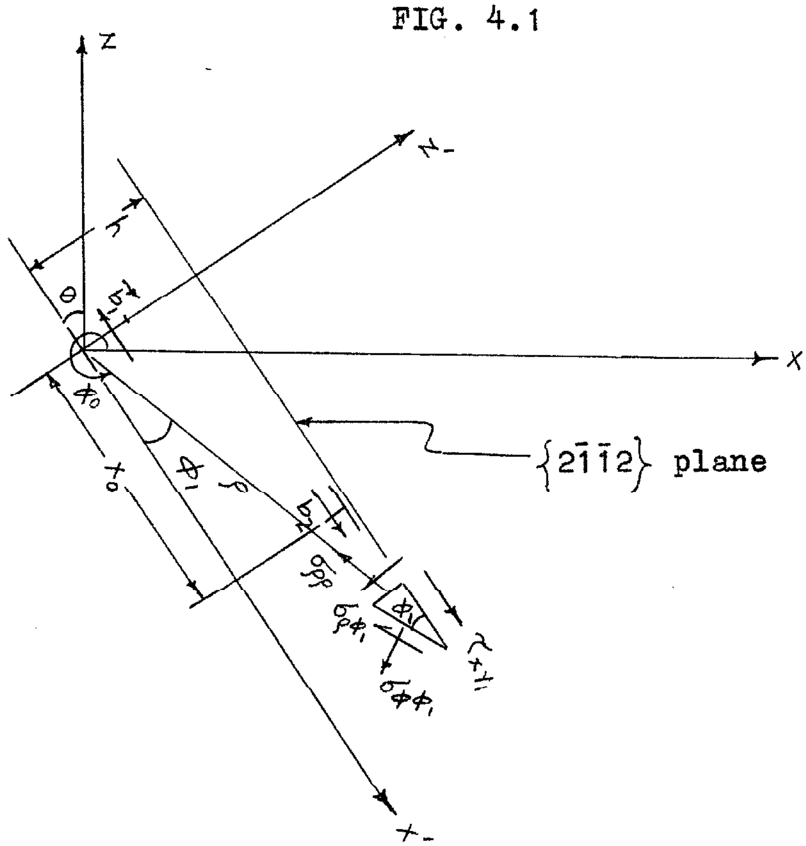
and for $R \gg r_o$

$$U=\left[\frac{\lambda_{1i} b_z^2 \ \mathrm{Sin}\,\phi_o}{4\pi(\lambda_{1i}D_{1r}-\lambda_{1r}D_{1i})} - \frac{b_x^2\lambda_{1i} \ \mathrm{Cos}\,\phi_o}{4\pi C_{1i}}\right]\left(\ln\frac{R}{r_o}\right) \quad (3.8)$$

CHAPTER IV: INTERACTION OF PARALLEL DISLOCATIONS WITH PARALLEL BURGER'S VECTORS

Figure 4.1 shows two edge dislocations of opposite sign, one lying at the origin of coordinates (x', z') and the other at $x' = x_0$, $z' = h$. $\tau_{x'y'}$ is the shear stress acting along the glide plane of the second dislocation

FIG. 4.1



due to the first one. Considering unit area on which $\tau_{x'y'}$ acts, equilibrium of forces yields

$$\tau_{x'y'} = \sigma_{\rho\rho_1} \sin\phi_1 \cos\phi_1 - \sigma_{\phi\phi_1} \sin\phi_1 \cos\phi_1 - \sigma_{\rho\phi_1}(\sin^2\phi_1 - \cos^2\phi_1) \quad (4.1)$$

The stress field of a single dislocation along $\phi = \phi_0$

is given by

$$\sigma_{\rho\rho} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left\{\frac{-b_z \, \mathrm{Cos}\,\phi_0}{4\pi \bar{S}_{33}} - \frac{b_x \mathrm{Sin}\,\phi_0}{4\pi \bar{S}_{11}}\right\}$$

$$\sigma_{\phi\phi} = \left(\frac{1}{\rho} - \frac{3\rho}{R^2}\right)\left\{\frac{-b_z \, \mathrm{Cos}\,\phi_0}{4\pi \bar{S}_{33}} - \frac{b_x \mathrm{Sin}\,\phi_0}{4\pi \bar{S}_{11}}\right\} \qquad (4.2)$$

$$\sigma_{\rho\phi} = \left(\frac{1}{\rho} - \frac{\rho}{R^2}\right)\left\{\frac{-b_z \, \mathrm{Sin}\,\phi_0}{4\pi \bar{S}_{33}} + \frac{b_x \mathrm{Cos}\,\phi_0}{4\pi \bar{S}_{11}}\right\}$$

$$\sigma_{\rho y} = \sigma_{y\phi} = 0$$

for the case where the elastic constants are related by

$$(2\bar{S}_{13}+\bar{S}_{55})^2 = 4\bar{S}_{11}\bar{S}_{33}$$

This is true for zinc at 31°C and this relationship is assumed in this chapter.

Substituting equations (4.2) into (4.1) and making use of $\phi_0 = 360^0 - (90^0 - \theta - \phi_1)$

where

$$\mathrm{Cos}\ \theta = \frac{c}{\sqrt{a^2+c^2}}$$

$$\mathrm{Sin}\ \theta = \frac{a}{\sqrt{a^2+c^2}}$$

the shear stress $\tau_{x'y'}$ is given by

$$4\pi\sqrt{a^2+c^2}\ \tau_{x'y'} = \frac{1}{\rho}(\mathrm{Sin}^2\phi_1 - \mathrm{Cos}^2\phi_1)\left[\frac{b_z}{\bar{S}_{33}}(a\mathrm{Sin}\,\phi_1 - c\mathrm{Cos}\,\phi_1) - \frac{b_x}{\bar{S}_{11}}(a\mathrm{Cos}\,\phi_1 + c\,\mathrm{Sin}\,\phi_1)\right]$$
$$+\frac{\rho}{R^2}\left[\frac{-b_z}{\bar{S}_{33}}(a\mathrm{Sin}\,\phi_1 + c\mathrm{Cos}\,\phi_1) - \frac{b_x}{\bar{S}_{11}}(a\mathrm{Cos}\,\phi_1 - c\mathrm{Sin}\,\phi_1)\right] \qquad (4.3)$$

For an isotropic elastic medium

$$\bar{S}_{11} = \bar{S}_{33} = \frac{1}{E}(1-\nu^2)$$

and

$$\tau_{x'y'} = \frac{Gb}{2\pi(1-\nu)} \cos\phi_1 \left[\frac{1}{\rho}(\cos^2\phi_1 - \sin^2\phi_1) - \frac{\rho}{R^2}\right]$$

which is recognized as that obtained from isotropic elasticity theory

At any point $x'=x_o$, $z'=h$

$$\sin\phi_1 = \frac{h}{\rho} \quad , \quad \cos\phi_1 = \frac{x_o}{\rho} \quad , \quad \rho^2 = x_o^2 + h^2$$

where x_o is measured along the glide plane of the first dislocation. Substituting these into (4.3)

$$4\pi\sqrt{a^2+c^2}\,\tau_{x'y'} = \left| \frac{-b_{z_1}}{\bar{S}_{33}h} \frac{\left(\frac{x_o}{h}\right)^2-1}{\left(\frac{x_o}{h}\right)^2+1} \left(a-\frac{cx_o}{h}\right) + \frac{h^2}{R^2}\left(a+\frac{cx_o}{h}\right)\bar{e}_z + \frac{b_{x_1}}{\bar{S}_{11}h} \frac{\left(\frac{x_o}{h}\right)^2-1}{\left[\left(\frac{x_o}{h}\right)^2+1\right]^2} \left(\frac{ax_o}{h}+c\right) - \frac{h^2}{R^2}\left(\frac{ax_o}{h}-c\right)\bar{e}_x \right| \qquad (4.4)$$

where $\bar{e}_z$ and $\bar{e}_x$ are the unit vectors in the z and x directions respectively and the modulus of the quantity on the right hand side is taken.

The component of the force exerted on unit length of the second dislocation in its glide plane by the stress field of the first one is

$$F = b_2 \cdot \tau_{x'y'}\Big|_{x=x_o}$$

Substituting from (4.4)

$$4\pi\sqrt{a^2+c^2}\;F = \frac{-b_{z_1}\cdot b_{z_2}}{\bar{S}_{33}h}\left[\frac{\left(\frac{x_o}{h}\right)^2-1}{\left\{\left(\frac{x_o}{h}\right)^2+1\right\}^2}\left(a-\frac{cx_o}{h}\right)+\frac{h^2}{R^2}\left(a+\frac{cx_o}{h}\right)\right]$$
$$+\frac{b_{x_1}\cdot b_{x_2}}{\bar{S}_{11}h}\left[\frac{\left(\frac{x_o}{h}\right)^2-1}{\left\{\left(\frac{x_o}{h}\right)^2+1\right\}^2}\left(\frac{ax_o}{h}+c\right)-\frac{h^2}{R^2}\left(\frac{ax_o}{h}-c\right)\right] \quad (4.5)$$

The interaction force can now be specialised into that for a dislocation dipole where there are two edge dislocations of opposite sign gliding on consecutive glide planes. If $b_1 = -b_2 = \vec{b}$ equations (4.5) reduce

$$4\pi\sqrt{a^2+c^2}\;F = \frac{b_{z_1}\cdot b_{z_2}}{\bar{S}_{33}h}\left[\frac{\left(\frac{x_o}{h}\right)^2-1}{\left[\left(\frac{x_o}{h}\right)^2+1\right]^2}\left(a-\frac{cx_o}{h}\right)+\frac{h^2}{R^2}\left(a+\frac{cx_o}{h}\right)\right]$$
$$-\frac{b_{x_1}\cdot b_{x_2}}{\bar{S}_{11}h}\left[\frac{\left(\frac{x_o}{h}\right)^2-1}{\left\{\left(\frac{x_o}{h}\right)+1\right\}^2}\left(\frac{ax_o}{h}+c\right)-\frac{h^2}{R^2}\left(\frac{ax_o}{h}-c\right)\right] \quad (4.6)$$

For most crystals $R \gg h$ and equation (4.6) becomes

$$4\pi\sqrt{a^2+c^2}\;F = \frac{b_{z_1}\cdot b_{z_2}}{\bar{S}_{33}h}\left[\frac{\left(\frac{x_o}{h}\right)^2-1}{\left\{\left(\frac{x_o}{h}\right)^2+1\right\}^2}\left(a-\frac{cx_o}{h}\right)\right]$$
$$-\frac{b_{x_1}\cdot b_{x_2}}{\bar{S}_{11}h}\left[\frac{\left(\frac{x_o}{h}\right)^2-1}{\left\{\left(\frac{x_o}{h}\right)^2+1\right\}^2}\left(\frac{ax_o}{h}+c\right)\right] \quad (4.7)$$

For dislocations on the same glide plane the interaction force is given by equations (4.6) for the limiting case $h \to 0$

$$4\pi\sqrt{a^2+c^2}\ F \to \left(\frac{cb_z^2}{\bar{S}_{33}} + \frac{cb_x^2}{\bar{S}_{11}}\right)\left(\frac{-1}{x_o} + \frac{x_o}{R^2}\right) \qquad (4.8)$$

Consider

$$F' = \frac{F}{\dfrac{1}{4\pi h\sqrt{a^2+c^2}}}$$

Let $\frac{x_o}{h} = m$

Then F' is an extremum when $\frac{dF'}{dm} = 0$. Differentiation of (4.7) shows this happens when

$$m^4 + \frac{2c-2ap}{a+pc}\,m^3 - \frac{6cp+6a}{a+pc}\,m^2 + \frac{6ap-6c}{a+pc}\,m + 1 = 0 \qquad (4.9)$$

where

$$p = \frac{\dfrac{b_z^2}{\bar{S}_{33}}}{\dfrac{b_x^2}{\bar{S}_{11}}}$$

For zinc at 31°C

$$b_x = -0.47423\ \vec{b}$$

$$b_z = 0.88031\ \vec{b}$$

$$\bar{S}_{11} = 8.377 \times 10^{-13}\ cm^2/dyne$$

$$\bar{S}_{33} = 21.648 \times 10^{-13}\ cm^2/dyne$$

$$\frac{c}{\sqrt{a^2+c^2}} = 0.88031$$

$$\frac{a}{\sqrt{a^2+c^2}} = 0.47423$$

Then equation (4.9) becomes

$$m^4+0.4959m^3-6m^2-1.4877m+1=0$$

This is a fourth degree equation in m whose roots are determined by Newton's method of iteration. They are found to converge to

$$m=0.3068$$
$$m=2.3053$$
$$m=-.554$$
$$m=-2.55$$

The interaction force when the dislocations are so disposed is given by equation (4.7)

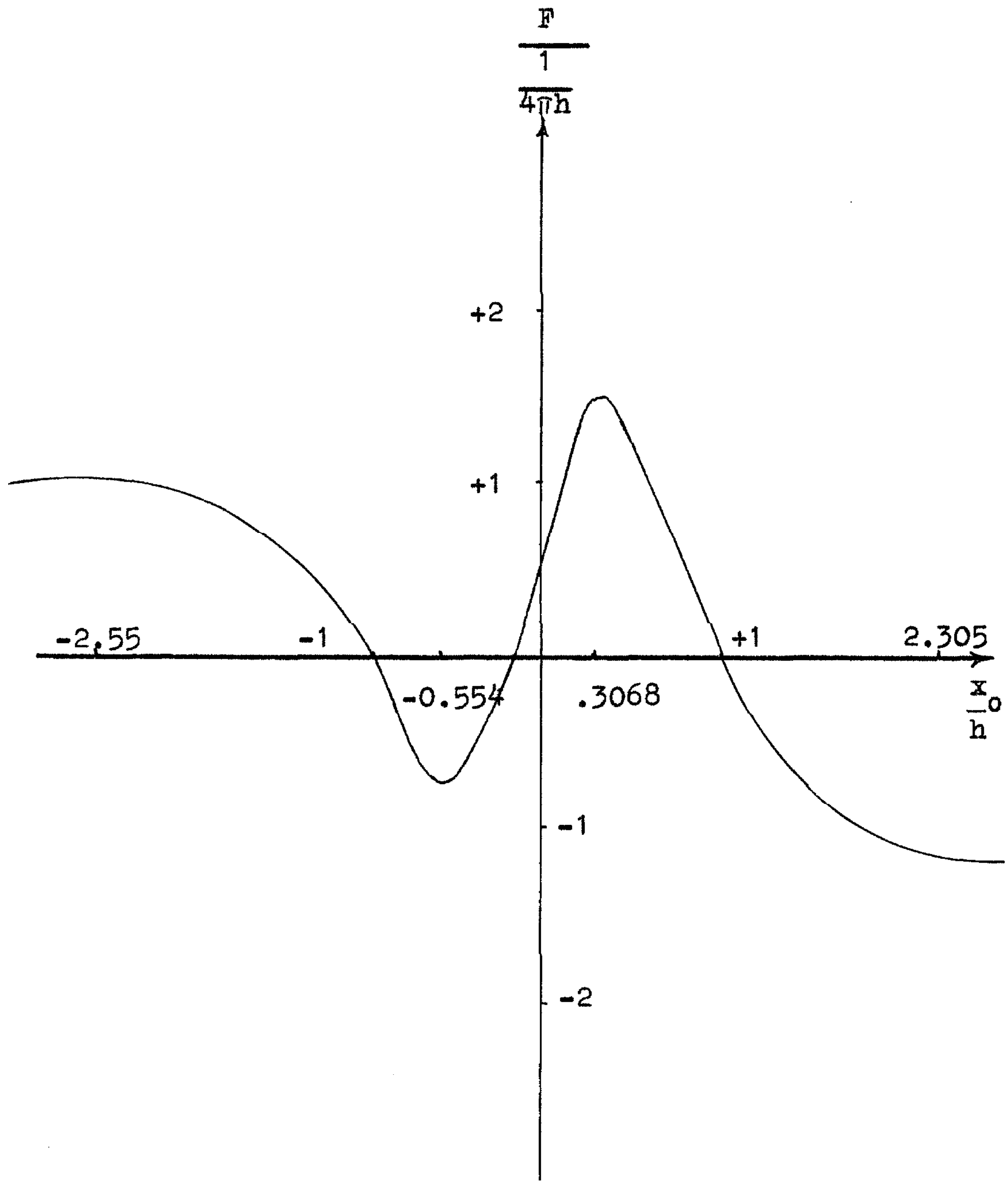
$$\begin{aligned} F(0.3068) &= 1.53076 \times 10^{11} \frac{b^2}{4\pi h} \text{ dynes/cm} \\ F(2.3053) &= -1.17563 \times 10^{11} \frac{b^2}{4\pi h} \text{ dynes/cm} \\ F(-0.554) &= -0.7245 \times 10^{11} \frac{b^2}{4\pi h} \text{ dynes/cm} \\ F(-2.55\ ) &= 1.03783 \times 10^{11} \frac{b^2}{4\pi h} \text{ dynes/cm} \end{aligned} \qquad (4.10)$$

The applied resolved shear stress τ_r required to make the dislocations glide past one another is given by

$$\tau_r b = F_{max}.$$

From (4.10)

FIGURE 4.3. Force diagram between two dislocations of opposite sign



$$\tau_{r\ max} = 1.53076 \times 10^{11} \frac{b}{4\pi h} \text{ dynes/cm}^2$$

or

$$\tau_{r\ max} = 1.0378 \times 10^{11} \frac{b}{4\pi h} \text{ dynes/cm}^2$$

depending on the direction of motion of the second dislocation.

For an equilibrium position, the interaction force τ_{xy_1} between the two dislocations vanishes. From equations (4.7) with numerical values of b_x, b_z etc., inserted such positions are given by

$$m = \pm 1, -0.15043$$

The equilibrium positions are stable when $m = \pm 1$, or $x_o = \pm h$ because any deviation of m from this position induces a force in the direction that tends to move the dislocation back towards $\frac{x_o}{h} = \pm 1$. It follows similarly that the equilibrium is unstable when $m = -0.15043$.

The force diagram between the dislocations is as in figure 4.3.

CHAPTER V. STRAIN ENERGY OF A DISLOCATION DIPOLE

The total elastic energy per unit length along the pair of dislocations is the sum of their self energies and their interaction energy.

The elastic energy per unit length of dislocation 1 when it is alone in the body was given in chapter 111, equations (3.2), (3.3) and (3.4)

The interaction energy is the work done by the stress field of the first dislocation when a suitable cut is formed in the body and its two surfaces displaced with respect to each other so as to form the second dislocation. Three cases are to be considered as before depending on the temperature and the inter-relationship between the various elastic constants. For the special case

$$(2\bar{S}_{11}+\bar{S}_{55})^2 = 4\bar{S}_{11}\bar{S}_{33}$$

the interaction force was studied in Chapter Iv. Accordingly this case is considered first.

Case (2): $(2\bar{S}_{11}+\bar{S}_{55})^2 = 4\bar{S}_{11}\bar{S}_{33}$

A convenient cut is along the glide plane of the second dislocation extending from (x_o,h) to $(\sqrt{R^2-h^2},h)$ in the coordinate system (x',z').

The tractions applied to the surfaces of the cut due to the stress field of the first dislocation are

$$\bar{T}_{-} = \tau_{xy_1} \bar{e}_x'$$

$$\bar{T}_{+} = -\tau_{xy_1} \bar{e}_x'$$

+ and - refer to top and bottom surfaces respectively. These tractions are to be applied in order to prevent spontaneous displacements from occurring and are maintained constant while the second dislocation is being formed.

In order to form the second dislocation the necessary displacements of the top and bottom surfaces are

$$\bar{U}_{-} = + \tfrac{1}{2} b_2 \bar{e}_x'$$

$$\bar{U}_{+} = - \tfrac{1}{2} b_2 \bar{e}_x'$$

The work done by the tractions T through the displacements $\bar{U}_{\pm}$ is the interaction energy U_{12} and is

$$U_{12} = \int_{x'=x_0}^{\sqrt{R^2-h^2}} (\bar{T}_{+} \cdot \bar{U}_{+} + \bar{T}_{-} \cdot \bar{U}_{-})\,dx$$

Substituting for $\bar{T}_{\pm}$, $\bar{U}_{\pm}$

$$U_{12} = \int_{x'=x_0}^{\sqrt{R^2-h^2}} b_2 \tau_{xy_1}\,dx$$

This yields after substitution from (4.6) and integration

$$4\pi\sqrt{a^2+c^2}\; U_{12} = \left[\ln\frac{R}{h} - \tfrac{1}{2}\ln\left(1+\frac{x_0^2}{h^2}\right) - \frac{1}{1+\frac{x_0^2}{h^2}} + \frac{3}{2}\frac{h^2}{R^2} - \tfrac{1}{2} + \tfrac{1}{2}\left(\frac{x_0}{R}\right)^2\right]\left[\frac{b_{z_1} b_{z_2} c}{\bar{S}_{33}} + \frac{b_{x_1} b_{x_2} a}{\bar{S}_{11}}\right] + \left[\frac{\frac{x_0}{h}}{1+\left(\frac{x_0}{h}\right)^2} - \frac{x_0 . h}{R.R}\right]\left[\frac{-b_{z_1} b_{z_2} a}{\bar{S}_{33}} + \frac{b_{x_1} b_{x_2} c}{\bar{S}_{11}}\right] \qquad (5.1)$$

The interaction energy given by (5.1) is perfectly general and holds for dislocations of the same sign or for those of opposite sign. For dislocations of opposite sign, namely for a dislocation dipole, $\vec{b}_1 = -\vec{b}_2 = b$, and equation (5.1) becomes

$$4\pi\sqrt{a^2+c^2}\ U_{12} = \left[\ln\frac{R}{h} - \tfrac{1}{2}\ln\left(1+\frac{x_0^2}{h^2}\right) - \frac{1}{1+\frac{x_0^2}{h^2}} + \frac{3}{2}\frac{h^2}{R^2} - \tfrac{1}{2} + \tfrac{1}{2}\left(\frac{x_0}{R}\right)^2\right]\left[\frac{-b_z^2 c}{\bar{S}_{33}} - \frac{b_x^2 a}{\bar{S}_{11}}\right]$$
$$+\left[\frac{\frac{x_0}{h}}{1+\left(\frac{x_0}{h}\right)^2} - \frac{x_0 h}{R.R}\right]\left(\frac{b_z^2 a}{\bar{S}_{33}} - \frac{b_x^2 c}{\bar{S}_{11}}\right) \qquad (5.2)$$

In addition to the interaction energy work has to be done to overcome the stress field of the second dislocation during its own formation. This is the self energy of the second dislocation.

At a certain stage during the formation of the second dislocation when the relative displacement across the cut is b_2' the shear stress across the cut due to the second dislocation is given by

$$4\pi\sqrt{a^2+c^2}\ \tau_{xy_2} = \left(\frac{c b_{z_2}}{\bar{S}33} + \frac{a b_{x_2}}{\bar{S}11}\right)\left(-\frac{1}{x'-x_0'} + \frac{x'-x'}{R^2}\right) \qquad (5.3)$$

The tractions associated with this stress on the upper and lower surfaces of the cut are

$$\bar{T}_{\pm} = \pm\,\tau_{xy_2}\, e_x' \qquad \text{respectively}$$

Similarly the displacements associated with db_2' are

$$d\bar{U}_{\pm} = \pm \tfrac{1}{2}\, db_2'\bar{e}_x' \qquad \text{respectively}$$

The increment of work

$$dU_2 = \int_{x'=x_0'+r_0}^{\sqrt{R^2-h^2}} \tau_{xy_2} \cdot db_2' dx'$$

Hence the self energy of the second dislocation is

$$U_2 = \int_{b_2'=0}^{b_2} \int_{x'=x_0'+r_0}^{\sqrt{R^2-h^2}} \frac{1}{4\pi\sqrt{a^2+c^2}} \left(\frac{cb_{z_2}}{\bar{S}_{33}} + \frac{ab_{x_2}}{\bar{S}_{11}}\right)\left(\frac{-1}{x'-x_0'} + \frac{x'-x_0'}{R^2}\right) db_2' dx'$$

Integration will yield U_2 as the sum of U_1, the self energy of the first dislocation plus correction terms due to the position of the second dislocation along its glide plane. In this theory these correction terms are neglected and the self energy of the second dislocation U_2 is assumed as the same as U_1, the self energy of the first dislocation.

Thus for $\vec{b}_1 = -\vec{b}_2 = \vec{b}$

$$U_2 = U_1 = \left[\frac{-b_z^2 \operatorname{Sin} \phi_0}{8\pi \bar{S}_{33}} + \frac{b_x^2 \operatorname{Cos} \phi_0}{8\pi \bar{S}_{11}}\right]\left[\ln\frac{R}{r_0} - \tfrac{1}{2} + \tfrac{1}{2}\frac{r_0^2}{R^2}\right] \qquad (5.4)$$

The total elastic energy per unit length along the dislocation dipole is

$$U_{\pm} = U_1 + U_{12} + U_2$$

$$4\pi\sqrt{a^2+c^2}\,U_{\pm} = \left\{\ln\frac{h}{r_o} + \tfrac{1}{2}\ln\left(1+\frac{x_o^2}{h^2}\right) + \frac{1}{1+\frac{x_o^2}{h^2}} - \frac{3}{2}\frac{h^2}{R^2} - \tfrac{1}{2}\left(\frac{x_o}{R}\right)^2 + \tfrac{1}{2}\left(\frac{r_o}{R}\right)^2\right\}\left\{\frac{b_z^2 c}{\bar{S}_{33}} + \frac{b_x^2 a}{\bar{S}_{11}}\right\}$$

$$+\left[\frac{\frac{x_o}{h}}{1+\left(\frac{x_o}{h}\right)^2} - \frac{x_o}{R}\,\frac{h}{R}\right]\left[\frac{b_z^2 a}{\bar{S}_{33}} - \frac{b_x^2 c}{\bar{S}_{11}}\right] \qquad (5.5)$$

The energy associated with a dislocation dipole in an infinite body is thus finite. For a given x_o, when $R \gg h$, equation (5.5) becomes

$$4\pi\sqrt{a^2+c^2}\;U_{\pm} = \left\{\ln\frac{h}{r_o} + \tfrac{1}{2}\ln\left(1+\frac{x_o^2}{h^2}\right) + \frac{1}{1+\frac{x_o^2}{h^2}}\right\}\left\{\frac{b_z^2 c}{\bar{S}_{33}} + \frac{b_x^2 a}{\bar{S}_{11}}\right\}$$

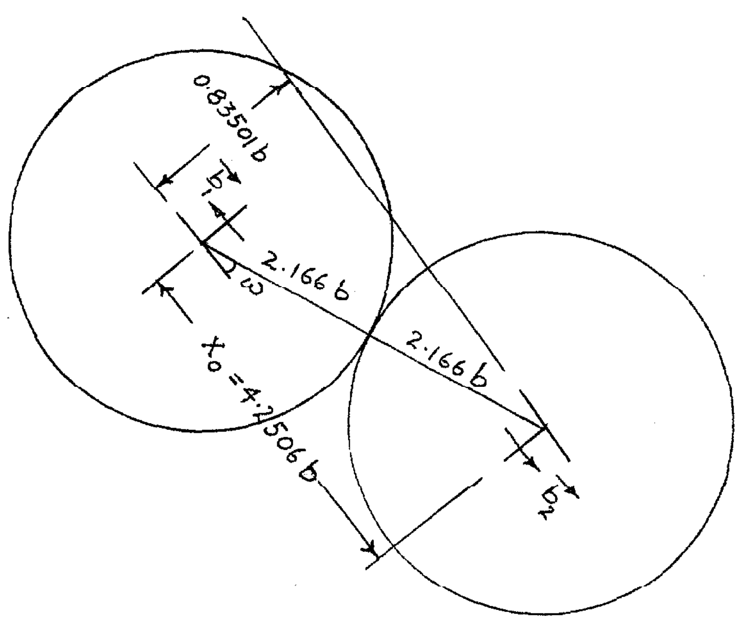
$$+\left[\frac{\frac{x_o}{h}}{1+\left(\frac{x_o}{h}\right)^2}\right]\left[\frac{b_z^2 a}{\bar{S}_{33}} - \frac{b_x^2 c}{\bar{S}_{11}}\right] \qquad (5.6)$$

From equation (4.7) the stable equilibrium positions of the dislocations are given by $x_o = \pm h$ and from Chapter II, $r_o = 2.166b$. Substitution for the various terms yields for zinc at $31^\circ C$,

$$U_{\pm} = 0.18 \text{ electron volts/atom length 'a'}$$

However the core radius $r_o = 2.166$ b so that as the dislocations approach each other there is a hardening effect due to the overlapping of cores. Physically a more realistic equilibrium position for the dislocations is when the cores just touch each other. Referring to figure 5.1, h is the component of one of the two Burger's Vectors in the direction perpendicular to the other one and hence is the value of h that results when a dislocation dipole is formed by the intersection of two gliding dislocations of at least partially screw orientation on a $\{11\bar{2}2\}$ pyramidal plane.

FIG. 5.1



Corresponding to this configuration

$$h = b \sin 2\theta = 0.83501\ b$$

x_o=4.2506 b

Substituting these into equation (5.6)

$U_{\pm}$=0.74 electron volts per atom length "a"

It follows that in any actual physical situation the position of the dislocations will lie somewhere in between the theoretical value of $x_o = \pm h$ and the assumed configuration where the cores touch each other so that the total elastic energy per unit length along the pair of dislocations should lie between 0.74 and 0.18 electron volts per atom length. The total energy per unit length of the dipole trail also includes the energy of the cores of the two dislocations. This is about 2 electron volts per atom length per dislocation so that the total energy of the dipole is about 5 ev/atom length.

The energy of an interstitial atom in zinc is about 25 eV. Thus a dipole trail corresponding to a row of interstitial atoms will remain a dipole trail rather than spontaneously converting itself into a row of interstitial atoms because its energy is much less than the energy of the interstitial atom unless work is done by the external forces to overcome the energy differential.

Case (1): $(2\bar{S}_{13}+\bar{S}_{55})^2 > 4\bar{S}_{11}\bar{S}_{33}$

λ_1 and λ_2 are real and the self energy of either dislocation was given in equation (3.2) as

$$U_1=U_2=\left[\frac{-\lambda_1\lambda_2 b_z^2 \ \mathrm{Sin}\,\phi_o}{4\pi\bar{S}_{33}(\lambda_1+\lambda_2)} + \frac{b_x^2 \ \mathrm{Cos}\,\phi_o}{4\pi\bar{S}_{33}(\lambda_1+\lambda_2)}\right]\left(\ln\frac{R}{r_o} - \frac{1}{2} + \frac{1}{2}\frac{r_o^2}{R^2}\right)$$

As indicated at the outset the theory was motivated by the experimental work of Stoffel and Wood [1] which was conducted at temperatures of 25^oC and -77^oC. To provide a correlation between theory and experiment it was deemed useful to construct the theory at 25^oC, -77^oC and 139^oC, providing results at not only the room temperature but also at two temperatures equally spaced from it. Thus the results following are for zinc at a temperature of 139^oC.

The self energy and the interaction energy change with temperature are not due only to the changes in the elastic constants S_{ij} but are due also to the thermal expansion of the crystal lattice. The variation in the coefficients of thermal expansion of zinc with temperature is highly nonlinear. The computations are further complicated by the fact that this variation is different along a direction in the basal plane and the hexagonal crystallographic axis. For the present investigation the following thermal expansion coefficients as furnished by the New Jersey Zinc Co [12] are used.

Between $0^{o}C$ and $100^{o}C$

along 'a' axis $\alpha_a = 15 \times 10^{-6} / {}^{o}C$

along 'c' axis $\alpha_c = 61.5 \times 10^{-6} / {}^{o}C$

It is further assumed that these coefficients of expansion are constant between $-77^{o}C$ and $139^{o}C$.

The lattice dimensions at $25^{o}C$ are

a=2.6595 Angstroms

c=4.9368 Angstroms

At any other temperature T

$$a_T = \left\{ 2.6595 + \alpha_a (T-25^{o}C) \right\} A$$

$$c_T = \left\{ 4.9368 + \alpha_c (T-25^{o}C) \right\} A$$

Hence at $139^{o}C$

$$a = 2.661 \times 10^{-8} \text{ cms}$$

$$c = 4.9431 \times 10^{-8} \text{ cms}$$

$$\text{Cos } \theta = \frac{c}{\sqrt{a^2+c^2}} = 0.8795$$

$$\text{Sin } \theta = 0.4735$$

It is seen that the inclination of the pyramidal plane to the c-axis as defined by θ changes with temperature.

The elastic constants S_{ij} and $\bar{S}_{ij}$ are

$$S_{11} = 9.05 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$S_{33} = 29.88 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$s_{12} = 0.596 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$s_{13} = -8.075 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$s_{14} = 28.5 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$\bar{s}_{11} = s_{11} - \frac{s_{12}^2}{s_{11}} = 9.011 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$\bar{s}_{33} = s_{33} - \frac{s_{13}^2}{s_{11}} = 22.64 \times 10^{-13} \text{ cm}^2/\text{ dyne}$$

$$\bar{s}_{55} = s_{44} = 28.5 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

$$\bar{s}_{13} = \bar{s}_{31} = 0.5567 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

α_1 and α_2 are the roots of

$$\bar{s}_{33}\alpha^2 - (2\bar{s}_{13} + \bar{s}_{55})\alpha + \bar{s}_{11} = 0$$

Substituting for the $\bar{s}_{ij}$

$$\alpha_1 = 18.714$$

$$\alpha_2 = 10.898$$

By definition

$$\lambda_1 = \alpha_1^{-\frac{1}{2}} = 0.23148$$

$$\lambda_2 = \alpha_2^{-\frac{1}{2}} = 0.3.3$$

The orientation of the dislocation is defined by

$$\mathrm{Sin}\,\phi_o = -0.8795$$

$$\mathrm{Cos}\,\phi_o = +0.4735$$

Burger's Vector $b = 5.62 \times 10^{-8}$ cms

Core radius $r_o = 12.17 \times 10^{-8}$ cms

For $R \gg r_o$, equation (3.4) is used for U_1 and U_2. Substituting these various numbers

for $R = 10^{-3}$ cms., $U_1 = U_2 = 8.103 \times 10^{10} b^2$ ergs/cm

for $R = 10$ cms, $U_1 = U_2 = 16.38 \times 10^{10} b^2$ ergs/cm

Thus for 10^{-3}cms $< R < 10$ cms

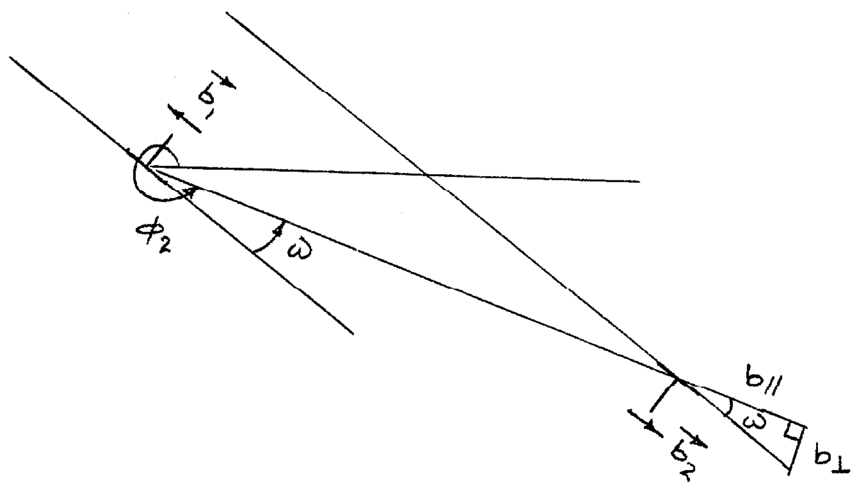
$$8.103 \times 10^{10}\, b^2 < U_1 < 16.38\, b^2 \times 10^{10} \text{ ergs/cm} \quad (5.7)$$

or

$$4.22 < U_1 < 8.53 \text{ eV/atom length 'a'}$$

To determine the interaction energy U_{12} for this case, an equilibrium configuration of dislocations as in figure 5.1 is assumed. Referring to figure 5.2 a radial cut is made along $\phi = \phi_2$ and the two sides of the cut displaced with respect to each other so that the component of this displacement along the glide plane of the second dislocation is b_2. This is a convenient cut to make as the expression for U_{12} then needs to be

FIG. 5.2



integrated only with respect to ρ. Work has to be done against the stress components $\sigma_{\rho\phi}$ and $\sigma_{\phi\phi}$ corresponding to which are the displacements

$$b_{//} = b_2 \operatorname{Cos}\omega = 0.981 \ b_2$$
$$b_{\perp} = -b_2 \operatorname{Sin}\omega = -0.193 \ b_2 \qquad \text{respectively}$$

so that

$$U_{12} = \int_{r_0}^{R} (b_{//} \ \sigma_{\rho\phi} - b_{\perp} \ \sigma_{\phi\phi}) d\rho \tag{5.8}$$

The stresses $\sigma_{\rho\phi}$, $\sigma_{\phi\phi}$ for a given angle $\phi = \phi_2$ are given by equations (2.27) and (2.26) respectively with ϕ replaced by ϕ_2.

Substitution and integration yields

$$U_{12}=b_2\text{Cos }\theta_1\left\{\frac{-\lambda_1\lambda_2 b_{z_1}\text{ Sin}\phi_2}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)}+\frac{b_x\text{ Cos }{}_2}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right\}\left(\ln\frac{R}{r_o}-\tfrac{1}{2}+\tfrac{1}{2}\frac{r_o^2}{R^2}\right)$$

$$-b_2\text{Sin }\theta_1\left\{\frac{-\lambda_1\lambda_2 b_{z_1}\text{ Cos}\phi_2}{2\pi\bar{S}_{33}(\lambda_1+\lambda_2)}\qquad\frac{b_{x_1}\text{ Sin}\phi_2}{2\pi\bar{S}_{11}(\lambda_1+\lambda_2)}\right\}\left(\ln\frac{R}{r_o}-\frac{3}{2}+\frac{3r_o^2}{2R^2}\right)$$

(5.9)

It is observed from figure 5.2 that

$$\phi_2=360^\circ-(90^\circ-\theta-\omega)$$

so that

$$\text{Cos }\phi_2=\text{Sin }\theta\text{ Cos}\,\omega+\text{Cos }\theta\text{ Sin}\,\omega=0.639$$

$$\text{Sin }\phi_2=-\text{Cos }\theta\text{Cos}\,\omega-\text{Sin }\theta\text{ Sin}\,\omega=-0.953$$

The total strain energy is then

$$U_{\pm}=2U_1+U_{12}$$

Substituting the various numbers, for $R \gg r_o$

$$U_{\pm}=0.8041\text{ eV/atom length 'a'}$$

Case (3): $(2\bar{S}_{13}+\bar{S}_{55})^2<4\bar{S}_{11}\bar{S}_{33}$

λ_1 and λ_2 are complex conjugates.

Following the same procedure as for case (1), the lattice dimensions a and c for $T=-77^{\circ}C$ are

$$a = 2.6579 \times 10^{-8} \text{cms}$$

$$c = 4.9302 \times 10^{-8} \text{cms}$$

The orientation of the dislocation is given by

$$\cos\theta = 0.8788$$

$$\sin\theta = 0.4738$$

The various elastic constants are

$$S_{11} = 8.0 \times 10^{-13} \text{cm}^2/\text{dyne}$$

$$S_{33} = 27.1 \times 10^{-13} \text{cm}^2/\text{dyne}$$

$$S_{12} = 0.5525 \times 10^{-13} \text{cm}^2/\text{dyne}$$

$$S_{13} = -7.15 \times 10^{-13} \text{cm}^2/\text{dyne}$$

$$S_{44} = 24.0 \times 10^{-13} \text{cm}^2/\text{dyne}$$

$$\bar{S}_{11} = 7.962 \times 10^{-13} \text{cm}^2/\text{dyne}$$

$$\bar{S}_{33} = 20.71 \times 10^{-13} \text{cm}^2/\text{dyne}$$

$$\bar{S}_{55} = 24.0 \times 10^{-13} \text{cm}^2/\text{dyne}$$

$$\bar{S}_{13} = \bar{S}_{31} = 0.5144 \times 10^{-13} \text{cm}^2/\text{dyne}$$

From Chapter II

$$\alpha_1 = \alpha_2 = \sqrt{\frac{\bar{S}_{11}}{\bar{S}_{33}}} = 0.62$$

$$K_1^2 = K_2^2 = 2\left(\frac{\bar{S}_{11}}{\bar{S}_{33}}\right) - \left(\frac{2\bar{S}_{13} + \bar{S}_{55}}{\bar{S}_{33}}\right) = 0.4396$$

Hence by definition

$$\delta_1 = \frac{-K_1}{\alpha_1 + 1 + 2(\alpha_1 - \frac{1}{4}K_1^2)^{\frac{1}{2}}} = 0.217 = -\delta_2$$

$$\gamma_1 = \frac{\alpha_1 - 1}{\alpha_1 + 1 + 2(\alpha_1 - \frac{1}{4}K_1^2)^{\frac{1}{2}}} = -0.124 = \gamma_2$$

$$\lambda_1 = \frac{1 - \gamma_1 - i\,\delta_1}{1 + \gamma_1 + i\,\delta_1} = 1.152 - i\,0.533 = \bar{\lambda}_2$$

$$C_1 = \bar{S}_{11}\lambda_n^2 - \bar{S}_{13} = (7.79 + i9.78)10^{-13}\ \text{cm}^2/\text{dyne} = \bar{C}_2$$

$$D_1 = \frac{1}{\lambda_1}(\bar{S}_{13}\lambda_1^2 - \bar{S}_{33})$$

$$= (-14.217 - i17.124)10^{-13}\text{cm}^2/\text{dyne}$$

$$= \bar{D}_2$$

$\bar{\lambda}_2$, $\bar{C}_2$, $\bar{D}_2$ are the complex conjugates of λ_2, C_2, D_2 respectively.

The self energy of a single dislocation was given in equations (3.5) and (3.6). Varying the dimensions of the crystal R from 10^{-3}cms to 10 cms, substitution of the various numbers yields

$$7.14 \times 10^{10} b^2 < U_1 < 14.43 \times 10^{10} b^2 \text{ ergs/cm} \qquad (5.10)$$

or

$$3.72 < U_1 < 7.51 \text{ eV/atom length 'a'}$$

The interaction energy is determined as before as the work done when a cut is made along $\phi = \phi_2$ and the second dislocation is formed by displacing the two sides of the cut by $\pm \frac{1}{2}$ b.

$$U_{12} = \int_{r_o}^{R} (b_{\parallel} \sigma_{\rho\phi} - b_{\perp} \sigma_{\phi\phi}) d\rho$$

The stresses $\sigma_{\rho\phi}$, $\sigma_{\phi\phi}$ are given by equations (2.48) and (2.49) with ϕ replaced by ϕ_2.

Substitution for the stresses and integration yields

$$U_{12} = b_2 \cos\theta_1 \left\{ \frac{b_{z_1} \lambda_{1i} \sin\phi_2}{2\pi(\lambda_{1i}D_{1r} - \lambda_{1r}D_{1i})} - \frac{b_{x_1}\lambda_{1i}\cos\phi_2}{2\pi C_{1i}} \right\} \left(\ln\frac{R}{r_o} - \frac{1}{2} + \frac{1}{2}\frac{r_o^2}{R^2} \right)$$
$$- b_2 \sin\theta_1 \left\{ \frac{b_{z_1}\lambda_{1i}\cos\phi_2}{2\pi(\lambda_{1i}D_{1r} - \lambda_{1r}D_{1i})} + \frac{b_{x_1}\lambda_{1i}\sin\phi_2}{2\pi C_{1i}} \right\} \left(\ln\frac{R}{r_o} - \frac{3}{2} + \frac{3r_o^2}{2R^2} \right)$$

(5.11)

For $R \gg r_o$, substitution of the various numbers into equations (5.11) and (5.10) and addition yields

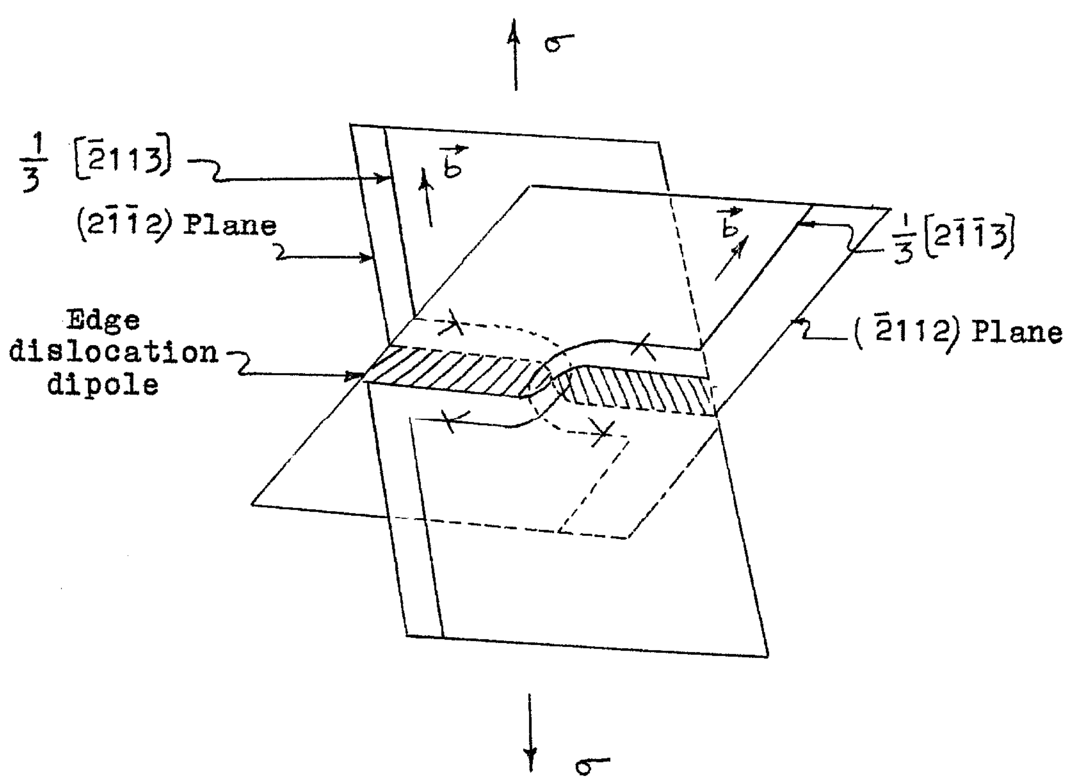
$U_{\pm} = 0.7046$ electron volts /atom length 'a'

Comparison of this value for $U_{\pm}$ at $-77^{\circ}C$ with the values for the energy of the dipole obtained before, namely, $U_{\pm}$ =0.74 eV/atom length 'a' at $31^{\circ}C$ and $U_{\pm}$=0.8041 eV/atom length 'a' at $139^{\circ}C$ shows that the variation in the elastic strain energy of an edge dislocation dipole on a $\{11\bar{2}2\}$ pyramidal plane in a single zinc crystal is confined to $\pm$ 10% from that at room temperature within the temperature range investigated. For most practical applications, therefore, the elastic strain energy of such a dipole, where the dislocation cores touch each other as in figure 5.1 between $-75^{\circ}C$ and $+140^{\circ}C$ could be taken as 0.75 eV/ atom length 'a'.

CHAPTER VI. A THEORY OF STRAIN HARDENING IN A SINGLE ZINC CRYSTAL

As indicated at the outset, experiments conducted by Stoffel and Wood [1] showed that the probable mechanism of yielding for a single zinc crystal subjected to uniaxial tension involved the motion of dislocations on the pyramidal planes. Consider figure 6.1. Two $\frac{1}{3}\langle 2\bar{1}\bar{1}3\rangle$ dislocations moving on two intersecting $\{2\bar{1}\bar{1}2\}$ planes intersect and leave behind a trail of edge dislocation dipoles. There are six such planes of type $\{2\bar{1}\bar{1}2\}$ and simultaneous motion of dislocations on two or more of them results in strong interlocking due to the formation of these dipole trails. Such dipoles

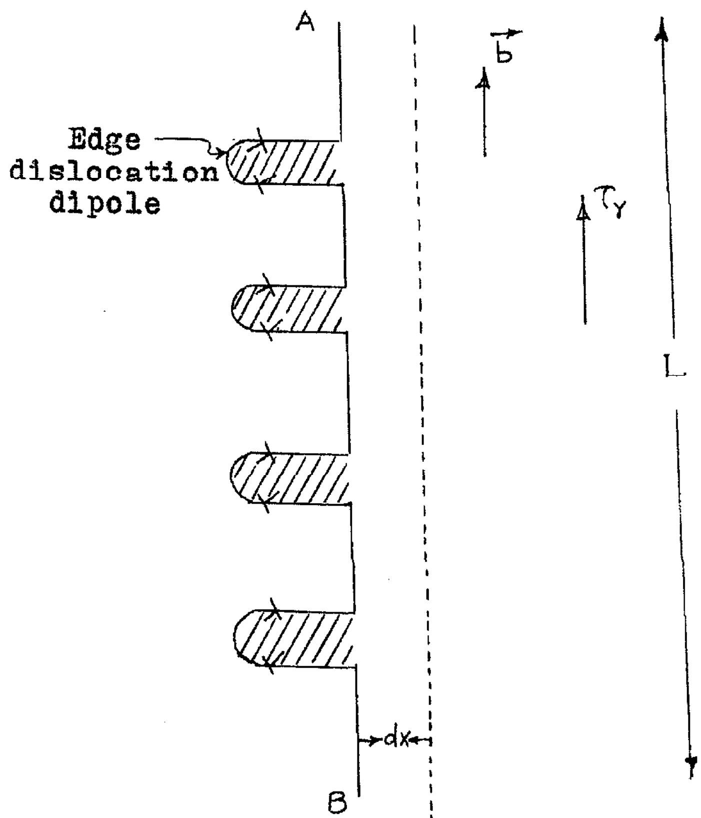
FIG. 6.1



act as a drag on the moving dislocations. The energy of their formation has to be supplied by the work done by the applied force on the moving dislocations. As plastic flow proceeds more and more dislocations cut across each other, the density of the edge dislocation dipoles increases. This increased density of dipoles increases the drag on the moving dislocations proportionately. Thus the crystal strain hardens.

Figure 6.2 shows only a section AB of one of the dislocations in figure 6.1, a $\frac{1}{3}\langle 2\bar{1}\bar{1}3\rangle$ dislocation

FIG. 6.2



moving on a $\{\bar{2}112\}$ plane. Let the length of this section of the dislocation be L, $\vec{b}$ be its Burger's Vector.

The uniaxial tensile stress σ results in a resolved shear stress τ_r on the glide plane of this dislocation.

$$\tau_r = \sigma \cos \theta \qquad (6.1)$$

where θ is defined in figure 2.1

Due to τ_r there is a force $\tau_r b$ on the dislocation normal to the dislocation line.

As this section of the dislocation moves it intersects other dislocations on $\{\bar{2}112\}$ planes and leaves behind a trail of edge dislocation dipoles.

Let d be the linear density of such dipole trails.

When this section of the dislocation AB moves through a distance dx, work is done by the applied forces. It is given by τ_rb.dx.L.

This work is expended on the dipole trails. The energy of these dipole trails increases by

$$U_{\pm} dxLd$$

Since the energy is conserved

$$\tau_r \, b \, dx \, L = U_{\pm} \, dx \, L \, d \qquad (6.2)$$

Hence the density of edge dislocation dipole trails is given by

$$d = \frac{\tau_r \; b}{U_{\pm}} \qquad (6.3)$$

All the variables on the right hand side of this equation are known. The Burger's Vector b is known from physical considerations. The expressions for the energy of a dipole trail have been developed in this thesis. A uniaxial stress strain curve yields τ_r as a function of the uniaxial tensile strain $\mathcal{E}_c$. Thus equation (6.3) determines the density of dipole trails as a function of the uniaxial tensile strain. For the present investigation the uniaxial stress-strain curve as given in figure 1.1 is used and d is determined as a function of $\mathcal{E}_c$ at two temperatures 25°C and -77°C.

At 25°C,

$$\cos \theta = 0.88031$$

$$b = 5.607 \times 10^{-8} \text{ cms}$$

$$U_{\pm} = 0.445 \times 10^{-4} \text{ ergs/cm.}$$

Hence from equation (6.3)

$$d = 1.1092 \times 10^{-3} \sigma \text{ /cm} \qquad (6.4)$$

where σ is expressed in dynes/cm^2.

or

$$d = 0.765 \times 10^{2} \sigma \text{ /cm} \qquad (6.5)$$

where σ is expressed in psi.

The values of d as a function of σ and $\mathcal{E}_c$ are given in table 6.1.

TABLE 6.1

σ psi	ε_c per cent	d no/cm
0.25×10^3	0.012	1.91×10^4
0.40×10^3	0.02	3.06×10^4
0.46×10^3	0.03	3.52×10^4
1.15×10^3	0.2	8.79×10^4
2.00×10^3	0.4	15.30×10^4
2.35×10^3	0.445	17.89×10^4

Similarly at $-77^\circ C$

$$\cos \theta = 0.8788$$

$$b = 5.609 \times 10^{-8} \text{ cms}$$

$$U_{\pm} = 0.424 \times 10^{-4} \text{ ergs/cm}$$

Hence

$$d = 1.1625 \times 10^{-3} \sigma \qquad (6.6)$$

where σ is in dynes/cm

or

$$d = 0.8017 \times 10^{2} \sigma \qquad (6.7)$$

where σ is in psi.

Table 6.2 indicates the relationship between d and ε_c.

These results are plotted in figure 6.3.

This quantitative relationship between the density of edge dislocation dipole trails and the uniaxial tensile

TABLE 6.2

σ psi	ε_c per cent	d no/cm
0.25×10^3	0.012	2.0×10^4
0.40×10^3	0.02	3.2×10^4
0.55×10^3	0.03	4.41×10^4
2.50×10^3	0.2	20.04×10^4
4.15×10^3	0.4	33.27×10^4
5.50×10^3	0.6	44.09×10^4
6.35×10^3	0.675	50.91×10^4

strain could be subjected to direct experimental observation. If the density of these dipole trails as a function of ε_c is observed by X-ray diffraction, for example, and the experimental results confirm the theoretical results, then it follows that the factor governing the motion of dislocations on pyramidal planes in a single zinc crystal is the formation of these dipole trails. Should the experimental results indicate otherwise then it would prove conclusively that some other factor apart from the formation of dipole trails governs their motion.

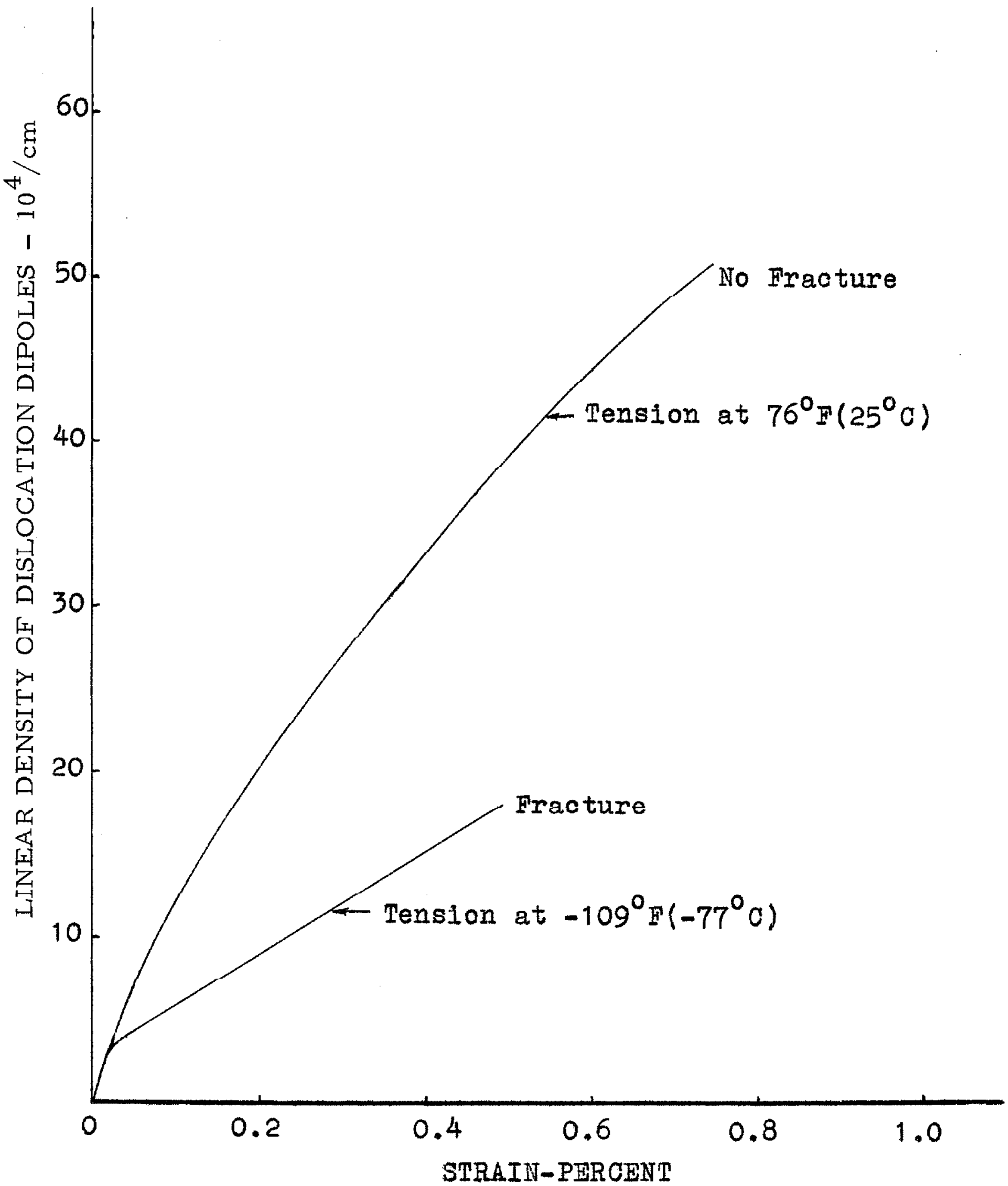


FIGURE 6.3. Linear density of dislocation dipoles as a function of uniaxial percent strain.

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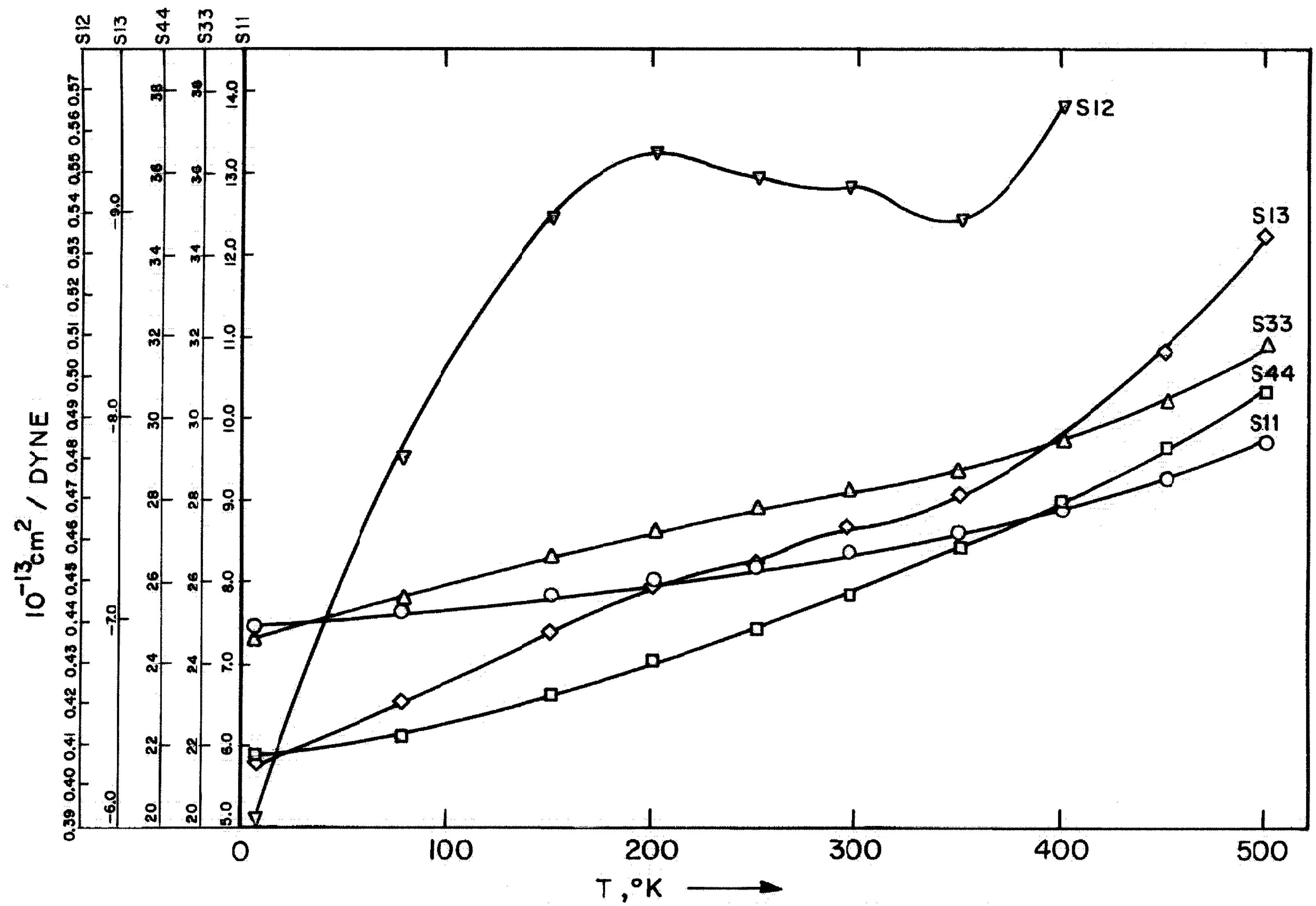

FIGURE 2.3. Elastic constants of zinc vs temperature.