Interaction of Dislocations with an Applied Stress in Anisotropic Crystals*

G. deWit and J. S. Koehler
University of Illinois, Urbana, Illinois
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The equilibrium shape of a dislocation segment between two pinning points in the same glide plane is calculated. The assumption is made that the dependence of the dislocation self-energy on the geometry of the dislocation line can be expressed by using an energy per unit length, E, which is a function only of the angle, θ, between the Burgers vector and the tangent to the dislocation. Only glide of the dislocation, not climb, is considered. The results obtained are compared with those for elastically isotropic crystals. It is found that the character of the dislocation shape is altered considerably if $E+d^2E/d\theta^2$ can be negative. It is suggested that the change in sign of this quantity is associated with diffusionless phase changes.

I. INTRODUCTION

IN this paper, anisotropic elasticity theory is used to study the interaction of dislocations with an externally applied stress in a single crystal.

In Sec. II, the self-energy of a dislocation is considered. The results of a method for calculating the elastic energy per unit length of a long straight dislocation[1] are given. The other contributions to the self-energy of an arbitrarily shaped dislocation are also discussed briefly.

The equilibrium of a single pinned dislocation segment under an applied stress is studied in Sec. III. The differential equation for the shape of the deformed dislocation is derived and it is shown how the solution depends on the self-energy function.

A comparison is made between the results obtained in this paper and those obtained when isotropic elasticity theory is used. The type of self-energy function found for some of the various crystal types is discussed. In addition, some experimental evidence linking dislocation behavior with diffusionless phase changes is presented.

II. SELF-ENERGY OF A DISLOCATION

A. Introductory Remarks

It is desired to obtain an expression for the self-energy of an arbitrarily shaped dislocation in an anisotropic crystal. Since this is a very general problem, attention is first focused on the elastic energy of a straight dislocation. Even for this simpler problem an analytic solution does not exist for an arbitrary orientation of the dislocation in an anisotropic crystal, but a numerical solution can be obtained for any particular orientation. In what follows a number of special cases are considered where the Burgers vector is fixed and the dislocation is confined to a certain plane in the crystal. For these cases, numerical results are used to obtain a function which approximately gives the dependence of the elastic energy per unit length on the dislocation orientation for a straight dislocation. This is then employed as an approximation to the total self-energy per unit length of a curved dislocation.

B. Elastic Energy of a Long Straight Dislocation

Foreman[1] shows that in an elastically anisotropic crystal, E, the elastic energy per unit length of a long straight dislocation, is given by

$$E=[b^2/4\pi][\ln(R/r_0)][K], \tag{1}$$

where b is the magnitude of the Burgers vector, R has the dimensions of the crystal if there is only one dislocation in the crystal, r_0 is the radius of the dislocation core, and K is a function of the elastic constants of the crystal and the orientation with respect to the crystal axes of both the Burgers vector and the dislocation. For an isotropic crystal, K can be expressed as a function of the angle θ between the Burgers vector and the dislocation as follows:

$$K=[\tfrac{1}{2}\mu/(1-\nu)][(2-\nu)-\nu\cos 2\theta], \tag{2}$$

where μ is the shear modulus and ν is Poisson's ratio. For an arbitrary orientation of the dislocation in an anisotropic crystal, K must be found numerically.

Later in this paper it will be useful to know how K varies when the Burgers vector remains fixed and the dislocation changes its direction on a particular plane. For this case, the orientation of the dislocation in the crystal is determined if θ is specified, and thus K can be represented by the series

$$K=\sum_{n=0}^{\infty}[\alpha_n\cos n\theta+\beta_n\sin n\theta], \tag{3}$$

where α_n and β_n are functions only of the elastic constants of the crystal, not of θ.

Values of K for various values of θ have been found numerically, using experimentally determined elastic constants, for each of the materials Cu, Pb, and Li. The results are summarized in Table I. For Cu and Pb, which are face-centered cubic crystals, the calculations were carried out for the Burgers vector along a $\langle 110\rangle$ direction and the dislocation in a (111) plane, while for body-centered cubic Li, the calculations were carried

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[1] A. J. E. Foreman, Acta Met. 3, 322 (1955).

TABLE I. Summary of numerical calculations of K.

Crystal	Temp.	C_{11}[a]	C_{12}[a]	C_{44}[a]	$\frac{2C_{44}}{(C_{11}-C_{12})}$	Source for C_{ij}	Type of slip plane	Direction of Burgers vector
Cu	Room	17.10	12.39	7.56	3.21	Lazarus[b]	(111)	⟨110⟩
Pb	Room	4.76	4.03	1.44	3.95	Goens and Weerts[c]	(111)	⟨110⟩
Li	78°K	1.48	1.25	1.08	9.31	Nash and Smith[d]	(110)	⟨111⟩

Pb		Cu		Li	
θ	K[a]	θ	K	θ	K
0	0.725	0	4.21	$-\pi/2$	0.712
$\pi/12$	0.798	$\pi/6$	5.19	-2ψ[e]	0.663
$\pi/6$	0.958	$\pi/3$	6.74	$-\psi$	0.481
$\pi/4$	1.142	$\pi/2$	7.45	0	0.241
$\pi/3$	1.326			$\pi/2-2\psi$	0.363
$5\pi/12$	1.444			$\pi/3-\psi$	0.421
$\pi/2$	1.479			ψ	0.539
				$\pi/2-\psi$	0.699
				$\pi-3\psi$	0.724
				$2\pi/3-\psi$	0.719
				$\pi/2$	0.712

[a] K and C_{ij} are in units of 10^{11} dynes/cm².
[b] D. Lazarus, Phys. Rev. **76**, 545 (1949).
[c] E. Goens and I. Weerts, Physik. Z. **37**, 321 (1936).
[d] H. C. Nash and C. S. Smith, J. Phys. Chem. Solids **9**, 113 (1959).
[e] $\psi=\sin^{-1}(1/\sqrt{3})$.

out for the Burgers vector along a ⟨111⟩ direction and the dislocation in a (110) plane. These values of K were then used to obtain the coefficients in a truncated form of (3), as follows:

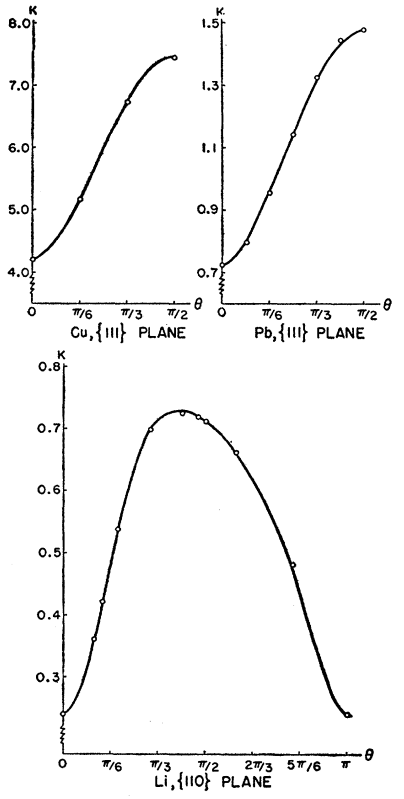

FIG. 1. Results of numerical calculations of K (in units of 10^{11} dynes/cm²) as a function of θ.

Cu

$$K=(5.93-1.60\cos2\theta-0.08\cos4\theta-0.02\cos6\theta+0.01\cos8\theta)\times10^{11}\text{ dynes/cm}^2,$$

Pb

$$K=(1.128-0.374\cos2\theta-0.020\cos4\theta-0.030\cos6\theta-0.006\cos8\theta)\times10^{11}\text{ dynes/cm}^2,$$

Li

$$K=(0.534-0.226\cos2\theta-0.057\cos4\theta-0.010\cos6\theta+0.044\sin2\theta-0.014\sin4\theta-0.008\sin6\theta)\times10^{11}\text{ dynes/cm}^2. \quad (4)$$

These curves are shown in Fig. 1, together with the values of K from Table I. The calculations also show that for a {111} slip plane and a ⟨110⟩ Burgers vector in any cubic crystal, the following is true

$$\alpha_{2n+1}=0, \quad \beta_n=0, \quad (5)$$

while for a {110} slip plane and a ⟨111⟩ Burgers vector in any cubic crystal, these relations hold:

$$\alpha_{2n+1}=0, \quad \beta_{2n+1}=0. \quad (6)$$

C. Some Other Contributions to the Self-Energy of a Dislocation

In the above, some relationships have been presented which give E, the elastic energy per unit length of a long straight dislocation. Equation (1) summarizes the results of Foreman and shows how E is related to K, which gives the orientation dependence. Equations (5) and (6) show what general form K takes when consideration is restricted to a particular direction of b and a particular slip plane. Equation (4) gives K by means of numerical coefficients calculated for particular crystals.

According to Nabarro,[2] if there are many dislocations in the crystal, R should be taken as the average distance to the nearest dislocation of opposite sign. This effectively cuts off the integration of the energy density at R.

In what follows, (1) is used to approximate the energy of a curved dislocation. According to Friedel,[3] at distances closer to the curve than the radius of curvature, the stresses, and thus the energy density, are much the same as those of a straight dislocation. Thus if the radius of curvature of the dislocation line is larger than the distance between dislocations, there will be little trouble with the approximation. Some measure of the error can be obtained by considering a simple example for the case where trouble might begin, i.e., where the radius of curvature is equal to the values used for R. If the exact expression for the energy of a circular dislocation or radius R in an isotropic crystal is compared with the result obtained from (1), the error is about 6% if the distance between dislocations is 10^{-3} cm and the core radius is 5×10^{-8} cm.

One more qualification must be mentioned before (1) can be used to represent the self-energy of an arbitrary dislocation segment. This expression does not include the core energy, that is, the energy associated with that part of the crystal closer to the dislocation than r_0. Within the core, linear elasticity theory does not apply, and more detailied information about atom to atom interactions is needed.

III. EQUILIBRIUM OF A PINNED DISLOCATION SUBJECT TO AN APPLIED STRESS

A. Statement of the Problem

There is considerable interest in the problem of what happens when a stress is applied to a segment of dislocation between two pinning points. The Frank-Read[4] source is based on such a situation. Therefore, the work that follows considers the differential equation of equilibrium of such a dislocation segment for the case of a uniform applied stress. The solution of this differential equation gives information about the equilibrium shape of the dislocation and also about the "critical stress" above which no equilibrium is possible.

B. Derivation of the Differential Equation of Equilibrium

If a stress is applied to a crystal, a dislocation in the crystal will be subject to a force, and a segment between two pinning points will tend to bow out. Since the external stress will do work on the dislocation, there will be an interaction energy. The self-energy will also change as the dislocation bows out, and the equilibrium will be determined by minimizing the total energy. This paper will consider the motion of the dislocation only in its slip plane, and when it is necessary to be more specific, the observed slip planes in the face-centered cubic and body-centered cubic crystals will be used.

Let the x-y plane be the slip plane and the Burgers vector be along the x axis. With no external stress, the dislocation segment lies along the line

$$y=x\tan\theta_0.$$

The equilibrium shape of the segment when there is a constant applied stress may be taken as the curve

$$x=x(u),\quad y=y(u), \tag{7}$$

where u is a parameter which increases in the positive sense of the dislocation. The curve must pass through the pinning points

$$\begin{aligned} &x(u_1)=0, && y(u_1)=0,\\ &x(u_2)=l\cos\theta_0, && y(u_2)=l\sin\theta_0. \end{aligned} \tag{8}$$

See Fig. 2. The problem is to find the functions referred to in (7).

In order to derive the differential equation which the curve x *versus* y, (7), must satisfy, a slight modification of the methods of the variational calculus will be used. Consider that the dislocation moves from

$$x=x(u),\quad y=y(u), \tag{9}$$

to

$$x=x(u)+\delta x(u),\quad y=y(u)+\delta y(u),$$

where δx and δy are small, and

$$\delta x(u_1)=\delta y(u_1)=0,\quad \delta x(u_2)=\delta y(u_2)=0.$$

Otherwise δx and δy are arbitrary. If F is the force per unit length due to the external stress, it will do work

$$\delta W_F=\int_{u_1}^{u_2}[F_x\delta x+F_y\delta y]ds(u),$$

where ds is the element of length, and F_x and F_y are components of F. In order for (7) to represent the equilibrium position of the dislocation, W_F must be

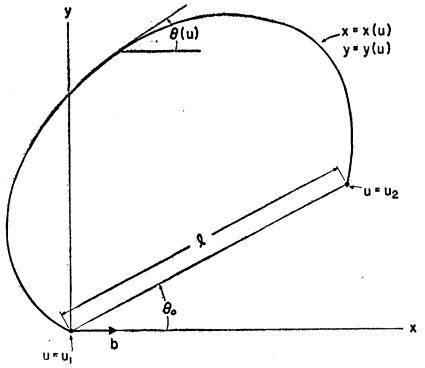

FIG. 2. An illustration of the quantities used in the equilibrium problem.

[2] F. R. N. Nabarro, *Advances in Physics*, edited by N. F. Mott (Taylor and Francis, Ltd., London, 1952), Vol. 1, p. 335.
[3] J. Friedel, *Les Dislocations* (Gauthier-Villars, Paris, 1956), pp. 20–23.
[4] F. C. Frank and W. T. Read, Phys. Rev. **79**, 722 (1950).

balanced by the change in the self-energy

$$\delta W_S=\delta\int_{u_1}^{u_2} E ds(u), \tag{10}$$

where E is given by (1), and the change in the functional $\int E ds$ is evaluated according to the usual variational procedures. Thus

$$\delta W_F-\delta W_S=0. \tag{11}$$

In order to evaluate δW_F, it is necessary to know the force acting on a dislocation due to an applied stress. From Peach and Koehler,[5] this is given by

$$\mathbf{F}=-\boldsymbol{\nu}\times(\boldsymbol{\sigma}\cdot\mathbf{b}), \tag{12}$$

where $\mathbf{F}$ is the force per unit length of dislocation, $\boldsymbol{\nu}$ is the unit vector tangent to the dislocation in the positive sense of the dislocation, $\boldsymbol{\sigma}$ is the stress dyadic, and $\mathbf{b}$ is the Burgers vector of the dislocation. According to (7), the dislocation is confined to the x-y plane, its slip plane, and thus it would be inconsistent to consider a force which would tend to cause climb (motion perpendicular to the slip plane). Examination of (12) shows that only σ_{xz} causes a force in the x-y plane. Thus, in what follows only σ_{xz} is considered, and the results are valid whenever σ_{xx} and σ_{xy} vanish or whenever climb is difficult. If Eq. (9) is used to evaluate $\boldsymbol{\nu}$ and ds, δW_F becomes

$$\delta W_F=\sigma_{xz}b\int_{u_1}^{u_2}[-y'\delta x+x'\delta y]du, \tag{13}$$

where

$$x'=dx/du,\quad y'=dy/du.$$

In order to evaluate δW_S it is necessary to note that E is a function of θ. Since θ is completely defined by (see Fig. 2)

$$\begin{aligned}\sin\theta&=y'/[(x')^2+(y')^2]^{\frac{1}{2}},\\ \cos\theta&=x'/[(x')^2+(y')^2]^{\frac{1}{2}},\end{aligned} \tag{14}$$

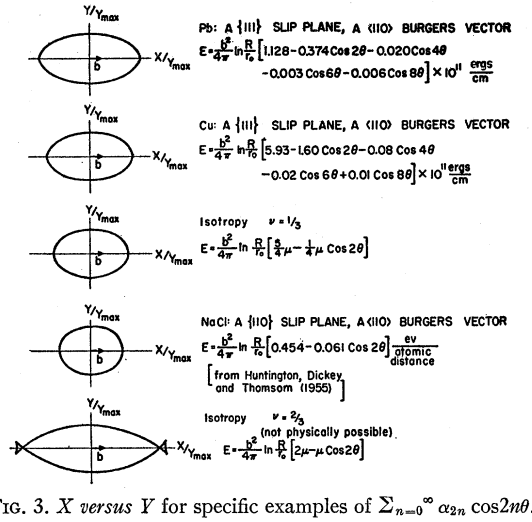

FIG. 3. X *versus* Y for specific examples of $\Sigma_{n=0}^{\infty}\alpha_{2n}\cos 2n\theta$.

[5] M. Peach and J. S. Koehler, Phys. Rev. **80**, 436 (1950).

for the purposes of (10), E can be taken as

$$E=E(\theta)=E(x',y').$$

In (14), the fractional exponent indicates the positive square root of the quantity in parentheses. By the standard methods of variational calculus, δW_S becomes, using the above

$$\delta W_S=\int_{u_1}^{u_2} du\{[\delta x][dF_{x'}/du]+[\delta y][dF_{y'}/du]\},$$

where

$$\begin{aligned}F&=[E(x',y')][(x')^2+(y')^2]^{\frac{1}{2}},\\ F_{x'}&=\partial F/\partial x',\quad F_{y'}=\partial F/\partial y'.\end{aligned} \tag{15}$$

If the equilibrium condition (11) is to be satisfied for arbitrary δx and δy, then from (13) and (15), the following must be true:

$$dF_{x'}/du-\sigma_{xz}by'=0,\quad dF_{y'}/du+\sigma_{xz}bx'=0. \tag{16}$$

Under equilibrium, the segment of the dislocation between the two pinning points must follow a curve which satisfies the differential equations (16). However, there may be other curves, or other parts of one curve which satisfy (16) but do not represent the shape of the dislocation. Therefore, in the following, the general solution of the differential equation is examined first. Then the part of the solution which represents the bowed out dislocation is determined.

C. General Solution of the Differential Equation of Equilibrium

Equations (16) can immediately be integrated to yield

$$F_{x'}-\sigma_{xz}b(y-C_1)=0,\quad F_{y'}+\sigma_{xz}b(x-C_2)=0.$$

By using (14), it is easy to verify that the following satisfies the above equations

$$\begin{aligned}C_1+Y=y=C_1+(\sigma_{xz}b)^{-1}&\\ \times\{[\cos\theta][E(\theta)]-[\sin\theta][dE/d\theta]\},&\\ C_2+X=x=C_2-(\sigma_{xz}b)^{-1}&\\ \times\{[\sin\theta][E(\theta)]+[\cos\theta][dE/d\theta]\}.&\end{aligned} \tag{17}$$

It should be noted that a change in the magnitude of the applied stress σ_{xz} has no effect on the curve X *versus* Y other than a change of scale. A change in the sign of σ_{xz} reflects the curve through the origin.

It will be recalled that in order to derive the differential equation and its solution, (17), it was not necessary to assign any properties to the self-energy per unit length E, other than that it was a function of θ which could be differentiated. The curve cannot be plotted, of course, until more is said about the properties of this function $E(\theta)$.

In Fig. 3, X *versus* Y is plotted using the relations for E found previously for Pb and Cu. The isotropic case is also plotted in Fig. 3, using $\nu=\frac{1}{3}$ and $\nu=\frac{2}{3}$. The latter is physically unrealizable since ν has an upper bound of $\frac{1}{2}$. The calculations of Huntington, Dickey,

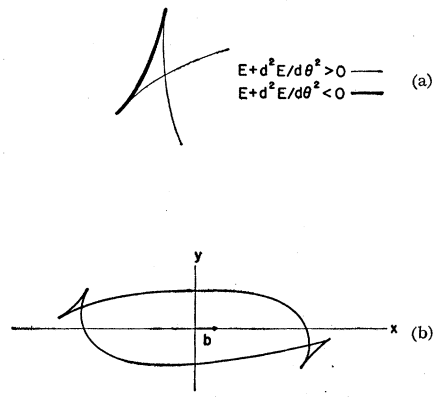

FIG. 4. (a) Feature which will occur on curve X *versus* Y when $E+d^2E/d\theta^2<0$ over some range of θ. (b) X *versus* Y for a {110} plane in Li with Burgers vector along a [111] direction.

and Thomson[6] show that for NaCl also, the energy E can be represented by a cosine series. Their results have been used to obtain the curve of X *versus* Y shown in Fig. 3. In Fig. 4, the curve is plotted using the function $E(\theta)$ calculated for Li.

It is possible to obtain information about the curve X *versus* Y even if all the characteristics of the function $E(\theta)$ are not known. This can be done by determining where X and Y, as given by (17), and $dX/d\theta$ and $dY/d\theta$, as given below, are positive, negative, and zero.

$$\begin{aligned} dX/d\theta &= -(\cos\theta)(b\sigma_{xz})^{-1}(E+d^2E/d\theta^2), \\ dY/d\theta &= -(\sin\theta)(b\sigma_{xz})^{-1}(E+d^2E/d\theta^2). \end{aligned} \tag{18}$$

Table II lists the properties of X *versus* Y which result if certain properties are assigned to $E(\theta)$. For dislocations in the observed slip systems of face-centered cubic crystals (a {111} slip plane and a ⟨110⟩ Burgers vector), E is given by

$$E=\sum \alpha_{2n}\cos 2n\theta,$$

according to (5). In this case the curve X *versus* Y will be symmetric with respect to the X and Y axes, and thus will have the general characteristics of the first four curves in Fig. 3, provided that

$$E+d^2E/d\theta^2>0, \tag{19}$$

for all θ. For dislocations in the observed slip systems of the body-centered cubic crystals (a {110} slip plane and a ⟨111⟩ Burgers vector), E is given by

$$E=\sum (\alpha_{2n}\cos 2n\theta+\beta_{2n}\sin 2n\theta),$$

TABLE II. Dependence of X *versus* Y on the function $E(\theta)$.

Property of $E(\theta)$	Resulting property of X *versus* Y
$E(\theta+2\pi)=E(\theta)$	Closed curve
$E(\theta+\pi)=E(\theta)$	Curve symmetric with respect to origin
$E(n\pi-\theta)=E(\theta)$ n an integer	Curve symmetric with respect to X and Y axes
$E+d^2E/d\theta^2>0$ for all θ	Curve has no cusps and does not cross itself

[6] Huntington, Dickey, and Thomson, Phys. Rev. **100**, 1117 (1955).

according to (6). In this case the curve X *versus* Y will not be symmetric with respect to the X and Y axes, but will be symmetric with respect to the origin. If (19) is not satisfied, i.e., if

$$E+d^2E/d\theta^2<0, \tag{20}$$

for some range of θ, then the curve will have a "handle" as shown in the last curve in Fig. 3 and in Fig. 4.

D. Shape of Dislocation

The curve X *versus* Y is the solution to the differential equations of equilibrium derived previously. What must still be done is to determine what part of this curve represents the bowed out dislocation. To do this, the constants of integration must be determined so that the curve passes through the fixed points of the dislocation given by (8). It is not in general possible to obtain explicit expressions for these constants, but many of the properties of the bowed out dislocations can be found. It will also be useful to inquire about the direction of increase of the parameter u, since this determines the positive sense of the dislocation.

The discussion will first be confined to those cases for which

$$E+d^2E/d\theta^2>0 \quad \text{for all } \theta.$$

The illustrations will be drawn using a solution of the type found for the face-centered cubic crystals, but the reader should have no difficulty in applying the remarks to other cases.

The direction in which the dislocation will tend to bow out is determined by the direction of the force as given in (12). Figure 5 shows that there are two portions of the curve X *versus* Y which might represent the dislocation, and compares them as $\sigma_{xz}\to 0$, for the case that $\sigma_{xz}>0$. The positive sense of the dislocation is

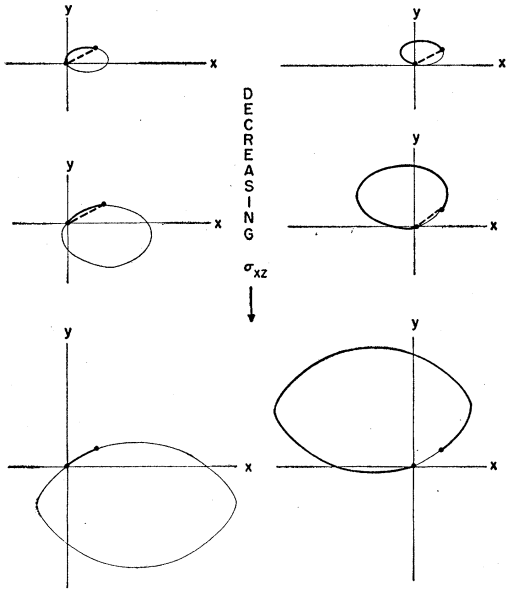

FIG. 5. Comparison of two possible dislocation shapes as $\sigma_{xz}\to 0$.

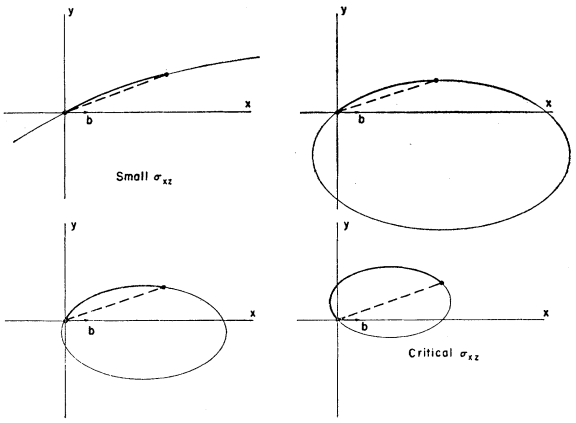

FIG. 6. Effect of increasing σ_{xz}.

away from the x-y origin. From (17), it is seen that the curve X *versus* Y does not change in shape, but only in scale. As $\sigma_{xz} \rightarrow 0$, the curve X *versus* Y becomes larger and larger. The case shown on the left in Fig. 5, i.e., the case where the dislocation is represented by the smaller portion of the closed curve, reduces to the original straight line segment as $\sigma_{xz} \rightarrow 0$. The other case approaches a bowed out dislocation of infinite extent. Another way to express this is that the case where the dislocation is represented by the smaller portion of the closed curve gives the shape which the dislocation would assume if σ_{xz} is gradually increased from zero. Only this case is considered in what follows.

The shape of the bowed out dislocation can now be examined as a function of σ_{xz}, the length l of the original segment, and the angle θ_0 between the original segment and the Burgers vector. In doing this, only $\sigma_{xz}>0$ will be considered.

As σ_{xz} increases, the curve X *versus* Y becomes smaller, as shown in Fig. 6. In the last illustration in Fig. 6 the line which represents the original dislocation passes through the center of the curve X *versus* Y, and thus the two cases shown in Fig. 5 would coincide. It is easy to see that if σ_{xz} were increased any more, and thus if the curve X *versus* Y became any smaller, it would not be possible for the curve to pass through the two fixed points of the dislocation. Thus this value of σ_{xz}, which will be referred to as the critical stress, is the largest for which there will be an equilibrium position for the bowed out dislocation.

The critical stress depends, of course, on the length l of the original dislocations segment and the angle θ_0 between it and the Burgers vector. Figure 7 shows several dislocation segments with the same l, but different θ_0, each under critical stress. The fact that the intercepts of the closed curve with the X and Y axes are inversely proportional to σ_{xz} [see (17)] gives some idea of the dependence of the critical stress on θ_0.

It is also interesting to examine how the shape of the dislocation varies when θ_0 changes, but σ_{xz} and l are constant. This is shown in Fig. 8.

Consideration will next be given to the case where (20) is satisfied for some range of θ. The solution to the differential equation, X *versus* Y, will thus have a handle as shown in the last part of Fig. 3 and in Fig. 4.

The first comment which should be made concerning this case is that the curve X *versus* Y is of a much more complex character than those previously considered. There is some doubt as to the validity of the results in this case, since (1) may not represent the self-energy accurately enough.

Some care must be used in drawing the curve representing the dislocation when $E+d^2E/d\theta^2$ goes negative. To see what happens substitute from (14) for $\sin\theta$ and $\cos\theta$ in (18). Both equations become:

$$1=-(b\sigma_{xz})^{-1}(E+d^2E/d\theta^2)(d\theta/du)[(x')^2+(y')^2]^{-\frac{1}{2}}.$$

Since the positive square root is required, this equation can only be satisfied if:

$$(b\sigma_{xz})^{-1}(E+d^2E/d\theta^2)d\theta/du<0.$$

Hence the sign of $d\theta/du$ is determined once the signs of σ_{xz} and $(E+d^2E/d\theta^2)$ are given.

Figure 9(a) shows the direction of increase of u near a handle. It will be noted that if θ_0 is outside the range where (20) is satisfied, then there is nothing particularly unusual about the shape of the bowed out dislocation. This is shown in Fig. 9(b). If θ_0 is in the range where (20) is satisfied, there are three possibilities for the shape of the dislocation which preserve the positive sense of the dislocation, as shown in Fig. 9(c). Each of these possibilities has some unusual aspects. The two possibilities shown to the left of Fig. 9(c) show the dislocation bowing out against the applied force instead of in the direction of the applied force. The two possibilities shown on the right of Fig. 9(c) would reduce to a bent line segment instead of a straight line segment as $\sigma_{xz} \rightarrow 0$.

The next consideration is whether this case ever occurs in real crystals, and if so, when does it occur.

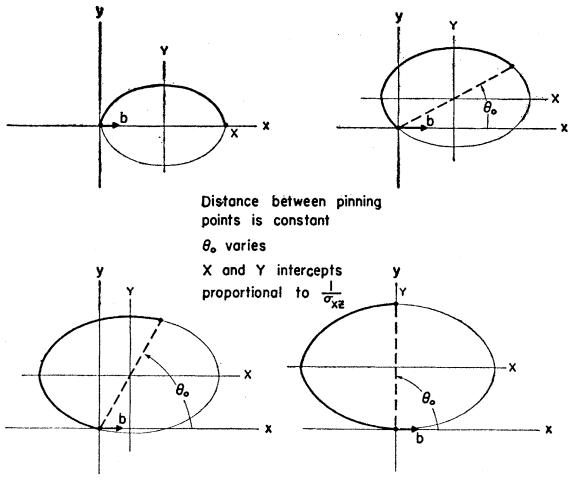

FIG. 7. Several dislocations subject to critical stress.

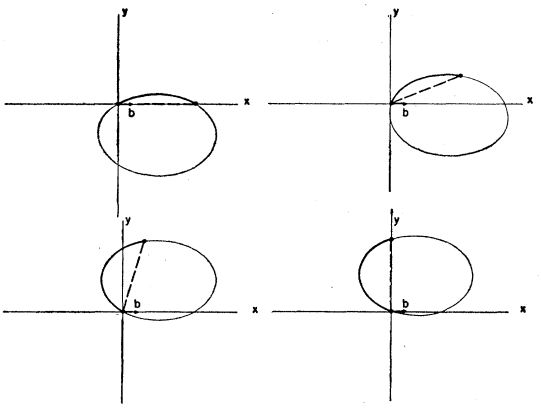

FIG. 8. Effect of changing angle between initial dislocation segment and Burgers vector for constant σ_{xz} and l.

For the isotropic form of $E(\theta)$, [see (2)], the relation given in (20) can be satisfied only if $\nu > \frac{1}{2}$. This is ordinarily not considered possible, since a sample of such a material would expand under pressure.[7] It might be expected that there would be some corresponding limit for anisotropic crystals. For Cu and Pb, the relation in (20) evidently is not satisfied since there are no handles on the curves shown in Fig. 3. However, Li has a handle at 78°K, as shown in Fig. 4.

IV. FINAL REMARKS

A. Summary

Before proceeding further, the results obtained for the problem of the equilibrium of a pinned dislocation subject to an applied stress will be reviewed.

A simpler treatment of this problem is often given which assumes a constant self-energy per unit length. The results thus obtained is that the dislocation assumes the shape of a segment of a circle. It is easily seen from (17) that the solution to the differential equation of equilibrium obtained in this paper (X *versus* Y) reduces to a circle if $dE/d\theta=0$. However, Fig. 3 shows that even the simple isotropic case (with $\nu=\frac{1}{3}$) yields a curve significantly different than a circle.

When E takes the form $\sum \alpha_{2n} \cos 2n\theta$, the curve X *versus* Y has the same symmetry as for the isotropic case. However, for Pb and Cu there is a greater relative difference between the X and Y intercepts, and so it might be said that these crystals have a "less circular" solution. But for NaCl, Fig. 3 shows that the X and Y intercepts are more nearly equal than in the isotropic case. It is interesting to note that the anisotropy factor, $2C_{44}/(C_{11}-C_{12})$, is greater than unity for Pb and Cu and less than unity for NaCl. This factor is greater than unity for metals and usually less than unity for alkali halides.

The body-centered cubic case has different symmetry properties and so is not only quantitatively but also qualitatively different from the isotropic case, and is also quite different from the case $E=$constant.

It has been shown that the critical stress and the shape of the bowed out dislocation are functions of θ_0, the angle between the Burgers vector and the original dislocation segment (see Figs. 7 and 8).

B. A Look Ahead

In this section, a possible generalization of the results of this paper will be presented, for the case that $E+d^2E/d\theta^2$ is negative for some range of θ. Then a suggestion will be made about what physical phenomena may be associated with the peculiar aspects of the solution in this case.

First, the following general ideas are suggested by the specific results of this paper:

If $A \gg 1$, where

$$A = \text{anisotropy factor} = 2C_{44}/(C_{11}-C_{12}),$$

then $E+d^2E/d\theta^2$ approaches zero or becomes negative for some values of θ.

If $E+d^2E/d\theta^2<0$, then the dislocation segment will be bent lines even for zero applied stress.

Each of the above possibilities will be discussed below.

The real crystals considered in this paper are, in order of increasing A: NaCl, Cu, Pb, and Li. If the approximate numerical expressions for $E(\theta)$ for these crystals are examined [see (4) and Figs. 1 and 3], it is found that, for the first three examples, $E+d^2E/d\theta^2$ near $\theta=\pi/2$ is closer to zero for the crystals with higher A. For Li there is a region where $E+d^2E/d\theta^2$ is negative. Thus, at least for these specific examples,

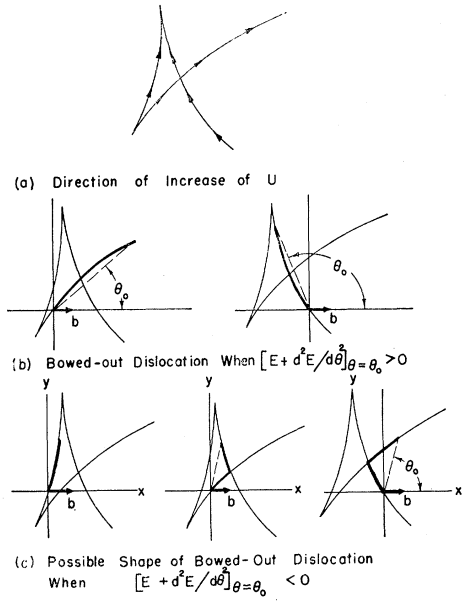

FIG. 9. Some aspects of the solution when $E+d^2E/d\theta^2$ changes sign.

[7] A. E. H. Love, *A Treatise on the Mathematical Theory of Elasticity* (Dover Publications, New York, 1944), fourth edition, p. 104.

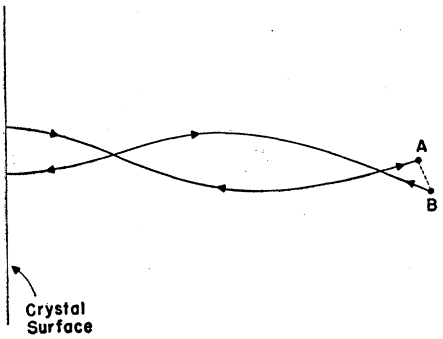

FIG. 10. A possible dislocation configuration when $E+d^2E/d\theta^2<0$.

$E+d^2E/d\theta^2$ is positive unless A, the anisotropy factor, is large.

The shape of the bowed out dislocation when $E+d^2E/d\theta^2<0$ is shown in Fig. 9(c). If the two possibilities to the left are ruled out because the dislocation has not moved in the direction of the applied force, then the remaining solution has a cusp. As the applied stress approaches zero, the solution becomes a bent line segment instead of a straight line segment. If (1) is used to evaluate the energy of this bent line segment, it is less than the energy of the straight line joining the two pinning points. Thus, it is possible that, when $E+d^2E/d^2<0$, a straight dislocation segment will be unstable and will assume the shape of a bent line segment.

Second, what physical phenomena are associated with the anomalous shapes? We would like to suggest that diffusionless phase changes are associated with situations in which anomalous shapes can be produced by changing some physical parameter such as the temperature or pressure. Consider the following experimental findings:

Nash and Smith[8] and Quimby and Siegel[9] measured the elastic constants of lithium and of sodium, respectively. Their results are shown in Table III. If the generalizations presented in the preceding paragraphs are valid, then from the dislocation calculations one would predict the onset of instability as T is decreased. Moreover, one would expect instability at a higher temperature in lithium than in sodium.

Barrett[10] has observed a phase transformation in lithium when this material is cooled below 70°K. The body-centered cubic crystal changes to a very imperfect hexagonal or face-centered cubic crystal. Barrett also found that the transformation occurs at higher temperatures in plastically deformed specimens. This seems reasonable if dislocations are involved. Barrett[11] has recently observed a similar behavior in sodium, however, the transformation temperature is 36°K or lower. This is in accordance with the lower anisotropy of sodium.

TABLE III. Elastic constants of sodium and lithium

T	$A=2C_{44}/(C_{11}-C_{12})$ Li	Na
78°K	9.24	8.20
150°K		7.98
155°K	8.98	
195°K	8.85	
200°K		7.60

Cobalt zirconium and thallium[12] show similar transformations going from hexagonal close packed at room temperature to face-centered cubic at high temperature. At present not enough elastic constant data are available; nor has a dislocation calculation been carried through for hexagonal crystals.

Gold cadmium alloys[13] with about 50% cadium are body-centered cubic at high temperature and undergo a phase transformation near room temperature. Again the elastic anisotropy is about ten and increases as the temperature decreases.[14] β brass shows similar behavior.[15]

A final theoretical suggestion might be made concerning a possible dislocation arrangement for a solid in which $(E+d^2E/d\theta^2)$ is negative over a portion of the values of θ. It is possible that the following arrangement is adopted (see Fig. 10). This has the advantage that none of the portion having $(E+d^2E/d\theta^2)$ negative is used. The arrangement is unusual in that it extends over a large distance, but perhaps that is a useful property if one is concerned with phase changes.

[8] H. C. Nash and C. S. Smith, J. Phys. Chem. Solids (to be published).
[9] S. L. Quimby and S. Siegel, Phys. Rev. **54**, 293 (1938).
[10] C. S. Barrett, *Phase Transformations in Solids* (John Wiley & Sons, Inc., New York, 1951), p. 343.
[11] C. S. Barrett, J. Inst. Metals **84**, 43 (1955).
[12] C. S. Barrett, *Structure of Metals* (McGraw-Hill Book Company, New York, 1952), second edition, p. 557.
[13] L. C. Chang and T. A. Read, J. Metals **3**, 47 (1951); L. C. Chang and T. A. Read, Acta Cryst. **4**, 320 (1951); L. C. Chang and T. A. Read, J. Appl. Phys. **22**, 525 (1951).
[14] A. Zirinsky, Acta Met. **4**, 164 (1956).
[15] See D. Lazarus [Phys. Rev. **76**, 545 (1949)] for elastic constants. A. B. Greninger and V. G. Mooradian, Trans. Am. Inst. Mining Met. Engrs. **128**, 337 (1938), have observed a transformation in a 62.5% zinc alloy.