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Experimental Determination of the Line Energy of a Basal Screw Dislocation in Zinc*

by

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ABSTRACT

The critical breakaway stress was measured for basal edge dislocations with strongly pinned ends and initial lengths which varied from 0.005 to 0.033 cm. A line energy of 2.9 dyne cm/cm for a screw-oriented dislocation which is parallel to, and approximately 0.5μ below, a free surface, is deduced from these measurements.

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1. INTRODUCTION

In analogy with an elastic string, a dislocation is considered to have a line tension tending to minimize its total energy and thereby, its length. Line tension is important in problems of static equilibrium or dynamic motion where curvature of the line is non-zero. Prominent among these cases for a dislocation are the vibratory motion of a line segment, the character of extended dislocation nodes used to estimate stacking fault energies, and the equilibrium configuration of a bowed-out line.

The longitudinal behavior of an elastic string is identical to that of a one dimensional elastic solid, and hence its line tension, $T = \frac{\partial W}{\partial \ell}$ is constant, where W is the elastic energy in the string and ℓ is the string length. For a dislocation, it is necessary to adopt a definition of T consistent with the fact that its energy is modified by interaction with other dislocations, by the presence of nearby surfaces, and by its own orientation in a particular crystal geometry. Thus the line tension of a dislocation segment must be defined locally. It is then equal to the change in total energy (of the dislocation configuration of which the segment is a part) for an infinitesimal increase in length of the segment.

In the most simple case of an isolated dislocation the line tension $T(\theta)$ is given by (DeWit and Koehler, 1959)

$$T(\theta) = E(\theta) + \frac{d^2E(\theta)}{d\theta^2} \qquad (1)$$

where θ is the angle between the dislocation line and its Burgers vector, and $E(\theta)$ is the orientation-dependent line energy of the dislocation. In many crystals the expression for line energy takes the form (DeWit and Koehler, 1959 and Spence, 1962)

$$E(\theta) = A - B\cos 2\theta \tag{2}$$

where A and B are constant ($E(\frac{\pi}{2}) = E_{edge} = A + B$, while $E(0) = E_{screw} = A - B$). We will restrict our considerations to dislocations whose line energy is given by eqn. (2). Correspondingly, eqn. (1) reduces to

$$T(\theta) = A + 3B\cos 2\theta. \tag{3}$$

The major difficulty encountered in the determination of line energy is calculation of the energy of the dislocation core, a region that cannot be treated by the continuum approximations of linear elasticity. This core or misfit energy has been estimated in several atomistic dislocation models, and commonly it is included in the expression for total line energy by modifying the linear elastic energy term, $K\ell n\left(\frac{R}{r_o}\right)$, to $K\ell n\left(\frac{\alpha R}{r_o}\right)$. Here K is the orientation-dependent term, R is a geometrical outer radius, r_o is the core radius denoting the limits of linear elasticity, and α is the misfit energy parameter. Usually α is between one and ten in magnitude and r_o is of the order of b, the dislocation Burgers vector. The misfit energy contributes only slightly to the total line energy when R is large (dislocations widely separated in bulk crystals) but increases in relative importance as the dislocation approaches other dislocations or a free surface.

In the experiment reported herein, we measured directly the line energy of basal screw dislocations in zinc lying within 1.5 microns of a free surface, and subsequently we deduced the magnitude of α.

2. THEORETICAL CONSIDERATIONS

In the following we outline an experimental method in which the line energy of a basal screw dislocation in zinc is found directly from measurement of the breakaway stress for an initially pinned length of basal edge dislocation.

Let us consider the response of an edge dislocation pinned at both ends to a sudden application of shear stress, τ, where τ is greater than the lattice friction stress, $\tau_R(\theta)$. In the following treatment we assume this τ_R is independent of dislocation orientation and less than τ. Neglecting inertial effects (Vreeland and Jassby, 1970) the equation of motion of an element of the expanding dislocation is

$$(\tau - \tau_R)b - B(\theta)v = K(\theta)\,T(\theta) \tag{4}$$

where $B(\theta)$ is the orientation-dependent viscous damping coefficient, v is the normal component of the element's velocity, and $K(\theta)$ is the curvature of the element. The product $K(\theta)\,T(\theta)$ is a maximum and equal to $(\tau - \tau_R)b$ at the pinning points where v is equal to zero. If the net stress, $\tau - \tau_R$, is less than the Frank-Read stress, the loop will come to equilibrium before the segments adjacent to the pinned points reach the screw orientation. No equilibrium configuration exists for the dislocation if the net stress exceeds the Frank-Read stress (Frank and Read, 1950), and the loop will continue to expand indefinitely. The Frank-Read stress, τ_c, is given by

$$\tau_c\, b\, \ell = 2E_{screw} \tag{5}$$

where ℓ is the distance between pinning points. The equilibrium shape of a loop at this stress has been discussed by DeWit and Koehler (1959), and is schematically shown in fig. 1, curve A. At some time during loop growth, when the net stress exceeds τ_c, a configuration shown schematically as curve B of fig. 1 is reached, where the elements closest to the pinning points are of screw character. If these elements cross-slip the dislocation is no longer constrained by the pinning points, but rather by the cross-slipped segments. Whether or not cross slip occurs, the loop will continue to expand.

Upon removal of the applied stress, the configuration of a loop will change as the curvatures decrease to their residual values which are obtained from eqn. 4, setting v = 0, and taking into account the change in direction of the friction stress,

$$\tau_R b = K_R(\theta)T(\theta) \tag{6}$$

Two equilibrium shapes (shown schematically in fig. 2) exist for the loop which satisfies eqn. 6. It can be shown that if the fastest moving point on the growing loop (midway between the two pinning points) does not extend beyond point A of fig. 2b when the applied stress is removed, then the dislocation collapses to the configuration of fig. 2a. If this same midpoint has moved farther than point A, all segments of the dynamic configuration will lie outside of the loop of fig. 2b at the moment the stress is removed. The dislocation then relaxes to a stable shape completely outside the loop of fig. 2b. In this case, the product $K(\theta)T(\theta)$ of the relaxed dislocation is equal to $K_R(\theta)T(\theta)$ near the pinning points, and is somewhat smaller around the midpoint. It should be noted that less time is required for the dislocation to reach the cross slip configuration of fig. 1 , than to reach a configuration which will not collapse to the stable loop of fig. 2a when $\tau > \tau_c > \tau_R$. According to eqn. 4, the normal velocity of a line element is greatest and consequently the time required to reach the critical configuration (fig. 1) is minimized when $B(\theta)$ is small. This made it desirable to carry out the experiment at low temperatures where $B(\theta)$ is considerably smaller than at room temperature (Pope and Vreeland, 1969; Jassby and Vreeland, 1971).

In light of the above, we can determine experimentally if the net stress has exceeded the Frank-Read stress for an isolated edge dislocation either by observation of a configuration indicating cross slip has occurred, or by observation of an expanded loop that has not collapsed to the configuration of fig. 1a. We obtain a direct measure of E_{screw} by determining the minimum applied stress required to obtain these observations (τ_R is determined from measurement of the residual curvature, and ℓ is measured directly).

3. EXPERIMENTAL TECHNIQUES

In our experiment cylindrical zinc single crystals, 1.27 cm in diameter by approximately 1 cm in length with a c-axis orientation were produced by acid-machining techniques. An end surface (basal plane) of each crystal was cleaved and the crystals were subsequently annealed for short periods. The annealing treatment left the end surfaces free of basal dislocations to a depth of at least 2.5 μ as determined by Berg-Barrett x-ray topography analysis (Co Kα radiation from $\{10\bar{1}3\}$ reflecting planes was used giving a penetration depth of 2.5 μ in zinc). The density of non-basal dislocations intersecting the end surfaces was determined to be between 10^2 and $10^3 cm^{-2}$.

Basal edge dislocations, with lengths between 0.005 and 0.033 cm, were introduced into the near surface of the cleaved end of each crystal by scratching this end with an alumina whisker. Scratches were directed along diameters which were perpendicular to the three basal Burgers vectors (fig. 3). Care was taken so that along any one diameter, all the scratches, and hence basal dislocations, were equal in length to within 5 percent. Also, the distance between successive scratches was kept to about 1/2 of the scratch length.

After preparing and scratching a crystal in the manner discussed above, it was then bonded to a testing machine (Pope, Vreeland and Wood, 1964), which is capable of producing a torsional stress state on the scratched crystal surface. The tests were carried out at either $44^{\circ}K$ or $88^{\circ}K$. Care was taken to ensure that the maximum torsional stress on the crystal surface (at the outer radius) would exceed the estimated critical stresses for the different dislocation lengths introduced.

Subsequent to the torsion test, the cleaved surface of the crystal was examined by Berg-Barrett x-ray topography. For each radial set of scratches, the critical applied stress was taken as the torsion stress at the midpoint of the first radial scratch for which unstable dislocation growth or cross slip was seen. Maximum values of residual dislocation curvature were then measured. Fifteen tests were performed and the results of these tests are presented in the next section.

4. EXPERIMENTAL RESULTS

4.1 Measurement of the Minimum Stress for Breakaway of an Edge Dislocation

Fig. 4 is an enlargement of an x-ray micrograph of a radial set of scratches on a crystal surface taken subsequent to testing. In fig. 4 a dislocation emitted by the third radial scratch from the center of the crystal has cross-slipped at one end to the free surface, while cross-slip at both pinning points has occurred for dislocations on the next two scratches. We note that residual dislocations left on the basal plane after cross-slip are approximately equal in length to the scratches. Those dislocations emitted by the two scratches beyond the fifth from the center of the crystal have combined, one from one scratch and a second from the neighboring one, which resulted in a large reacted length with a short remaining length joining the two scratches. The larger length has cross slipped at its extremities.

Evidence of cross-slip of the original loop at the lowest stresses, and of dislocation reaction followed by cross-slip of the resulting longer loops at the higher stresses were typically observed after each test. The stress acting at the midpoint of the first radial scratch from which dislocations were emitted by cross-slip was measured and plotted as a function of the length of the scratch in fig. 5. In a few tests, breakaway did not occur at all along a radial set of scratches, or occurred at a much larger stress than that indicated by the general trend. These points are not shown in fig. 5. In these particular circumstances, the x-ray micrographs showed that the scratching failed to introduce the usual distribution of dislocations.

The maximum residual curvature was found to be about $22\ cm^{-1}$ for edge dislocations and the minimum curvature was approximately zero.

4.2 Calculation of E_{screw}

The straight line of smallest slope drawn from the origin through the data points of the graph in fig. 5 represents for each scratch length the minimum applied stress required to cause dislocation breakaway by cross-slip under the conditions of the experiment. We pointed out previously that a pinned edge dislocation expanding outward with a net stress just equal to the Frank-Read stress, will attain an equilibrium configuration when the line elements at the pinning points are of screw character and they must reach this position in order to cross-slip. However, numerical calculations (Frost and Ashby, 1969) demonstrate that with this stress condition an infinite time is necessary to reach the equilibrium shape. In this experiment we were faced with an upper limit of 64 μsec imposed by the experimental apparatus. Therefore a dislocation expanding with the Frank-Read stress will not reach a shape amenable for cross-slip to occur, but rather will collapse when the applied stress is removed after 64 μsec. Consequently, a stress <u>greater</u> than the Frank-Read stress is needed to cause the dislocation to break away in 64 μsec.

Fortunately, numerical solution of the equation of motion of an expanding dislocation line pinned at both ends permits us to determine the line energy of the basal screw dislocation from the data of fig. 5.

The following procedure was used. A first estimate of E_{screw} was obtained by assuming that the net stress, $\tau - \tau_R$, was equal to the Frank-Read stress. Then, combining eqns. 2, 3, 5, and 6,

$$E_{screw} = \frac{\tau b \ell}{2\left[1 + \left(1 - \frac{1}{2\gamma}\right)\ell K_{ER}\right]} \tag{7}$$

where τ = applied torsion stress at breakaway

$\gamma = E_{screw}/E_e$ ($\gamma = 0.89$, Spence, 1962)

K_{ER} = maximum residual curvature for an edge-oriented dislocation

$= 22\text{cm}^{-1}$

But since $\tau - \tau_R$ is actually an overestimate for the Frank-Read stress, the estimate for E_{screw} is too large in value. A second, and slightly smaller choice for E_{screw} was made. With this new estimate of E_{screw}, eqn. 4 was solved numerically for the motion of the pinned dislocation. If the numerical solution indicated that the line elements at the pinning points were of screw character after 64 μsec (duration of the stress pulse), then the choice of E_{screw} was correct. If not, E_{screw} was given a new value and the calculations repeated. In this way E_{screw} was determined from $\ell = 0.005$cm. The first estimate for E_{screw} from eqn. 7 was 3.1×10^{-4} dynes cm/cm, and finally after numerical iteration, a corrected value of 2.9×10^{-4} dyne cm/cm was determined (a 6.7 percent correction).

5. DISCUSSION

5.1 Conditions for Cross Slip

Screw oriented segments experience "image stresses" tending to make them cross slip to the free surface. Evidence of cross slip was typically observed on the high stress end of the first scratch showing residual dislocation displacements. Higher stresses permitted some dislocations to bow into the screw orientation without cross slip, as evidenced by their residual configurations. We interpret this to imply that the probability for cross slip of a screw dislocation is reduced as the dislocation velocity is increased.

5.2 Accuracy of the Measurements

We estimate that the dislocations produced by scratching lie between 0.25 μ and 1.5 μ of the free surface. The line energy depends logarithmically on this distance, and we calculate that the line energy increases by about 17 percent for a sixfold increase in dislocation depth. Some of the scatter in critical stress values could be the result of differences in this depth from scratch to scratch. The minimum value of critical stress for a given scratch length then gives a measure of E_{screw} for the dislocations closest to the free surface. The proximity of the dislocations to the free surface makes basal dislocation-dislocation interactions negligible in these experiments, since dislocation spacings were large compared to 1.5 μ. Interactions between basal dislocations and the second order pyramidal dislocation forest could affect a few critical stress measurements, since the average spacing of forest dislocations was between 0.033 and 0.1 cm. However the number of tests made for each scratch length was sufficient to assure that these interactions do not influence the minimum critical stress which was measured.

The greatest uncertainty in applied stress is introduced by friction in the bearings of the torsion testing system, and we estimate this uncertainty to be 0.1×10^6 dynes/cm^2, or 2 percent of the maximum measured critical stress and 13 percent of the minimum. The same percentage of uncertainty is introduced into the values of E_{screw}.

The torsional stress state produces a linear stress gradient. The stress variation from end to end of the shortest scratch was 4 percent of the critical stress, and this variation was 38 percent for the longest scratch. Numerical solutions for the equilibrium shape of a loop in a stress gradient were generated, and they indicated that the critical stress for instability, taken at the mid-point of the longest scratch, is 1.6 percent less than the Frank-Read stress for the same scratch length. The decrease is less for the shorter scratches, so this effect of the stress gradient did not significantly influence the measured values of critical stress. Since the centers of the scratches were spaced at about $3\ell/2$, a radial set of scratches permitted testing for the critical conditions at only discrete stress levels. Several different sets of scratches of the same length were used on specimens in different tests so that the minimum critical stress values could be found.

The value of friction stress determined from measurements of the maximum residual curvature was 0.2×10^6 dynes/cm^2 which is about 5 percent of the highest critical stress and about 25 percent of the lowest. The origin of the friction stress is not known. Peirels forces may contribute to the friction stress. Interactions between basal dislocations and small faulted loops which grow near basal surfaces during aging in an oxidizing atmosphere (Hales, Dobson and Smallman, 1968) could also give rise to a friction stress. Loops smaller than about 1 μ in diameter would not be resolved in the x-ray topographs. Observations made in our previous experiments on zinc indicate that specimens tested after aging for several weeks at room temperature have a maximum residual curvature three times larger than the maximum value observed in the freshly prepared specimens used in this investigation. The possibility exists that the friction stress varies from 0 to 0.2×10^6 dynes/cm^2 in our experiments, and this gives rise to an uncertainty in the net critical stress of from 5 percent (shortest scratches) to about 25 percent (longest scratches).

The most accurate value of E_{screw} is obtained from the critical stress measurement for the shortest scratch, and the considerations discussed above limit this accuracy to within 7 percent.

5.3 The Misfit Energy Parameter

It can be shown that the line energy of a basal screw dislocation in zinc a distance h below a free surface is given by

$$E_{screw} = \frac{b^2}{4\pi}\left[\frac{C_{44}(C_{11}-C_{12})}{2}\right]^{\frac{1}{2}} \ln\left(\frac{\alpha h}{r_o}\right) \tag{8}$$

where C_{11}, C_{12} and C_{44} are the standard elastic constants (Hirth and Lothe, 1968, p. 428). A simple manipulation of eqn. 8 gives

$$\frac{r_o}{\alpha} = \frac{h}{\exp\left[\dfrac{4\pi E_{screw}}{b^2\left[\dfrac{C_{44}(C_{11}-C_{12})}{2}\right]^{\frac{1}{2}}}\right]} \tag{9}$$

The cut-off radius r_o is of the order of b, but since in most cases it is difficult to assess its exact magnitude, it is more convenient to define

$$\frac{r_o}{\alpha} = \frac{b}{\alpha'} \tag{10}$$

Employing the values of the elastic stiffnesses in zinc at 83°K (Neighbours and Alers, 1958), b for a basal dislocation, and E_{screw} equal to 2.9×10^{-4}

dyne cm/cm from this experiment, we find that r_o/α or b/α' lies between the limits

$$0.65\times10^{-8} < \frac{r_o}{\alpha} = \frac{b}{\alpha'} < 4.0\times10^{-8} \tag{11}$$

if $0.25\mu < h < 1.5\mu$. Then

$$0.57 < \alpha < 4.1 \tag{12}$$

The Peirerls model for a screw dislocation gives a value of α' equal to 2.9 (Hirth and Lothe, 1968, p. 202).

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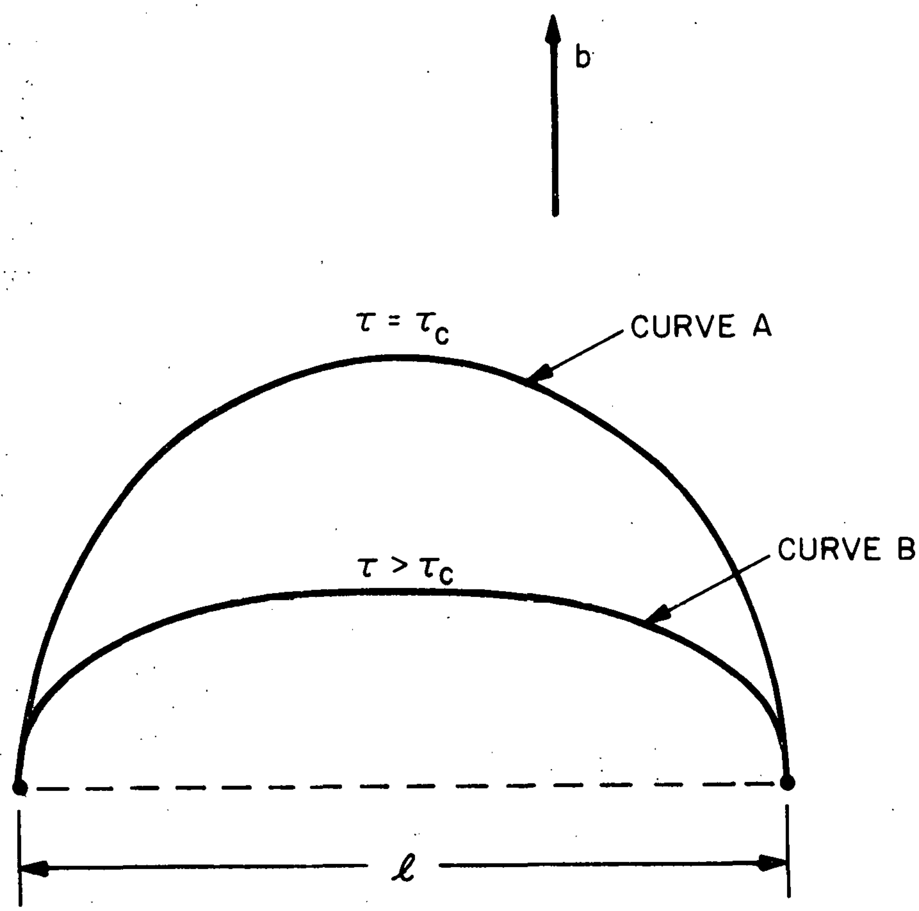
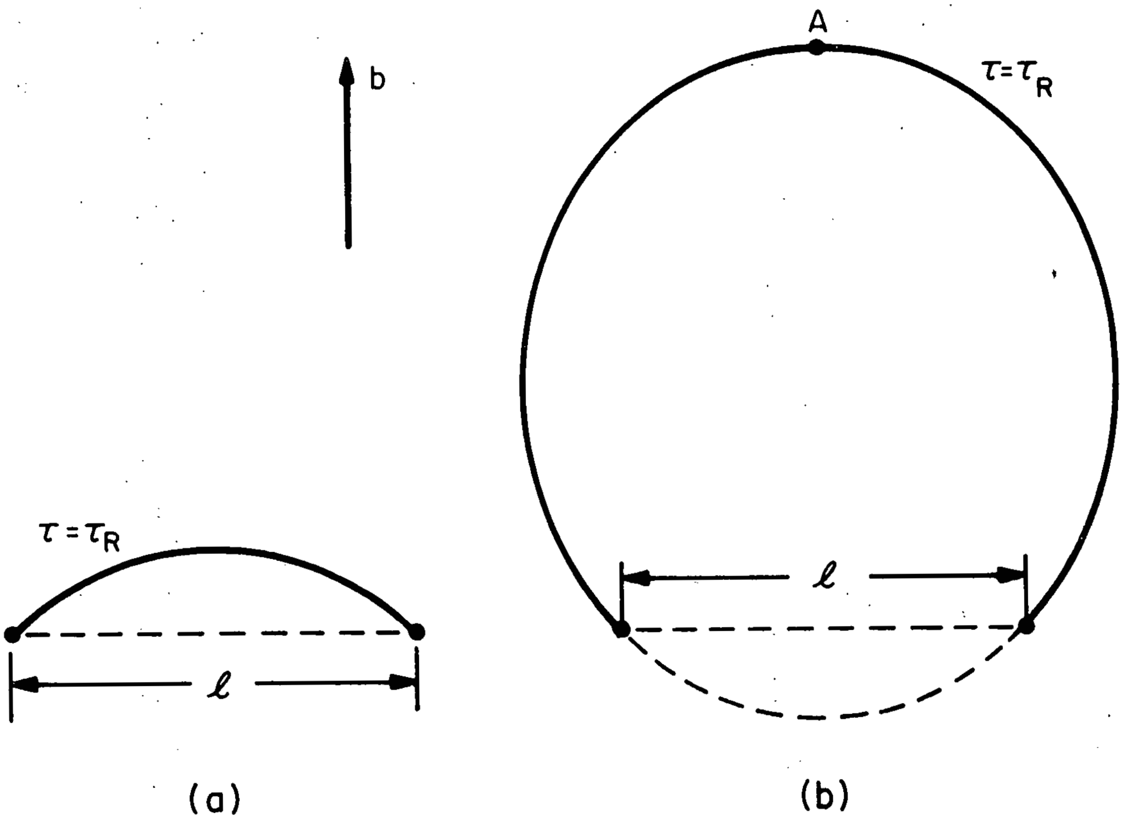
Fig. 1



Curve A - equilibrium shape of a dislocation line pinned at points a distance ℓ apart, with a net applied stress just equal to the Frank-Read stress. The dislocation elements at the pinning points are of screw character.

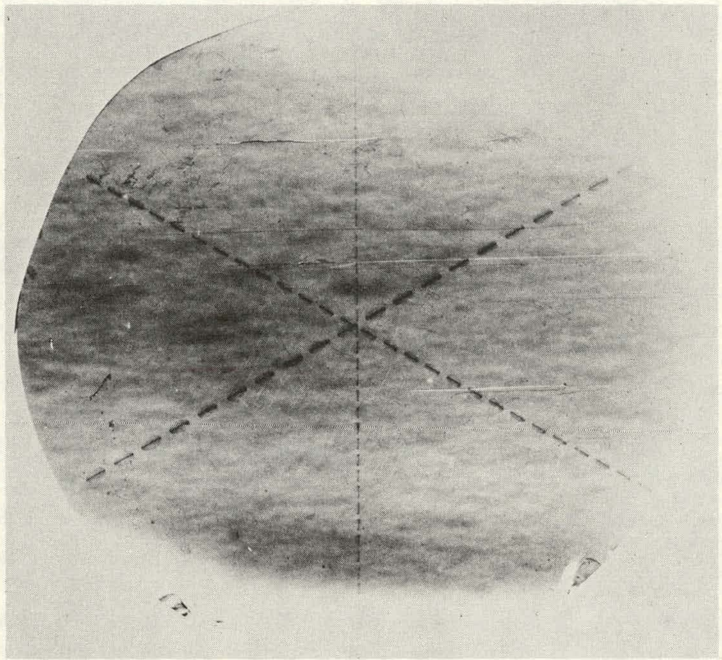
Curve B - the same dislocation expanding with a net applied stress greater than the Frank-Read stress. The loop is unstable and the line elements at the pinning points reach screw character before the midpoint of the dislocation line attains the distance of the midpoint of curve A (after Frost and Ashby, 1970).

Fig, 2



The two equilibrium configurations of a dislocation loop with an applied stress τ_R less than the Frank-Read stress (after de Wit and Koehler, 1959). (a) is stable while (b) is unstable.

Fig. 3

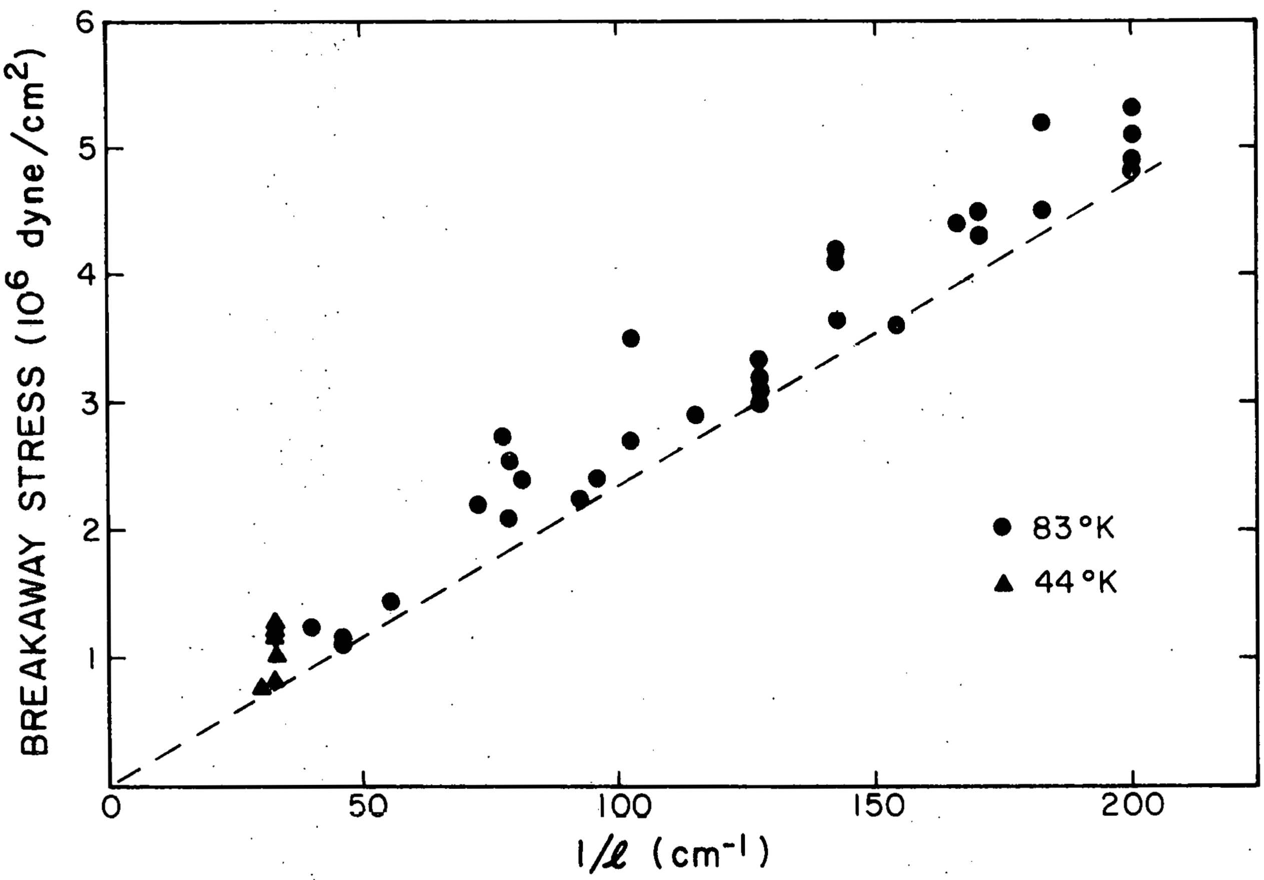


X-ray micrograph of a scratched crystal surface. The scratches are perpendicular to the three basal Burgers vectors. Magnification 7X.

Fig. 4

X-ray micrograph of a radial set of scratches after testing. The torsional stress increases linearly with distance from the center of the crystal, which in the micrograph is the point where the scratches intersect. Magnification 37X.

Fig. 5



Applied torsion stress required to cause dislocation breakaway plotted as a function of distance between pinning points.