

The Bowing of a Dislocation Segment

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ABSTRACT

The bowing under stress of a segment of an otherwise straight dislocation line has been determined for an isotropic solid. A digital computer is used to relax the dislocation to its equilibrium shape, using a variant of the Brown self-stress method. The critical stress required to make the dislocation become unstable has been determined for a wide range of segment lengths, and is in fair agreement with the predictions of the line tension model. The results are relevant to a Frank-Read source, since the elevation of the side-arms is shown to have a relatively minor effect on the critical bowing. The bowing of a screw dislocation between several attractive forest screw dislocations has also been considered.

§ 1. INTRODUCTION

THE bowing out of a dislocation between a pair of pinning points is of considerable interest in the theory of dislocations, especially in relation to dislocation multiplication processes and theories of hardening or internal friction. The detailed shape of the bowing has not hitherto been calculated with any great degree of precision, principally because of the difficulty in allowing for the elastic interaction between different parts of the dislocation line. In the present paper the results of a series of computer calculations of the bowing of a segment of an otherwise straight dislocation are presented, which fully take into account this elastic interaction.

The conventional 'elastic string' approximation regards the dislocation as having a constant line tension of the order of $\frac{1}{2}\mu b^2$, where μ is the shear modulus and b is the magnitude of the Burgers vector. To this approximation the critical stress required to make the segment become unstable is $\mu b/L$, where L is the length of the segment, and the shape of the critical segment is a semicircle. This model was refined by de Wit and Koehler (1959), who took into account the variation of the line tension between the edge and screw configurations and showed that the critical segment was oval in shape. They also calculated the equilibrium shapes of bowing segments in elastically anisotropic solids on the basis of the line tension approximation, and this has been discussed further by Ashby (1966). These authors all recognized that the effective line tension is a logarithmic function of the segment length, as was first pointed out by Mott and Nabarro (1948).

Several authors have attempted to investigate the bowing of a dislocation segment without having to make recourse to the line tension approximation. Brown (1964) introduced the concept of the 'self-stress'

of a dislocation, and showed that for an isotropic solid the effective line tension of a slightly bowed segment differs by a factor of four between the edge and screw orientations, with the screw being the stiffer of the two. This conclusion was supported by the work of Hirth *et al.* (1966), who derived analytic expressions for the energies of segments with various polygonal shapes. However, neither of these treatments allowed the dislocation to relax to its equilibrium shape and the approach to the critical configuration was not discussed. The line tension model of de Wit and Koehler predicts that the factor of four difference for small bowings reduces to a factor of about two near the critical point, and the present work seeks to test the validity of this conclusion.

In the present calculations a digital computer relaxes the segment to its equilibrium shape and the treatment is reasonably precise for an isotropic solid, apart from the usual approximation regarding the core energy†. The Brown self-stress is calculated at many evenly spaced points along the segment and the shape is repeatedly relaxed until the total stress at each point is negligible. Brown successfully used this procedure to calculate the equilibrium shapes of various extended nodes in face-centred cubic crystals, but it does not appear to have been widely used in other dislocation problems such as the bowing of a segment under stress.

In § 2 the procedure adopted in the computer calculation of the self-stress is outlined and in § 3 the results for the bowing of edge, mixed, and screw dislocations are described, including bowing to the critical (unstable) configuration. The effect of the stress fields of attractive forest screw dislocations on the bowing is also described in § 3.

§ 2. COMPUTATION OF SELF-STRESS

The self-stress at a point (x_0, y_0) on an arbitrarily curved dislocation lying in the xy plane is given by:

$$\sigma_s(x_0, y_0) = \frac{\mu b}{4\pi(1-\nu)} \int_{\text{line}} \frac{Y dx - X dy}{R^3} \left\{ 1 + \nu - 3\nu \left(\frac{Y}{R} \cos \alpha - \frac{X}{R} \sin \alpha \right)^2 \right\},$$

. . . (1)

where

$$X = x_0 - x, \quad Y = y_0 - y, \quad R^2 = X^2 + Y^2,$$

ν is Poisson's ratio and α is the angle that the Burgers vector makes with the x -axis. This is the result derived by Brown (1964) except for the sign of the $X \sin \alpha / R$ term, which was stated in error‡.

The dislocation segment is divided into a number of small sections, hereafter termed *divisions*, and the self-stress is calculated at each

† The core energy is of the order of one-tenth of the total energy of a dislocation and some allowance for this can be made by setting the core radius equal to b .

‡ The author wishes to thank Dr. D. J. Bacon for bringing this to his attention. The result as given by Brown is not invariant for a rotation of the reference axes.

dividing point. The contributions to the self-stress from the two straight semi-infinite parts of the dislocation, which are to be called the *side-arms*, are given in analytic form by Brown. The line integral along the segment is evaluated numerically and in the present work the following procedure is used: (i) divisions distant from (x_0, y_0) are regarded as infinitesimal integration segments, (ii) divisions near to (x_0, y_0) are taken to be straight sections of finite length, and (iii) the two divisions immediately adjoining (x_0, y_0) are treated as a uniformly curved section. The essential feature of this computational procedure is that it achieves the desired accuracy with a minimum of complication.

The contribution (iii) to the self-stress may be evaluated analytically for a short section of dislocation and is given by:

$$\sigma_s^{(3)}(x_0, y_0) = \frac{\mu b}{4\pi(1-\nu)R_c} \left\{ (1+\nu-3\nu\sin^2\alpha') \log\left(\frac{2\lambda}{r_0}\right) - \nu\cos 2\alpha' \right\}, \quad (2)$$

at the centre of a uniformly curved section of length 2λ , where R_c is the radius of curvature, r_0 is the core radius and α' is the angle that the Burgers vector makes with the section. It is assumed in deriving (2) that $\lambda \ll R_c$ and $r_0 \ll \lambda$, but terms of order 1 are retained in addition to those of order $\log(\lambda/r_0)$ since their contribution is not negligible. The Brown definition of self-stress is used in deriving (2), i.e. the average of values at r_0 to either side of the dislocation line. This definition appears to be equivalent to calculating the energy of the dislocation by the shear cut method; the work done by the core tractions is small for this case (Bullough and Foreman 1964) and will be neglected here.

The errors in the above procedure arise mainly from neglecting the curvature of divisions near to (x_0, y_0) . The size of these errors may be conveniently determined by using the same computational procedure to calculate the self-stress at points around a closed circular shear loop, for which the exact result is known (Brown 1964). The errors are found to be almost independent of the size of the divisions and are everywhere less than 1%, which is considered entirely acceptable in view of the uncertainties regarding the value of the core energy.

The dislocation segment is initially taken to lie on an arc of a circle whose radius is chosen to give a good fit to the expected final configuration, and subsequent relaxations are made radially by amounts proportional to the total stress at each dividing point. All points are relaxed simultaneously and this is repeated until the stress at every point is reduced to about 1% of the applied stress. An economy in computing time was achieved by starting with only a few divisions and repeatedly doubling their number after relaxing to equilibrium, since in this way gross changes in shape are made with only a few points to be relaxed. Furthermore, the change in calculated shape with number of divisions provides a good measure of the overall accuracy of the calculation, and it was found that the differences between results obtained with 24 and 48 divisions was negligible in most cases (see §3).

The procedure described above proved entirely satisfactory for dislocations of edge, mixed, and screw character, and for all applied stresses including the determination of the critical bowing. The computing was performed by Atlas II and IBM 7030 machines.

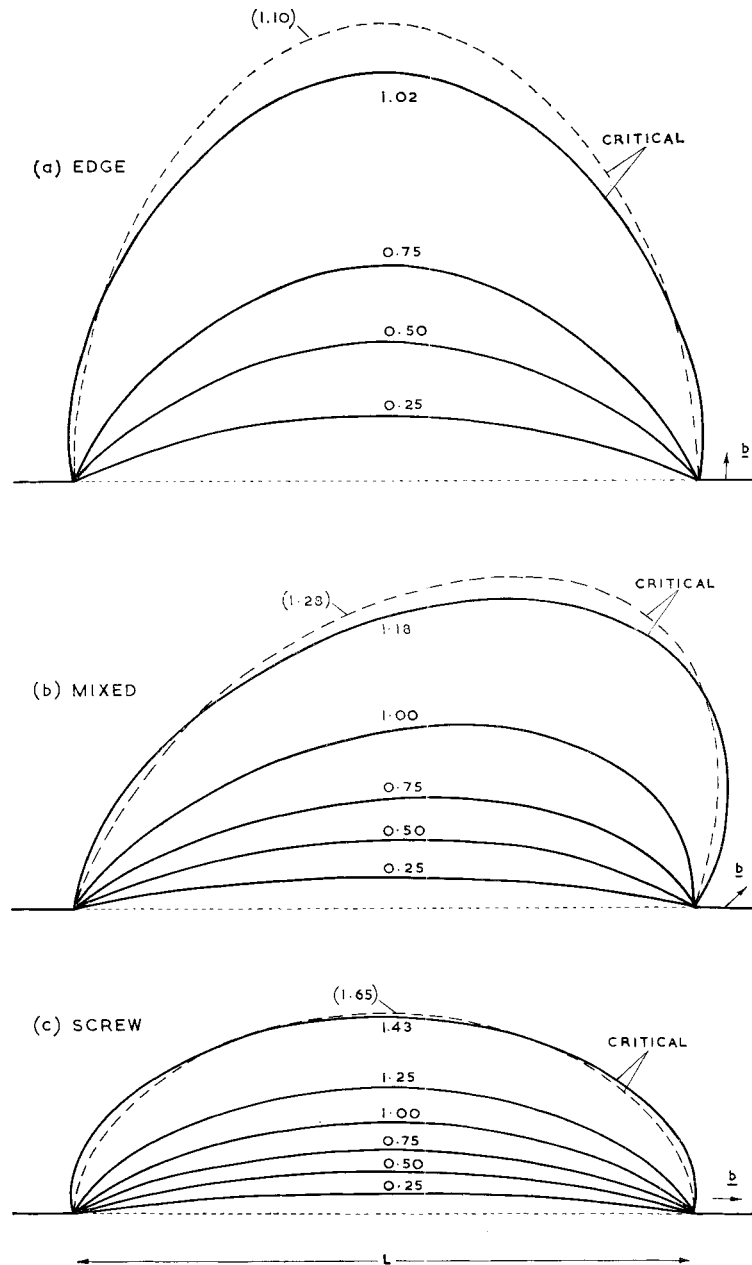
§ 3. DISLOCATION BOWING AND CRITICAL STRESS

Figure 1 shows the calculated equilibrium bowing of a dislocation segment of length $1000r_0$ that is initially edge, mixed, or screw in character. For small stresses the bowing is similar to that predicted by Brown (1964), with a difference of a factor 3.2 in amplitude of bowing between edge and screw segments under a stress of $0.25\mu b/L$, as compared with the factor 4 of Brown. The mixed dislocation bows into a characteristically asymmetric shape in an attempt to lie along the low energy screw direction as far as possible. The difference in the relative bowing of edge and screw dislocations decreases as the applied stress is increased and approaches a factor 2 near the critical configuration, which is similar to the predictions of the line tension model.

The critical configuration of the dislocation segment was determined by steadily increasing the stress in steps of $0.01\mu b/L$ until the instability occurred, and the shape shown is the last stable configuration that was obtained. The critical shape could not be obtained to a high degree of accuracy because the bowing is very sensitive to stress near the critical point. In addition it was found that near the critical configuration the bowing increased slightly as the number of divisions was increased, although this did not occur when the stress field of the side-arms was omitted. The explanation for this effect arises from the behaviour of the dislocation close to the pinning points. It is implicitly assumed in the present calculations that the obstacle responsible for the pinning will resist the mutual attraction between the dislocation arms over a distance from the pinning point comparable with the division length. Thus reducing the size of the divisions corresponds to reducing the effective size of the obstacle, thereby enhancing the 'pinching' effect between the dislocation arms. This proved to be a relatively small effect in the present work but will become important when the included angle between the dislocation arms is appreciably less than $\pi/2$.

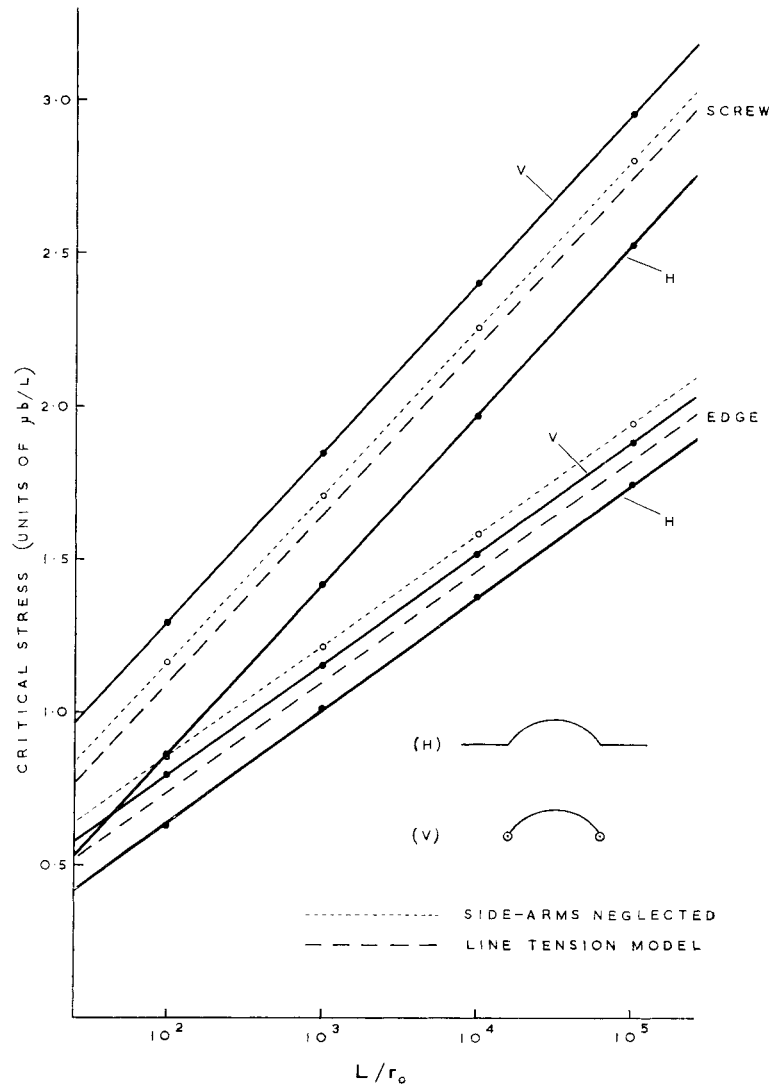
The shape of the critical segment is similar to that predicted by de Wit and Koehler (1959) on the basis of the line tension model, apart from the side-ways bowing near the pinning points, as shown in fig. 1. The variation of the critical stress with segment length is shown in fig. 2, for a wide range of lengths extending from heavily work-hardened materials to good single crystals. The discrepancy with the predictions of the line tension model is partly due to the effect of the dislocation side-arms, which assist the bowing of the segment, and the magnitude of this effect is illustrated in fig. 2 by showing the result obtained by omitting the stress field of the side-arms.

Fig. 1



The bowing of a segment of an otherwise straight dislocation line of (a) edge, $\alpha = \pi/2$, (b) mixed, $\alpha = \pi/4$, and (c) screw, $\alpha = 0$, character. The applied stress is given in units of $\mu b/L$ and Poisson's ratio is $\frac{1}{3}$. Results are shown for $L = 1000r_0$, where $r_0 \sim b$, but results for other lengths are similar if the units of stress are suitably scaled. Broken lines show the critical bowing predicted by de Wit and Koehler (1959) on the basis of the line tension approximation.

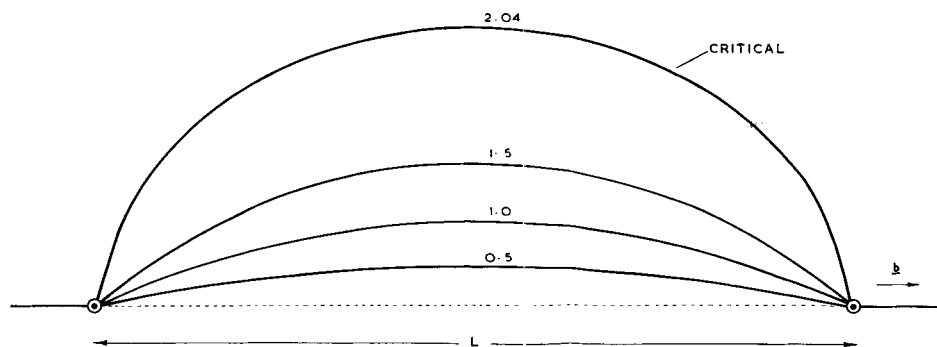
Fig. 2



Variation of the critical stress with segment length L (logarithmic scale) for an edge or screw segment (solid lines), for Poisson's ratio $\frac{1}{3}$. The dislocation arms are either horizontal (H) or vertical (V) to the glide plane of the segment (inset). Broken lines show the result predicted by de Wit and Koehler (1959) on the basis of the line tension approximation. Dotted lines show the result when the stress field of the dislocation side-arms is omitted. Segments were divided into 24 divisions for these computations.

Figure 2 also shows the critical stress when the two semi-infinite arms of the dislocation are normal to the glide plane of the segment, which is an approximate representation of a Frank-Read source. This configuration was attained by superimposing a pair of right-angled angular dislocations (Li 1964) so as to annul the present side-arms and replace them by vertical arms. The critical stress is independent of whether each arm lies above or below the glide plane, or indeed if arms of edge character should extend in both directions to form a nodal point, since one of the arms can always be annulled by adding a straight infinite edge dislocation without affecting the shear stresses on the glide plane. The 'pinching' effect found for horizontal side-arms did not occur in this case and the shape of the critical segment was similar to that predicted by the line tension model. The results for vertical arms are in good agreement with those obtained by Bacon (to be published) as part of a detailed study of the Frank-Read source. The arms of a source will in general be inclined to the glide plane at some intermediate angle and the critical stress should therefore lie between the results for horizontal and vertical arms shown in fig. 2.

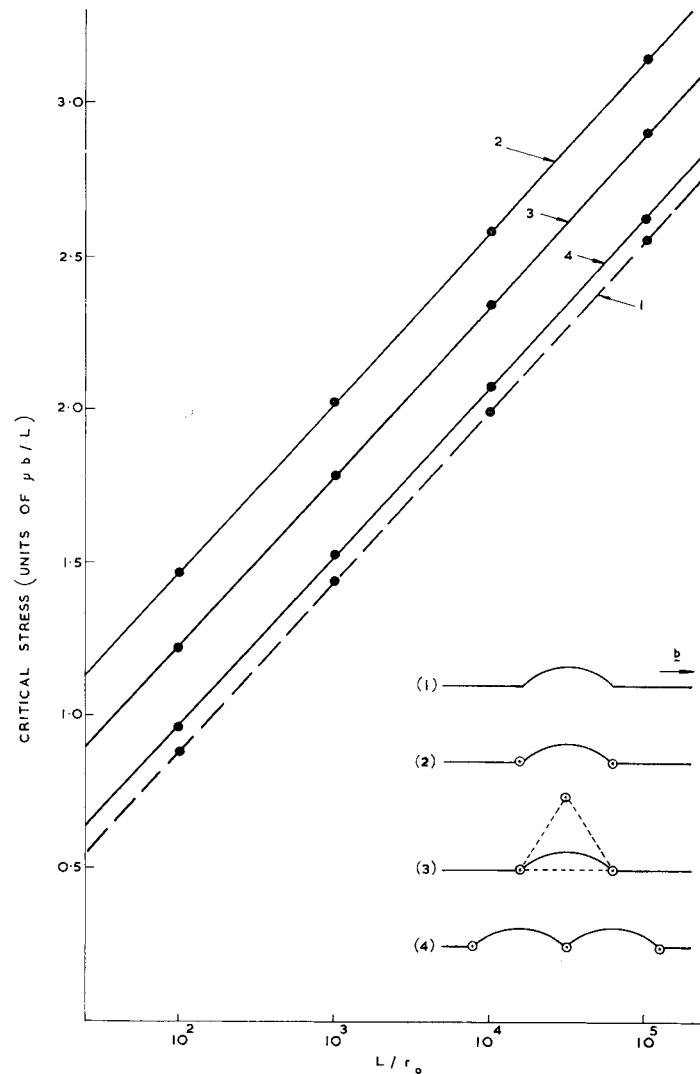
Fig. 3



A screw segment bowing between a pair of attractive forest screw dislocations, which are rigid and lie normal to the glide plane of the segment. The segment length is $1000r_0$, where $r_0 \sim b$, the applied stress is in units of $\mu b/L$, and Poisson's ratio is $\frac{1}{3}$.

The bowing of a segment of a glide dislocation will be modified if the obstacles responsible for the pinning exert long-range stress fields, as is the case for forest dislocations. This is illustrated in fig. 3, which shows a screw segment of length $1000r_0$ bowing between a pair of attractive forest screw dislocations (each of strength b) lying normal to the glide plane of the segment. It is assumed that the forest dislocations are rigid, and also that the gliding dislocation cannot penetrate them because of their local stress fields and the difficulty of moving a jogged screw dislocation. The adverse stress field of the forest screws appreciably

Fig. 4



Variation of the critical stress with segment length L (logarithmic scale) for an otherwise straight screw dislocation bowing between attractive forest screws (inset), for Poisson's ratio $\frac{1}{3}$. Curves 2 and 4 show the results for one and two bowing segments respectively and curve 3 is for an equilateral configuration of forest screws. Broken line (curve 1) is the result in the absence of forest dislocations. In case 4 the dislocation is restrained from pinching together close to the middle pinning point (see text).

reduces the bowing under a given applied stress, as shown by a comparison of figs. 3 and 1(c). The 'pinching' effect noted earlier does not occur in this case because the shear stresses exerted on the glide plane by the forest screws more than compensate by holding the dislocation arms apart near the pinning points. The critical stress is shown in fig. 4 as a function of the segment length, and is appreciably increased by the adverse stress field of the forest screws. Figure 4 also shows the critical stress for a segment bowing towards a third attractive forest screw, which is positioned in the equilateral configuration and assists the bowing of the segment.

The critical stress for two adjacent segments bowing between three uniformly spaced forest screws is also shown in fig. 4. The 'pinching' effect noted earlier was very pronounced at the middle pinning point and the critical stress steadily decreased as the divisions were made smaller. The result shown in fig. 4 assumes that an additional obstacle is present to resist the pinching within a distance of $L/40$ (one division length) from the forest screw. A calculation of the pinching forces for a V-shaped dislocation suggests that the middle forest screw unaided can only restrain the arms of the dislocation from pinching together close to the pinning point if the included angle is greater than 115° . This would restrict the bowing and reduce the critical stress by about a further 20%, unless an additional obstacle is present to inhibit the pinching.

§ 4. DISCUSSION

It will be seen from figs. 2 and 4 that in all cases so far considered the critical stress takes the form:

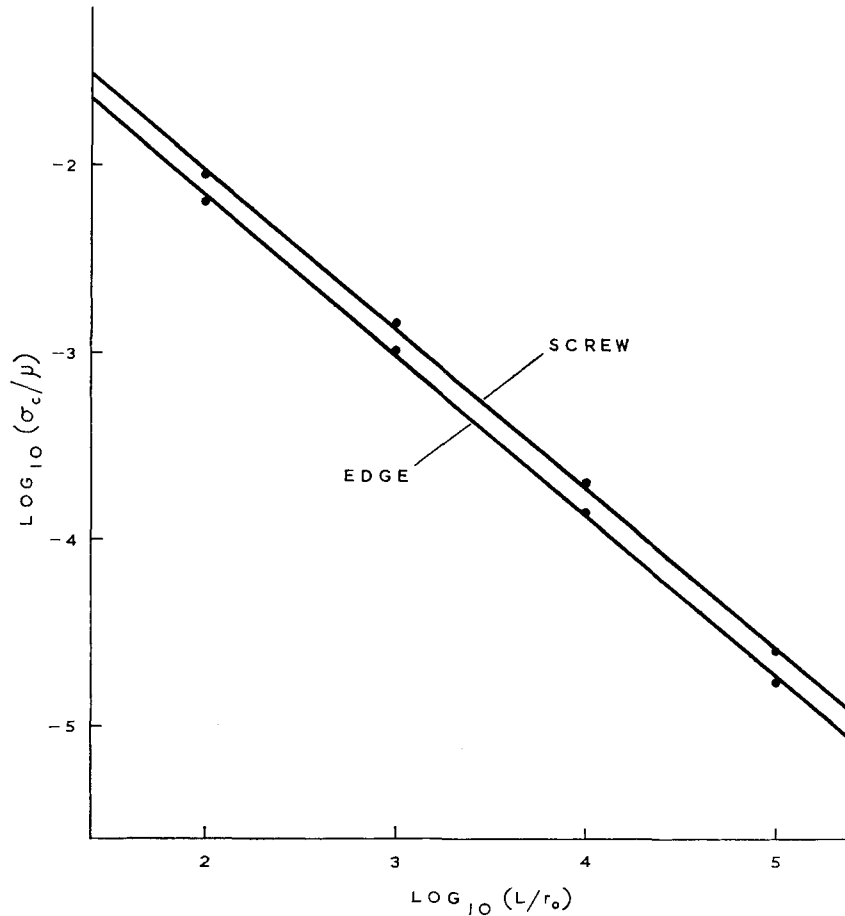
$$\sigma_c = A \frac{\mu b}{2\pi L} \left[\log \left(\frac{L}{r_0} \right) + B \right] \quad . \quad . \quad . \quad . \quad . \quad (3)$$

to a good approximation, where A is almost 1 for edge and 1.5 for screw segments (for $\nu = \frac{1}{3}$) as predicted by the line tension model. The constant B varies appreciably between different cases and clearly depends on the orientation of the side-arms and the presence of local stress fields, although in the line tension model it is difficult to estimate and is commonly set to zero. A surprising feature of the present results is the accuracy of (3), which nevertheless does not appear to be mathematically exact. It cannot be derived simply by scaling up L and λ throughout the calculation, because the self-stress does not scale uniformly around the segment. A slight change in shape occurs to compensate for this but it is too small to cause any significant deviation from (3) within the range of interest.

The shapes of the bowing segments are similar to the predictions of de Wit and Koehler (1959) on the basis of the line tension model, and this is especially the case when the arms of the dislocation are vertical and have been completely neglected. This suggests that the line tension approximation is very good locally but requires correction for interactions with the more distant parts of the dislocation. It is particularly important to

establish the validity of the line tension model because at present this is the only method available for treating an arbitrarily curved dislocation in an elastically anisotropic solid. Anisotropy will change the relative energies of edge and screw dislocations, and their relative bowings will

Fig. 5



The variation of $\log \sigma_c$ with $\log L$ for edge and screw segments with horizontal side-arms, shown for $r_0=b$ and Poisson's ratio $\frac{1}{3}$. The critical stress σ_c varies approximately as L to the power -0.85 for both edge and screw (solid lines).

therefore be different in almost every material. The present results are directly applicable to a metal such as aluminium, which is almost elastically isotropic, and they may be of assistance in understanding electron microscope observations of dislocations bowing under stress.

The difference between the bowing of edge and screw dislocations should mean that the screw parts of a dislocation line will find it more difficult to progress through a distribution of obstacles, assuming that a screw dislocation is effectively pinned by the obstacles and cannot avoid them by cross-slip. This will introduce some anisotropy into the local hardening, as for example in the computer calculations of dislocation movement through random arrays of obstacles made by Foreman and Makin (1966). For weak obstacles the dislocation line remains relatively straight and the effective line tension appropriate to its orientation should be used. For strong obstacles the dislocation moves primarily by the Orowan mechanism of unstable segments expanding and it may be shown that under these conditions the anisotropy in the hardening is negligible.

The present work confirms that the effective line tension of a dislocation segment varies linearly with $\log L$, as proposed by Mott and Nabarro (1948), and it will therefore change appreciably if the concentration of obstacles is varied by several orders of magnitude as in irradiation and solution hardening. Figure 5 shows that the critical stress of a segment varies as $L^{-0.85}$ to quite a good approximation. In most hardening problems $L \propto N^{-1/2}$, where N is the density of obstacles, so that the critical stress varies as $N^{0.42}$ approximately. This effect is not relevant to weak obstacles, where breakaway can readily occur, but may nevertheless be a contributing factor to the (dose)^{1/3} variation of irradiation hardening observed by some workers.

To summarize, the bowing of a dislocation is described quite well by the line tension model, except that the constant B is not well defined. The critical stress of a Frank-Read source should lie between the values for horizontal and vertical arms and may be close to $B=0$. The bowing of adjacent segments of a glide dislocation will be affected by their mutual interaction, which will depend on the size of the obstacle (Ashby 1966). The effective line tension of a segment varies logarithmically with its length and the critical stress can be greater than the conventional value of $\mu b/L$ if the segment is very long or lies close to the screw orientation.

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