The size of a dislocation

THE SIZE OF A DISLOCATION

By R. PEIERLS, The University, Birmingham

ABSTRACT. Calculations are made of the size of a dislocation and of the critical shear stress for its motion.

It is generally supposed that the plastic deformation of crystals proceeds by means of the propagation of dislocations along the slip planes. Since a dislocation consists of a displacement of a great many atoms, it is obviously impossible to obtain a rigorous solution of the equilibrium conditions for all these atoms. Dr Orowan has shown me how to obtain an idealized model, which leads to equations that can be solved, of the forces in a dislocation, and in this note I shall report on the results.

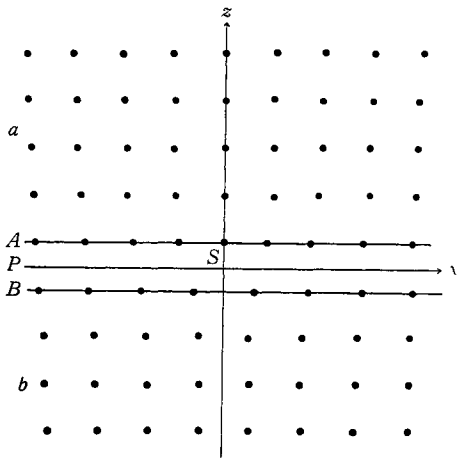

Figure 1.

The type of dislocation which I have investigated is sketched in figure 1. The slip plane P ($z=0$) divides the crystal into an upper part a and a lower part b. These are symmetrical about the vertical plane S ($x=0$). The central plane S lies in a net plane in the upper half-crystal a, and half way between two net planes in b.

The y axis at right angles to the plane of the figure (i.e. the line in which the plane S meets the slip plane P) is called the *dislocation line*. In the neighbourhood of this line the atoms of a are moved inwards and those of b are moved apart, so that at great distances from the dislocation line the two planes A and B which are immediately above and below the slip plane are again in correct alignment, A containing, however, one row of atoms more than B.

The atoms in the plane A are then subject to two forces: (i) The interaction

with other atoms in the half-crystal a. This force tends to spread the compression uniformly over the plane A, i.e. to extend the dislocation. (ii) The interaction with atoms in b, in particular with those in the adjacent layer B. This has a tendency to bring as many atoms of A as possible into correct alignment with B, i.e. to shorten the dislocation.

In equilibrium these two forces balance.

If the extension of the dislocation is large compared with the atomic distance d, both the horizontal displacement u and the vertical displacement w of the atoms in A vary slowly from atom to atom. The relative displacement of neighbouring atoms within each half-crystal is then much smaller than d. In these circumstances we may consider each half-crystal as an elastic continuum. Moreover we assume it to be an isotropic continuum, for the sake of simplicity. Then the force (i) is simply the force that has to be applied to the plane surface of an elastic continuum in order to make its horizontal displacement at the surface equal to $u(x)$. This force can be obtained by the usual methods of the theory of elasticity.

To the same degree of approximation, we may assume that the horizontal component of the force (ii) depends only on the horizontal displacement of the atoms of A relatively to the atoms of B immediately underneath. If $u(x)$ and $\bar{u}(x)$ are the two displacements, the force acting on a surface element near x is a periodic function of $u-\bar{u}$ with the period d. We may expect it to be very nearly a simple periodic function, i.e. to have the form

$$\text{constant} \times \sin\{2\pi(u-\bar{u})/d\}. \qquad \ldots\ldots(1)$$

The constant can be found from the shear modulus, provided it is assumed that the force arising between two lattice planes in a state of shear is independent of the displacement of the other lattice planes. This assumption is not strictly correct, but it is probably a reasonable approximation.

Further, it is assumed that the vertical component of the force (ii) depends only on the relative vertical displacement in A with respect to that of B. Since it follows from symmetry that the vertical displacements of A and B are equal, the vertical force (ii) is then equal to zero. This assumption again is not actually correct, since in places where the atoms in the two planes are out of alignment the equilibrium value of their vertical distance will obviously be changed. A separate discussion is required in order to take this effect into account, but for this one would have to specify the type of crystal one is dealing with and the direction of the slip plane.

With these approximations, the condition for the balance between the forces (i) and (ii) can be expressed by the following equation:

$$\int_{-\infty}^{\infty} \frac{\left(\frac{d\phi}{dx}\right)_{x'}}{x-x'}\,dx' = \frac{1}{2(1-\sigma)}\sin\frac{2\pi\phi}{d}, \qquad \ldots\ldots(2)$$

in which σ is Poisson's ratio, and $\phi = u-\bar{u}$. The solution is

$$\frac{\phi}{d} = \frac{1}{\pi}\tan^{-1}\left\{\frac{x}{d}(1-\sigma)\right\}, \qquad \ldots\ldots(3)$$

which shows that the extension of the dislocation is small and that the displacement has reached half its maximum value at a distance of $d/(1-\sigma)$ from the central plane S. This result indicates that we were not actually justified in our fundamental assumptions, which took the extension of the dislocation to be large. But the dislocation cannot, in any case, be much larger than we have found, since the equations ought to be correct if it were.

The next question is that of the motion of a dislocation under an external stress. As long as we retain the approximation of an elastic continuum for the crystal, it is evident that any stress, however small, will set the dislocation into motion. The reason is that, in our approximation, the energy of a dislocation is independent of its position; thus the dislocation is always in neutral equilibrium, and will move under any force. An external stress produces indeed a force that tends to move the dislocation since, if the dislocation moves by δx, the distant parts of a and b move relatively by $\delta x/N$, N being the number of atoms contained in the width of the crystal.

On the other hand, if the atomic structure is taken into account, the energy of a dislocation must, in the absence of a stress, depend on its exact position, i.e. on whether the plane of symmetry passes through a row of atoms or not. Hence the dislocation will have a number of stable-equilibrium positions, and these will persist even under a stress until this exceeds a certain magnitude.

A very rough idea of the variation of the energy with the position of the dislocation, and hence the critical stress, may be obtained in the following way. As long as the forces within each half-crystal are elastic, it is possible to express the total energy as a sum of terms involving only the displacements of the atoms in the two surface layers A and B. These displacements are, at each point, very little different from the displacements at the same point of the elastic continuum, as given by equation (3). Whereas, however, the energy of the continuum is to be obtained by integrating over the slip plane, we must now sum it over all atoms in the slip plane. The sum depends on the exact position of the centre of the dislocation, whereas the integral does not. We are therefore concerned with the difference between the sum and the integral. Now it is known that in sums of this type, in which the summation extends from $-\infty$ to $+\infty$, and in which the summand is a smooth function of the variable, the difference between sum and integral is extremely small; moreover, it decreases rapidly with increasing size of the dislocation.

If one tries to estimate on this basis the critical shear stress σ_c in terms of the shear stress σ_t that would be required to make an undistorted lattice plane slip uniformly over the adjacent plane, one finds that this ratio is given approximately by

$$\frac{\sigma_c}{\sigma_t} \simeq \frac{4\pi}{1-\sigma} \{5{\cdot}8 - \log(1-\sigma)\}\, e^{-4\pi/(1-\sigma)}.$$

When $\sigma = 0{\cdot}4$, this is about 10^{-7}.

No reliance can be placed on the actual order of magnitude of this result, since it is extremely sensitive to the simplifying assumptions which have been made,

and an improved discussion may considerably alter the order of magnitude. In spite of this, it seems safe to draw the following conclusions: (i) The extension of a dislocation, i.e. the width which contains all atoms whose displacements with respect to their neighbours exceed, say, $d/4$, is not appreciably larger than the atomic distance, and depends on Poisson's ratio. (ii) Under the influence of an external shear stress the dislocation will move, provided that the shear stress exceeds a critical value. This value is smaller by several powers of ten than the so-called theoretical shear stress, i.e. the stress required for uniform slip. (iii) In our present approximation the critical shear stress depends strongly on Poisson's ratio. If the anisotropy of the crystal is taken into account, it will instead depend on some other combination of the elastic constants, different for each plane. It will, however, also be influenced by the anharmonic forces between the atoms, which have here been neglected, since the displacements near the dislocation line are large.