6. Crack Nucleation in Body-Centered Cubic Metals

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ABSTRACT

Detailed examination of the Cottrell mechanism of crack initiation in body-centered cubic crystals indicates that dissociation of the resultant dislocation is easier than crack formation. Grain boundaries and twin boundaries may provide barriers strong enough to enable crack nucleation to occur.

Introduction

In considering the initiation of a crack in the body-centered cubic structure, Cottrell [1] has suggested that the formation of dislocations with Burgers vectors $a[001]$ is important. Such dislocations can be formed by the combination of two ordinary slip dislocations; thus a dislocation with Burgers vector $\frac{1}{2}a[\bar{1}\bar{1}1]$ in the (101) slip plane and a dislocation with Burgers vector $\frac{1}{2}a[111]$ in the $(10\bar{1})$ slip plane (Fig. 1) can combine to give

$$\tfrac{1}{2}a[\bar{1}\bar{1}1] + \tfrac{1}{2}a[111] \rightarrow a[001] \qquad (1)$$

This reaction results in a net decrease in energy and so should readily occur. The final dislocation, $a[001]$, lies along the [010] direction and so is a pure edge with slip plane (100).

The above process is somewhat similar to the formation of a Cottrell-Lomer sessile dislocation in the face-centered cubic structure; but in the present case the dislocation formed is not sessile and so should glide under a suitable stress. Slip corresponding to the motion of a [001] dislocation is not, however, observed, and we conclude that the Peierls force must be particularly large for these dislocations.

Cottrell has also suggested that such [001] dislocations can act as barriers in the slip plane against which other dislocations can pile up. At

first it seems surprising that a dislocation which is not sessile will remain in a fixed position in spite of the concentrated stress at the head of the piled-up group. However, when we examine the nature of these stresses, we find that they do not tend to move the [001] dislocation. For example, consider a single dislocation and take co-ordinates such that the z-axis is along the dislocation line, and $y = 0$ is the slip plane. Then at any point in $y = 0$, the stress components σ_{xx} and σ_{yy} owing to the dislocation are zero. (This result, which is a familiar one for isotropic materials,

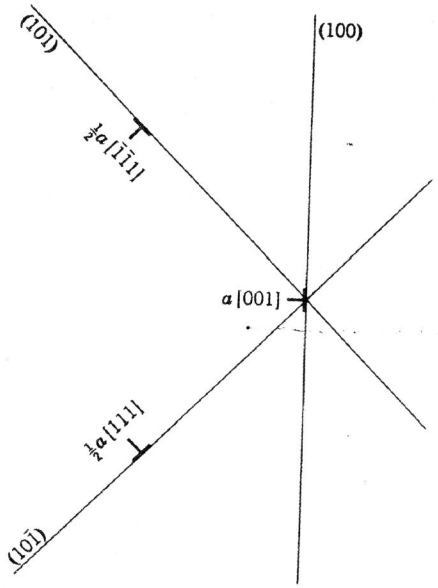

Fig. 1. Two slip dislocations combining to form a dislocation with Burgers vector $a[001]$.

remains true when, as in the present case, we have cubic symmetry.) It then follows, by a simple transformation of co-ordinates, that the shear stress on any plane meeting $y = 0$ at 45° is zero. Now applying this result to the case shown in Fig. 1, we see that the dislocations piled up in (101) (or equivalently in $(10\bar{1})$) do not produce any shear stress on the slip plane of the [001] dislocation and so have no tendency to move it. Thus this dislocation will be acted on only by the applied stress and the stresses resulting from dislocations other than those in the piled-up group; against such stresses, the large Peierls force, which we have already had to assume, will be sufficient to prevent its moving. Accordingly, the dislocation will be a good barrier, and we may expect that it will play a part in the work hardening of body-centered cubic metals similar to that played by Cottrell-Lomer sessiles in the face-centered cubic.

For sufficiently large piled-up groups, there remains the possibility of dissociation by the occurrence of the reverse of Reaction 1. The conditions under which this happens could be determined by the method used by Stroh [2] to investigate the dissociation of the Cottrell-Lomer sessile. However, we shall only consider here whether or not dissociation will occur before the piled-up group has grown large enough to initiate a crack.

Single Piled-Up Group

The dislocations may be piled up either in both the (101) and the $(10\bar{1})$ slip planes, or in only one of these planes. We consider first the simpler case in which they are piled up in a single plane, for example, the (101) plane.

To form a crack, the dislocations at the head of the piled-up group must be forced so close together that they form a single dislocation of large Burgers vector; when the Burgers vector has grown sufficiently large, the dislocation will become cracked. Calculations on a simplified model [3] indicate that the most difficult stage in this process is to combine the first two dislocations, and so we need consider only this stage.

Fig. 2. A group of dislocations piled up at an [001] dislocation A.

The force of repulsion between the $a[001]$ dislocation A at the head of the piled-up group and the $\frac{1}{2}a[\bar{1}\bar{1}1]$ dislocation B nearest it (Fig. 2) is

$$F_1 = Ga^2/4\pi(1-\nu)r \tag{2}$$

where r is the distance between the dislocations, G is the shear modulus, and ν is Poisson's ratio. When the dislocation [001] dissociates by the reverse of Eq. 1, the force between its components tending to reunite them is $Ga^2/8\pi r$. This force acts along the line joining these two dislocations. If, on dissociation, each is displaced the same distance, this force makes an angle of 45° with the slip plane; hence its component parallel to the slip plane is

$$F_2 = Ga^2/8\sqrt{2}\,\pi r \tag{3}$$

Comparing the forces for the same distance r between the dislocations and taking $\nu = \frac{1}{3}$, we obtain

$$F_1/F_2 = 2\sqrt{2}/(1-\nu) = 4.2 \tag{4}$$

In finding these forces we have used linear elastic theory which will certainly not be correct at very small distances. In fact, both F_1 and F_2 will have been overestimated, but the value of their ratio (Eq. 4) should be better than that of either of the forces separately.

Next we must consider what forces will occur in the piled-up group. Suppose that the dislocations other than A and B (Fig. 2) and the applied stress together produce a force F_A on A and F_B on B. Since the distance between A and B is small compared with the distance of either one from any other dislocation, we have approximately $F_A = F_B$. (In the case in which A and B have the same Burgers vector, we find from the calculations of Eshelby, Frank, and Nabarro [4] that $F_A = 0.84\, F_B$; the difference between this exact relation and the approximate relation $F_A = F_B$ is unimportant for the present application.) Since B is in equilibrium under the force F_B and the repulsion F_1 owing to A, we must have $F_B = F_1$. The force that A has to withstand is then

$$F_1 + F_A = F_A + F_B \simeq 2F_B$$

Thus the force tending to dissociate A is about twice the force tending to coalesce A and B and so to nucleate a crack. Combining this with Eq. 4, we see that to nucleate a crack would require a piled-up group about eight times as strong as the greatest the [001] dislocation can withstand. While this factor is admittedly subject to corrections because of nonlinear effects, it is difficult to believe that these corrections can be so great as to alter the conclusion that the [001] dislocation does not provide a strong enough barrier for fracture.

Two Piled-Up Groups

We reach a similar conclusion if the dislocations are piled up in both slip planes meeting the [001] dislocation. We may assume the two piled-up groups to be of equal strength, since the general case will be intermediate between this and that of a single piled-up group. Dislocations from each slip plane will now coalesce with the leading dislocation simultaneously. Since the $\frac{1}{2}a[111]$ and $\frac{1}{2}a[\bar{1}\bar{1}1]$ dislocations attract, the process is a little easier than before, and, allowing for this attraction, we find that Eq. 2 must be replaced by

$$F_1 = \frac{Ga^2}{4\pi r}\left(\frac{1}{1-\nu} - \frac{1}{4}\right)$$

Hence, with $\nu = \frac{1}{3}$, the ratio

$$F_1/F_2 = 3.5 \qquad (5)$$

On the other hand, the [001] dislocation is even more likely to dissociate because it now has to withstand two piled-up groups. A simple treatment such as was used previously shows that the force tending to dissociate the dislocation is more than three times that tending to coalesce the next dislocations with it. Combining this with Eq. 5, we find that now the piled-up group needed for fracture is ten times larger than the [001] dislocation can withstand, a result even more unfavorable for fracture than the previous case.

Discussion

The estimates just made of the strength of the [001] dislocation apply strictly only near the absolute zero, for the effect of thermal fluctuations has been neglected. Since thermal fluctuation can help appreciably the dissociation of a Cottrell-Lomer sessile dislocation which at 100°K may have only half the strength it has at 0°K,[2] a similar effect may be expected in the present case. On the other hand, it seems unlikely that thermal fluctuations can make crack nucleation much easier. Thus at any finite temperature, the [001] dislocation will prove an even less effective barrier.

The only barriers strong enough for crack nucleation appear to be grain boundaries and twin boundaries. Here there is the possibility of their giving way by the nucleation of slip in the perfect lattice. If we attempt to use the method of this paper to decide whether this is likely, we are led to no very definite conclusion. For if a pair of edge dislocations $\frac{1}{2}a[111]$ and $\frac{1}{2}a[\bar{1}\bar{1}\bar{1}]$ are formed, they must be separated against their mutual attraction, which is a force

$$F_3 = 3a^2G/8\pi(1-\nu)r$$

Hence from Eq. 2, the ratio of the forces for crack nucleation and slip nucleation is

$$F_1/F_3 = \tfrac{2}{3} \qquad (6)$$

Across a grain boundary, the shear stress on the most favorable slip plane will be less than the maximum shear stress by a factor depending on the change in orientation across the boundary. For a large-angle grain boundary, this factor may be of the order of $\frac{1}{2}$; that is, the stress tending to nucleate slip will be about half the stress on the leading dislocation A (Fig. 2). The stress will therefore be about the same as that tending to combine B with A. Combining this result with Eq. 6, we find that a crack should occur a little more easily than does slip in the perfect lattice. The two processes are of so nearly equal difficulty, however, that nonlinear effects are likely to be all-important here. Nevertheless, the cal-

culation does illustrate the great strength of a grain boundary as compared to a dislocation lock.

The experimental work of Biggs and Pratt [5] supports the idea that a twin boundary forms a suitable obstacle to slip for the nucleation of a crack, and they conclude that, in single crystals of iron, cracks are formed by dislocations piling up against twin boundaries.

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