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1961

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Abstract

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ON CLUSTERS OF DISLOCATIONS IN CRYSTALS CONTAINING IMPURITIES

(Presented by Academician A. V. Shubnikov, 2 VIII 1960)

According to current views, clusters of dislocations in slip bands play an important role in the processes of hardening and fracture of crystalline bodies. Many phenomena are determined by the nature of the distribution of dislocations at various obstacles in the slip plane.

Eshelby, Frank, and Nabarro ([1]), as well as Leibfried ([2]), carried out the corresponding calculations on the assumption that dislocations move freely in the slip plane. Experimental verification of the distribution of dislocations in clusters shows, however, a substantial deviation from the predictions of the theory. As a rule, agreement between theory and experiment is achieved only after several tens more dislocations, for some reason not detected experimentally, are artificially ascribed to the actually observed cluster on the side of the head of the cluster ([3,4]).

Fig. 1. Scheme of the formation of a cluster from dislocations blocked by impurities

The deviation of the observed distribution of dislocations from the theoretical one is possibly connected with the fact that in the theoretical schemes considered previously, the influence of impurities and defects, which may cause considerable resistance to the motion of dislocations in the slip plane, was in no way taken into account. On the other hand, the ideas about the formation of large clusters of freely gliding dislocations, which underlie certain theoretical notions concerning fracture of a crystal, have recently quite reasonably been subjected to serious doubt, owing to the improbability of the existence in a single crystal of strong barriers capable of withstanding the pressure of a large group of freely gliding dislocations.

Another scheme may be proposed, one that does not require excessively strong barriers for the formation of a cluster (Fig. 1). The role of the barrier may be reduced to initiating the formation of a cluster, which is held mainly by impurities that have settled on the dislocations*. If a dislocation, during its motion in the slip plane, is stopped by some obstacle, then after it has stopped, impurity atoms may accumulate around it, fixing its position. The blocking of a dislocation by impurities may prove to be very strong, especially in the case of precipitation of phase formations on dislocations.

* We note that all dislocation clusters examined experimentally were studied after removal of the stresses, i.e., they were obviously clusters of dislocations blocked by impurities.

The second dislocation, pressed toward the first by the tangential stress τ, will stop at a distance l_1, determined from the condition of equality of the external force τb and the force of interaction of the dislocations. If the distortion of the stress field around the first dislocation caused by impurity precipitation is neglected (far from the dislocation the stress practically does not change),

$$l_1 = \frac{Gb}{2\pi k\tau}, \tag{1}$$

where k, depending on the orientation of the Burgers vector, takes values from 1 (screw dislocations) to $1-\nu$ (edge dislocations).

After the position of the second dislocation has been fixed by impurities, the third dislocation stops at a distance l_2 from it, determined from the relation

$$\tau = \frac{G}{2\pi k}\left(\frac{1}{l_1+l_2}+\frac{1}{l_2}\right), \tag{2}$$

whence

$$\frac{1}{l_1} = \frac{1}{l_1+l_2}+\frac{1}{l_2}. \tag{3}$$

Fig. 2. Dependence of the cluster length L_n/l_1 and of the distance between dislocations $l_n/l_1 = a_n$ on n. The lines approximate functions (5) and (6); the points are the results of the numerical solution of system (4)

or

$$1 = \frac{1}{a_1+a_2}+\frac{1}{a_2}, \tag{3'}$$

where $l_i = a_i l_1$.

Continuing the process, we obtain, for determining the values a_i, the system of equations

$$1 = \frac{1}{a_1},$$

$$1 = \frac{1}{a_1 + a_2} + \frac{1}{a_2}, \tag{4}$$

$$1 = \frac{1}{a_1 + a_2 + a_3} + \frac{1}{a_2 + a_3} + \frac{1}{a_3},$$

$$\dots\dots\dots\dots\dots\dots\dots\dots$$

$$1 = \frac{1}{a_1 + \dots + a_n} + \frac{1}{a_2 + \dots + a_n} + \dots + \frac{1}{a_n}.$$

The results of a numerical solution of system (4) up to $n = 100$ are shown in Fig. 2.

To investigate the asymptotic behavior of a_n for large n, let us rewrite this system in the form

$$a_n = \sum_{m=0}^{n-1} \left[\sum_{p=0}^{m} (a_{n-p}/a_n) \right]^{-1}. \tag{4'}$$

and we shall solve it by the method of successive approximations. Setting in the right-hand side $a_{n-p} = a_n$, we obtain the first approximation

$$a_n^0 = 1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{n} \approx \gamma + \ln n,$$

where $\gamma = 0.5772157\dots$ is Euler' s constant.

The correction to the first approximation is found by estimating the difference

$$a_n - a_n^0 = \sum_{m=0}^{n-1} \left(\frac{a_n}{\sum_{p=0}^{m} a_{n-p}} - \frac{1}{m+1} \right) \approx \frac{1}{a_n^0} \sum_{m=1}^{n-1} \frac{1}{(m+1)^2} \sum_{p=1}^{m} (a_n - a_{n-p}) \approx$$

$$\approx \frac{1}{a_n^0} \sum_{m=1}^{n-1} \frac{1}{(m+1)^2} \ln \frac{n^{m+1}(n-m-1)!}{n!}.$$

Taking into account that the use of Stirling' s formula and the replacement of summation by integration for $n \gg 1$ gives

$$\sum_{m=1}^{n-1} \frac{1}{(m+1)^2} \ln \frac{n^{m+1}(n-m-1)!}{n!} \approx \frac{\pi^2}{6} - 1,$$

we finally obtain, for large n,

$$a_n \approx \gamma + \ln n + \frac{\pi^2/6 - 1}{\gamma + \ln n}, \tag{5}$$

whence the total length of the pile-up is

$$L_{n+1} = l_1 \sum_{m=1}^{n} a_m \approx \int_1^n dm \left(\gamma + \ln m + \frac{\pi^2/6 - 1}{\gamma + \ln m} \right) =$$

$$= l_1 \{ n \ln n + (n-1)(\gamma - 1) + (\pi^2/6 - 1) e^{-\gamma} [\mathrm{Ei}(\gamma + \ln n) - \mathrm{Ei}(\gamma)] \}, \tag{6}$$

where $\mathrm{Ei}(x)$ is the exponential integral function.

Figure 2 presents the general behavior of the approximating functions (5) and (6), showing good agreement with the values of a_n and L_n computed numerically up to $n = 100$ from algorithm (4).

Fig. 3. Comparison of the experimental distribution of dislocations in the slip plane in front of an obstacle with the results of the theory. a —α-brass, data of Haasen (3); b and c —cadmium, original data. The positions of dislocations corresponding to the model under consideration are indicated by hatching.

The application of this model is limited, on the one hand, by the necessity of matching the segregation rate of impurity atoms with the rate of pile-up formation and, on the other hand, by the requirement of high stability-

of fixing the positions of dislocations. Nevertheless, comparison of the experimental data on the distribution of dislocations in pile-ups, obtained by various authors, shows that in a number of cases the model considered describes the experimental results better than the model with freely gliding dislocations.

In Fig. 3 photographs are given of several pile-ups, with the positions of dislocations indicated as determined from the numerical solution of system (4). Some deviations may be explained by the fact that the blocking of dislocations by impurities is not completely rigid and by a small spreading of the head of the pile-up, which is not taken into account by the model. Small deviations of the experimental distribution from the calculated one may also be due to the influence of the stress field created by the obstacle.

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Received
22 VII 1960

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Note: Figure translations are in progress. See original paper for figures.