Quantitative Predictions from Dislocation Models of Crystal Grain Boundaries

W. SHOCKLEY AND W. T. READ
Bell Telephone Laboratories, Murray Hill, New Jersey
December 28, 1948

DISLOCATION models of grain boundaries have been discussed by numerous authors. This letter shows that these models have certain quantitative consequences which are directly susceptible to experimental test, so that theoretical and experimental investigations of grain boundaries may furnish a direct proof of the presence of particular arrays of dislocations in solids.

Of particular interest are grain boundaries between crystallites differing by a small angular rotation about an important crystallographic direction, such as that shown for a simple cubic model in Fig. 1(A). For this highly symmetrical case, the boundary is equivalent to a row of dislocations (B); if the boundary is parallel to the planes of the left grain, two types of dislocations will be required (C). For any such model there are simple relationships between the arrangement of the dislocations and the orientation of the grains and grain boundary. For Fig. 1(A) we have $\sin(\theta/2)=a/2L$ where a is the slip vector of the dislocation. For $\theta<1°$, L will be >100A so that the dislocation structure of small angle grain boundaries should be resolved by electron microscopy. The writers propose that such dislocation structures have already been optically resolved for very small angle boundaries. In connection with "veining" in aluminum, P. Lacombe[1] has observed that the veins separate regions of slightly different orientation (1.3×10^{-3} radian estimated from Fig. 3[1]); the veins are revealed by rows of similar etch pits. Assuming each etch pit originates on a dislocation, the spacing $L=3\times10^{-4}$ cm (estimated from Fig. 1[1]) gives $\theta=10^{-4}$ radian. The discrepancy of 13 is probably explained by the fact Figs. 1 and 3 correspond to different specimens. The veins shift radically after reannealing at 600°; although they are not straight where they intercept the surface, Fig. 1 shows they extend perpendicularly (within $<0.3°$) straight through the specimen—results consistent with arrays of dislocations.

For larger angle boundaries, minimum energy arrays should give definite interfacial energies; these arrays would be established at high temperatures by interactions between, and motions of, the dislocations and by vacancy diffusion. Figure 1 (A and B) represents the minimum energy array for the simple cubic model; for the approximation of an isotropic model with shear modulus μ and Poisson's ratio σ and for small θ, we find that the interfacial energy is

$$\gamma=[\mu a/4\pi(1-\sigma)]\theta(A-\ln\theta), \qquad (1)$$

where A is a constant depending upon the energy near the dislocation where Hooke's Law fails. (For Nabarro's[2] simple cubic model we find $A\doteq0.8$.) The coefficient of $\theta\ln\theta$ depends only on integrals where the strain is small; hence, it can be calculated without approximations, from the elastic constants and the slip vector "a" of the dislocation used. Similar results will hold for anisotropic materials and more complicated boundaries.

Thus experimental values of γ/θ should plot *versus* $\ln\theta$ as a straight line with slope $\mu a/4\pi(1-\sigma)$. Recently C. G. Dunn[3] of the General Electric Company has measured grain boundary energies on a relative scale in iron and finds that γ is approximately constant for $\theta>20°$ and for $\theta=8°$ $\gamma=0.6$ times the higher value. This data can be well approximated by a straight line for $A=0.5$ as shown in Fig. 2; surprisingly, the approximation fits the data even for angles as large as one radian. Using Eq. (1) (which is calculated for a simple cubic lattice), the elastic constants for iron, and $a=2.5$A, we estimate that Dunn's approximately constant value is 1300 ergs/cm².

We are indebted to J. H. Holloman of the General Electric Company and to C. S. Barrett and C. S. Smith of the Institute for the Study of Metals for stimulating discussions.

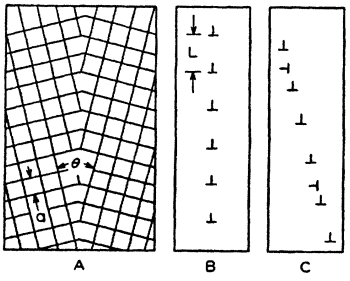

FIG. 1. Simple grain boundaries in cubic model: (A) symmetrical grain boundary, (B) equivalent array of dislocations, and (C) array for unsymmetrical grain boundary.

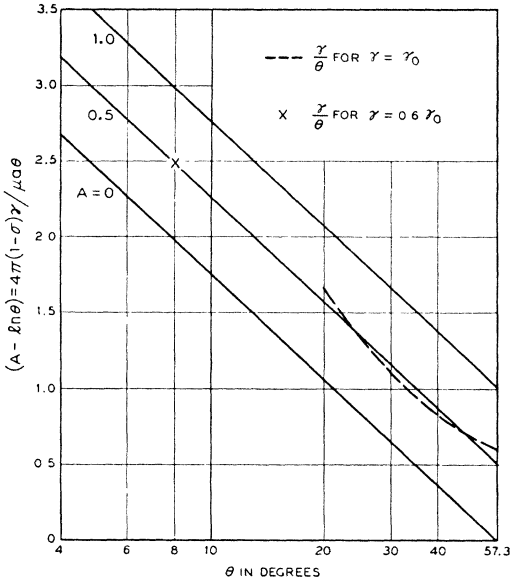

FIG. 2. Predicted dependence of interfacial energy γ upon orientation difference θ.

[1] P. Lacombe, *Report of Conference on Strength of Solids* (The Physical Society of London, 1948).
[2] F. R. N. Nabarro, Proc. Phys. Soc. **59**, 256 (1947).
[3] We are indebted to C. G. Dunn for this data which is scheduled for the February issue of Journal of Metals.