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THE MECHANISMS OF ACCOMMODATION OF DEFORMATION AT
GRAIN BOUNDARIES IN BCC MATERIALS

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ABSTRACT

Two possible mechanisms for the accommodation of deformation at grain boundaries in body-centered cubic materials are analyzed using transmission electron microscopy and diffraction. These include: the absorption of dislocations in a near-coincidence boundary and the structural rearrangements accompanying a change of grain boundary plane in a low angle boundary. The O-lattice crystallographic description of interfaces was used to model the structure of the grain boundaries. The relevance of these mechanisms to the mechanical behavior of a grain boundary is discussed.

INTRODUCTION

The processes of grain boundary sliding, grain boundary migration, the continuation of plastic flow or the accommodation of intergranular cracks, are all manifestations of the accommodation of deformation at grain boundaries. These are in turn, problems determined by the crystallography of each individual grain boundary (GB) (e.g., grain misorientation, GB plane, slip planes-GB plane intersections) as well as operating environmental conditions and stress state of the material. Although considerable progress has been made towards understanding the

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processes of plastic deformation in a crystalline matrix using fundamental concepts of crystal dislocations and diffusive fluxes, the applications of these concepts to grain boundaries has been somewhat slower. The first basic problem in understanding GB deformation is in fact the definition of both the perfect GB structure (the equivalent of the crystal lattice) and more complex GB structural defects (the equivalent of crystal dislocations and point defects).

Some success has been achieved in this respect through empirical-potential atomistic calculations (as in the case of crystal dislocations). The GB structure is shown to be a composite of basic structural units; random GBs are for example composed of proportional amounts of the structural units of nearby favoured GBs.\(^1\) In addition the validity of the O-lattice theory as a good approximation to the description of GB structure is confirmed by combined atomistic calculations and atomic resolution electron microscopy observations.\(^2\) Computer molecular statics calculations furthermore show a difference in vacancy structure at O-lattice sites and non O-lattice sites.\(^3\)

The geometrical O-lattice theory is based on the conservation of crystal structure and color symmetry at the GB.\(^4,5\) By definition, O points are coincidence points of internal coordinates; a favored boundary occurs where some O-points correspond to coincidences of lattice sites (i.e., a coincidence site lattice (CSL) where the fraction of common lattice points is \(1/2\)). A network of grain boundary dislocations (GBD) with Burgers vectors of the displacement-shift complete lattice (DSCL), that is one dimensional defects of the DSCL, is then associated with the CSL to accommodate a deviation from coincidence and effectively preserve the coincidence
orientation. The details of the matrix calculation of GB structure and dislocation reactions are shown elsewhere. The DSC lattice (of which the 0-lattice is a super-lattice with larger lattice parameter) is then the reference lattice to study the interaction of point and line defects responsible for deformation mechanisms at the GB. This paper presents some results on the study of the interaction of a matrix dislocation with the dislocation structure in a bcc material (molybdenum). This part of the work is in the same vein of other studies in fcc materials. In addition results of the accommodation of a change in GB plane in a low angle boundary are presented.

RESULTS AND DISCUSSION

Body-centered cubic materials are of interest in the study of GB deformation because of their technological importance and because of the paucity of observations of bcc GB structure. For this investigation, molybdenum was chosen as a representative bcc material that can be observed in the transmission electron microscope at high resolution. Samples of 99.99% pure Mo with traces of C (10ppm), Cr(20ppm), Fe(10ppm) and Ni (10ppm) as measured by a spectrographic examination were used. The material was cold rolled to 10 mils and annealed for 24 hours at 800°C in high vacuum (10^-8 torr) in order to avoid oxygen segregation to the GBs. Thin foils were electropolished in a double jet unit using a 4% vol. sulphuric acid-methanol solution at -55°C. As a result of cold rolling and the annealing treatment, a number of low angle boundaries and near-coincidence boundaries appeared in the thin foils.

Crystal lattice dislocations are known to interact with grain boundaries during the intermediate stages of plastic deformation and
during recrystallization; they dissociate forming a non-equilibrium configuration through reactions with the equilibrium dislocation network. A near-coincidence boundary with a misorientation near 55.9 °/(110) was studied in this work using transmission electron microscopy and diffraction because the decomposition products of matrix dislocations which had interacted with the GB during thermo-mechanical processing were present. The θ-lattice analysis of this boundary shows that the basis for the DSCL is

\[
\begin{align*}
\mathbf{b}_1 &= \frac{a}{82} [1 1 11] \\
\mathbf{b}_2 &= \frac{a}{41} [4 4 3] \\
\mathbf{b}_3 &= \frac{a}{41} [19 22 4]
\end{align*}
\]

This basis defines the shortest possible Burgers vectors for GBDs. Dislocations with Burgers vectors that are integral multiples of the basis are all geometrically possible; they include Burgers vectors equal to a crystal translation and a lattice dislocation. The GBD reaction

\[
\mathbf{b} = 3 \mathbf{b}_1 + \mathbf{b}_3
\]

\[
\frac{a}{2} [1 1 \bar{1}] = \frac{3a}{82} [1 1 11] + \frac{a}{41} [19 22 4]
\]

is marked in Figure 1 as "a". The three \(\mathbf{b}_1\) dislocations are so close that they appear as a single extrinsic dislocation. There are in the literature only two experiments where the smaller components of a reaction of this type have been distinguished as separate dislocation lines; the observation of Bollmann, et al., in a Σ = 29 boundary in stainless steel and the detailed study by Dingley and Pond of a dissociation in a Σ = 41 boundary in aluminum. The sites marked "b" (Figure 1) represent the
same dissociation for a trapped lattice dislocation that has retained its integrity in the GB region. A number of these dislocations (marked "c") do not dissociate in the boundary. The observations suggest the possibility of accommodation of transgranular flow in bcc materials through GBD reactions. An incoming glide dislocation can be redistributed in the boundary so as to create a favorable condition for slip in the other grain. This requires diffusion controlled climb of the GBDs and there is some evidence\textsuperscript{10} that this can occur even at room temperatures due to non-equilibrium effects. Eventually, the boundary will harden giving rise to dislocation pile-ups. The stresses at the head of the pile-up can then activate Frank-Read sources or prismatic loop sources in the GB.

It has also been suggested by Gleiter\textsuperscript{10} that when a trapped dislocation moves along the boundary plane, it will react at any sharp change of GB plane by emitting dislocations into a favorable slip plane (see e.g. Figure 2(d)). To study this phenomena, the structure and accommodation of a change in GB plane in a [101] low angle twist boundary was undertaken. A change in GB plane happens through a GB step, GB faceting or a GB curvature producing an effective change in the overall boundary plane. The structure of the boundary (Figure 2(a)) was imaged under strong excitation conditions (two beam conditions where either one or both grains are strongly diffracting) and weak excitation conditions (weak beam cases which induce more localized sampling of the strain fields of the GBDs). The dislocation structure is given by three sets of dislocations

\[ b_1 = \frac{a}{2} [1 1 1] \]
\[ b_2 = \frac{a}{2} [1 1 1] \]
\[ b_3 = a [0 1 0] \]
with line directions all parallel to the Burgers vector. A step in the GB is shown in Figure 2(b). The displacement of the extinction fringes occurs in free steps due to an effective change in thickness and also at extrinsic dislocations due to a change in the local deviation parameter. Steps at GBs are usually associated with a trapped GBD and thus show a dislocation character. Figure 2(c) shows the same GB faceted on the (111) plane. The facet is then in the pure tilt configuration and is accommodated by a set of edge dislocations with Burgers vector $b = \frac{a}{2} [1 1 1]$ and line directions $\gamma = [101]$.

Finally, as shown in Figure 2(e), the change in boundary plane from (101) to (112) was accommodated by the emission of dislocations onto the (110) plane. The stress concentration produced by the change in boundary plane is relieved by plastic flow. The curvature of the emitted dislocations show that they emanate from the boundary. As shown in the figure the foreign dislocation with the associated step discussed above was close to the boundary kink; if this trapped dislocation moves along the boundary plane it will react at the kink. In this case the dislocation would dissociate through the reaction

$$b = b_e + b_3$$

$$\frac{a}{2} [111] = \frac{a}{2} [111] + a [010]$$

The reaction is favorable because the products are free to glide on their respective planes while the extrinsic dislocation necessitated climb to move along the boundary plane.

CONCLUSIONS

The dissociation mechanisms presented here play an important role
in the continuation of plastic flow. Although detailed crystallographic analysis of these phenomena can be performed only in well-annealed specimens, the O-lattice theory provides an elegant method for the geometrical study of the resulting structures. In actual materials a high density of extrinsic GBD, might eventually cause the GB to harden depending on the loading rate. Whether the stresses will be relieved by activation of GB sources or creation of microcracks will depend on the availability of structural defects that can act as GB dislocation sources. Some possibility has in fact been raised concerning an intrinsic intergranular brittleness in materials where no interfacial segregation has occurred. Ultimately, the mechanical behavior of GBs will be understood through similar analyses of the fundamental mechanisms of deformation under well defined crystallographic and stress state conditions.

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REFERENCES


FIGURE CAPTIONS

Fig. 1. Grain boundary dislocation reactions in a near \( \Sigma = 41.55.9^\circ/ [110] \); "a" dissociation of a crystal dislocation; "b" dissociation of a trapped dislocation; "c" undissociated trapped dislocation.

Fig. 2. The structure and accommodation of a change in GB plane in a low angle twist boundary \( 4^\circ/[110] \). (a) GB structure; only the dislocation sets 2 and 3 are visible. (b) A GB step (indicated by black and white arrows); the step height is of the order of the dislocation spacings and there is no change in the dislocation structure (marked in the figure by the continuity of black lines). (c) A GB facet on the \( (11\bar{1}) \) plane is accompanied by a change in dislocation structure. (d) Gleiter's model\(^{10}\) for the emission of dislocations into a crystal from a GB kink. (e) A GB step associated with a trapped dislocation (straight arrows) moving towards a GB kink where it generates matrix dislocations (curly arrow).
Fig. 1
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