**STRUCTURE OF SMALL ANGLE TILT BOUNDARIES AND THEIR BEHAVIOR UNDER THE
APPLIED SHEAR STRESSES IN fcc METALS**

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Abstract A molecular statics study has been performed on $\langle 112 \rangle$ symmetrical tilt boundaries in fcc metals using pair potentials fitted to Cu and Ni. Boundaries are found to consist of a pair of walls of Shockley partials in both metals; distance between walls is much smaller than that between partials of an isolated extended dislocation. The separation between partial dislocation walls decreases with the increasing tilt angle and boundaries eventually come to have different structures from those observed in lower angle boundaries when the tilt angle exceeds a critical value depending on the potentials used. The critical shear strain for motion of the boundaries increases with the increasing tilt angle which is in good qualitative agreement with experimental observations so far reported.

1. Introduction

The small angle tilt boundary is one of the simplest type of boundaries and consists of a wall of edge dislocations. When the dislocations involved in the boundary are glissile or the temperature is high enough for even the sessile dislocations to climb, the small angle boundaries are expected to move under an applied shear stress. Washburn and Parker [1] were the firsts to show that small angle boundaries with tilt angles less than 2° in zinc actually moved under applied stresses and later Bainbridge et al. [2] showed that the velocity of boundary motion decreased with the increase in the tilt angle. Recently, Fukutomi and Horiuchi [3,4] examined the stress induced motion of various tilt boundaries with $\langle 100 \rangle$, $\langle 110 \rangle$ or $\langle 112 \rangle$ rotation axis using melt-grown aluminum bicrystals and found the same trend over a wide range of tilt angles up to a maximum of 30° depending on the tilt axis. This behavior is not straightforward as long as we assume that symmetrical tilt boundaries consist of a wall of one kind of edge dislocations.

In order to clarify atomic structures of small angle tilt boundaries and the mechanism governing their motion, a molecular statics study has been performed on $\langle 112 \rangle$ symmetrical tilt boundaries in fcc metals. We first show that the core structure of dislocations involved in the tilt boundaries is very different from that of an isolated dislocation in an otherwise perfect lattice. It is then shown that boundaries consist of a pair of walls of partial dislocations, the distance between which decreases with the increasing tilt angle. The core width of the individual partials becomes narrower with the decrease in the separation between walls of partial dislocations and the critical strain for the boundary motion under an applied stress increases rapidly with the increase in the tilt angle. This is in qualitative agreement with experimental observation and gives a possible mechanism for the stress-induced motion of the boundary described above.

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2. Method of calculation

Calculations have been made for the symmetrical tilt boundaries with $\{01\bar{1}\}$ median plane belonging to $\langle 21\bar{1} \rangle$ rotation axis, i.e. boundaries consisting of walls of edge dislocations with Burgers vector $1/2\langle 01\bar{1} \rangle$. Relaxation has been performed by the standard gradient method under the constant pressure, in which periodic border conditions are imposed both along the tilt axis and in the direction contained in the boundary plane and normal to the tilt axis. In the direction normal to the boundary plane, the bicrystal is chosen sufficiently large and bounded on both sides by perfect crystal blocks which are allowed to move. Two interatomic potentials were used in the calculations, empirical spline potentials fitted to copper [5] and nickel [6]; this choice was taken so as to see the effect of stacking fault energy on the boundary structure (unrelaxed stacking fault energies are 70mJ/m^2 for copper and 300mJ/m^2 for nickel and the fault width is calculated to be about two times wider in the former). The lowest energy configuration of the boundaries has been found by repeating relaxation starting from various initial configurations created by rigid translation parallel to the boundary plane of one grain relative to the other. Application of shear stress has been simulated by giving the bicrystal of the lowest energy configuration the homogeneous simple shear strain; a large strain is built up by repeating a small increment of shear strain and relaxation. The smallest strain needed for grain boundary to move one Burgers vector distance is taken as the critical shear strain for motion. The core structure of an isolated dislocation is calculated by the standard static relaxation with fixed border conditions and the critical strain for glide is determined in the same way as above.

3. Result

3.1 Structures of isolated dislocations and small angle tilt boundaries

Figs.1(a) and (b) show $(21\bar{1})$ projection of atoms for an isolated relaxed edge dislocation in copper and nickel, respectively; all the figures will be displayed in the same projections below. Six $(21\bar{1})$ planes are contained in one period along the dislocation line, however, they are displayed with same symbols with no distinction of their levels with respect to the plane of the figure. To show the distribution of disregistry of atom arrangements above and below the slip plane, several $(01\bar{1})$ traces are drawn in the figure. In the case of copper, atoms in $(01\bar{1})$ planes are arranged in straight lines across the slip plane on both extreme left and right sides of the figure, corresponding to atom arrangement of the perfect lattice. In the middle of the figure, there is also perfect alignment of atoms in $(01\bar{1})$ planes; this corresponds to the intrinsic stacking fault in the strictly perfect sense, width of which is about $3b$ (b is the magnitude of the Burgers vector). On either side of the stacking fault the partial core appears to spread widely, up to about $7b$. The same configuration of a dissociated edge dislocation calculated using the same potential was first found by Englert et al. [5] and later by Perrin et al. [7]. They describe this wide spread of partial dislocation cores simply as an increase in Peierls width

Fig.1 core configurations of isolated dislocations in copper (a) and nickel (b).

of the individual partials. This, however, is not simple spreading of partials but further splitting of individual partials into 'quarter' dislocations with the Burgers vector $1/12\langle 112 \rangle$; the γ -surface calculated from the potential used has a local minimum for the mid-point of the fault vector giving the intrinsic stacking fault. The regions where projected atom positions just above and below the glide plane are arranged like a series of isosceles triangles are corresponding stacking faults, the details of which will be reported elsewhere. In the case of nickel a total dislocation dissociates into partials with a stacking fault $1.5b$ wide in between.

Fig. 2 shows atomic configurations in symmetrical tilt boundaries with rotation angle 5.8° . With the help of $(01\bar{1})$ traces drawn the arrangement of dislocations along the boundary is clearly visualized; a boundary consists of a wall of dissociated dislocations in both cases of copper and nickel. Note here that 'quarter' dislocations observed in the dissociation of an isolated dislocation in copper shrink to form individual Shockley partials; the distance between walls of partials is $5b$ in copper and $2.5b$ in nickel whereas respective widths of individual partial cores are $4b$ and $1.5b$ as determined simply from the deviation of $(01\bar{1})$ traces from the straight line around the glide plane.

Fig.2 structures of 5.8° tilt boundaries in copper (a) and nickel (b)

When the tilt angle is increased to 17.4° , the difference between boundary structures in copper and nickel becomes vivid as shown in fig.3. The copper boundary still consists of a pair of walls of partials separated $3.5b$ apart, the width of the individual partial core being about $2.5b$, a little narrower than in the 5.8° boundary (cf. Fig.6) Note that the (111) planes are curved across the boundary and the orientation difference between crystals on both sides of the boundary is accommodated over a broad region. In nickel, on the other hand, dislocations lined up

Fig.3 Structures of 17.4° boundaries in copper (a) and nickel (b).

along the boundary are hardly dissociated; the width of dissociation may only amount to $1.5b$. The deviation of $(01\bar{1})$ traces from the straight line is very localized at the boundary. In consequence, the (111) planes on either side of the boundary are joined to each other at sharp angle. Therefore, boundary structure in nickel changes at about this tilt angle. In the case of copper, calculation was continued further for boundaries with a tilt angle up to 34.5° . At 23.1° the grain boundary keeps almost the same configuration as at 17.4° shown in fig.3(a). Fig.4 shows the boundary structure with a tilt angle 34.05° . It should be noted that the boundary structure at this rotation angle is very similar to that in 17.4° nickel boundary; the strain associated with the boundary dislocation is very localized and (111) planes bend abruptly across the boundary plane although the boundary may still be regarded as consisting of dissociated dislocations with partials separated $1.5b$ apart. There is no unique definition for the delimiting angle for the division between small and large angle boundaries, however, it is concluded from the above results that the delimiting angle should be different from metal to metal.

3.2 Behavior under applied shear stresses

Stresses have been applied to an isolated dislocation and boundaries in copper. In the case of an isolated dislocation, relaxation has been carried out after every successive increment of a shear strain of 0.002. It was found that the

Fig.4 Structure of 34.05° boundary in copper.

(a)

Fig.6 Width of partial cores and critical strain for boundary motion as a function of the tilt angle in copper.

(b)

Fig.5 Structures of boundaries under applied stresses in copper; 5.8° boundary at a strain of 0.005 (a) and 17.4° boundary at a strain of 0.02 (b).

dislocation begins to move at a strain of 0.004. For small angle boundaries, strain application was made by a step of 0.002 for a 5.8° tilt boundary. For other boundaries, however, strain increment of 0.005 was chosen.

Fig.5(a) shows atomic configurations of a 5.8° boundary under a shear stress applied parallel to the boundary plane in the sense that the boundary moves to the right. Fig.5(b) shows a 17.4° boundary which has moved at a strain of 0.02. The vertical dotted lines in the middle of each figure indicates the position at which there was the initial center line of the boundary under no stress. To a 34.05° boundary was applied a strain up to 0.025 but no perceptible motion of the boundary was detected. These results clearly show that the critical strain for grain boundary motion increases with increasing tilt angle as shown in Fig.6 where crosses mean that application of corresponding strains could not induce any boundary motion. The width of partial dislocation cores is also plotted against the tilt angle in Fig.6. The increasing Peierls stress with the increase in the tilt angle gives a possible explanation of grain boundary behavior under applied stresses described in Introduction.

4. Concluding Remarks

Since the work by Read and Shockley [8], several extensions of their model have been made. For example, Li and Chalmers [9] considered a boundary as a planar array of partial dislocations and showed that the distance between partial dislocation walls decreases with increasing dislocation density in the boundary. These modifications, however, can give no information about the resistance stress to the boundary motion. Bullough [10] treated a tilt boundary as a wall of Peierls dislocations and obtained an approximate solution for small tilt angles less than 5° ; he showed the decrease of Peierls width with increasing tilt angle and the consequent increase in the stress to cause glissile motion of the boundary. An atomistic study has shown above these two trends are also the case in the wide range where analytic treatment is not feasible. The result obtained gives a possibility that Peierls stress for dislocations in small angle boundaries can play an important role in the motion of the boundaries even in fcc metals where Peierls stress is negligibly small for isolated dislocations. More elaborations, however, will be needed on both experiments and theoretical models to explain the details of experimental observations.

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