Coupling of Sliding and Migration in the $\{1\bar{2}11\}$ Coincidence Boundary of Zn as an Evidence for the DSC Dislocation Model*

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Bicrystal experiments were carried out, in order to verify the DSC dislocation model of grain boundary sliding. Coupling of sliding and migration was observed in the $\{1\bar{2}11\}$ coincidence boundary of Zn. The amount of grain boundary migration was measured to be about twice as large as that of grain boundary sliding. The sliding-to-migration ratio as well as the migration direction were in agreement with those predicted by the DSC dislocation model.

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I. Introduction

The grain boundary dislocation model has acquired extensive evidence from electron microscopy⁽¹⁾⁻⁽³⁾. The grain boundary dislocation theory explains grain boundary sliding in terms of the motion of grain boundary dislocations⁽⁴⁾⁻⁽¹¹⁾. It has been predicted that grain boundary sliding should be accompanied by grain boundary migration⁽⁶⁾⁻⁽⁹⁾. The ratio of the amount of grain boundary migration to that of grain boundary sliding and the direction of grain boundary migration can be predicted geometrically.

If such a specific coupling of sliding and migration is actually realized, the correctness of the DSC dislocation theory can be verified, and at the same time, the grain boundary structure model might be justified as well.

In this study, a typical coincidence boundary to which the CSL and the DSC lattice can safely be applied was selected. Bicrystal experiments were carried out to see if the coupling of sliding and migration would occur on a

macroscopic scale.

II. Experimental

1. The material and the boundary crystallography

Grain boundary sliding may be produced by the motion of extrinsic grain boundary dislocations⁽¹²⁾. These dislocations are thought to be created in the dissociation reaction of crystal lattice dislocations which have run into the grain boundary during plastic deformation⁽⁹⁾. If one chooses h.c.p. metals in which the exclusive activity of basal slip is known, the crystal lattice dislocations which will be supplied into the grain boundary can be limited to the basal slip dislocations. Thus Zn is selected as the material.

In order to simplify the geometrical circumstances into a 2-dimensional illustration, a $\langle 10\bar{1}0 \rangle$ tilt boundary is selected. This type of a grain boundary has its grain boundary normal, slip plane normals and the Burgers vectors of the crystal lattice dislocations on one plane. For the purpose of verifying the DSC dislocation theory, a convenient grain boundary should be chosen, to which the CSL and the DSC lattice can definitely be applied. So, a $\langle 10\bar{1}0 \rangle$ symmetric tilt boundary (0.52 rad misorientation) as shown in Fig. 1 is selected,

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Fig. 1 Atomic configuration of a 0.526 rad $\langle 10\bar{1}0 \rangle$ symmetric tilt boundary in Zn. The grain boundary plane lies parallel to $\{1\bar{2}11\}$. Shaded atoms represent the coincidence sites on the grain boundary.

Fig. 2 $\Sigma 15$ near-CSL and its corresponding DSC lattice for a 0.526 rad $\langle 10\bar{1}0 \rangle$ symmetric tilt boundary in Zn.

whose boundary plane is parallel to $\{1\bar{2}11\}$ planes of both crystals. This boundary is thought to be of relatively low energy, from the experimental observations of grain boundary facettings of $\langle 10\bar{1}0 \rangle$ symmetric tilt boundary of Zn in the misorientation range of this boundary⁽¹³⁾⁽¹⁴⁾.

Figure 2 shows the coincidence plot, the near-CSL and the DSC lattice for the grain boundary in Fig. 1. The Σ value for this boundary is 15⁽¹⁵⁾, and the base vectors of the CSL are $a+2c$ and $7a-c$, where a and c are the base vectors of the crystal lattice. $a+2c$ is parallel to the grain boundary plane, and $7a-c$ is almost perpendicular to $a+2c$. The appearance of the CSL is, if seen in 2-dimension, a rectangle whose longer side is $(c/a)=1.856$ times as long as the shorter one. Accordingly, the base vectors of the DSC lattice are $(a+2c)/$

15 and $(7a-c)/15$. A 3-dimensional atomic configuration of the boundary will be considered in the discussion.

2. Experimental procedure

A high purity (99.999 mass%) Zn bicrystal plate containing a 0.52 rad $\langle 10\bar{1}0 \rangle$ symmetric tilt boundary was grown from the melt using seed crystals. The angular deviation from the ideal boundary orientation was within about 0.02 rad. A tensile specimen with dimensions of 5 mm $\times$ 4 mm $\times$ 50 mm was spark-cut. The grain boundary plane was inclined to the tensile axis by the angle of $\pi/4$. Then the specimen was electrolytically polished in a phosphoric acid-methanol solution (1 vol. to 1 vol.), and fiducial lines were inscribed on the $\{10\bar{1}0\}$ surface upon which the microscopic observation would be made. Grain boundary sliding behavior at elevated temperatures (553 to 633 K) was observed and photographed using a high temperature optical microscope equipped with a tensile stress loading apparatus.

III. Predicted Grain Boundary Sliding Behavior

Figure 3 depicts schematically the bicrystal specimen under tensile stress. The tensile axis makes an angle of $\pi/4$ with the normal of the grain boundary plane. The basal planes of the adjoining crystals 1 and 2 are inclined to the tensile axis by the angles of $\pi/6$ and $\pi/3$, respectively. The Schmid factors for both slip systems are equal, and the numbers of the crystal lattice dislocations activated in the crystals 1 and 2 are supposed to be equal. In this geometry, such crystal lattice dislocations

Fig. 3 Schematic representation of the Zn bicrystal specimen containing a 0.52 rad $\langle 10\bar{1}0 \rangle$ symmetric tilt boundary in Zn.

as shown in the figure would be activated to run into the grain boundary. On arriving at the boundary, these dislocations are assumed to be dissociated into DSC dislocations (grain boundary dislocations) in a dissociation reaction given by eq. (1).

$$a = (a+2c)/15 + 2 \cdot (7a-c)/15. \quad (1)$$

The $2 \cdot (7a-c)/15$ type DSC dislocation created from a crystal-1 dislocation and the one created from a crystal-2 dislocation have opposite signs to each other. So, it is assumed that this type of DSC dislocations will effectively cancel out by pair annihilation. Even if these dislocations might climb in the grain boundary before pair annihilation, they can make no contribution to the grain boundary sliding, since their Burgers vectors are normal to the boundary. Nor can they produce grain boundary migration, because they would cause no boundary steps by taking the Burgers vector twice as large as the base DSC vector⁽⁷⁾⁽⁸⁾⁽¹⁶⁾⁽¹⁷⁾.

Thus the net dislocations whose motion will produce grain boundary sliding are simply the DSC dislocations with the Burgers vector of $(a+2c)/15$. The magnitude of this Burgers vector is $0.26a$, where a is the nearest neighbors spacing.

Grain boundary sliding behavior can be predicted on a geometrical construction as shown in Fig. 4. In this figure, a DSC dislocation with Burgers vector of one base DSC vec-

tor, $(a+2c)/15$, is shown schematically. This DSC dislocation can be activated to glide in the boundary plane from lower left to upper right by the externally applied stress. In the region where the DSC dislocation has swept, atoms in the lower crystal, including the atoms on the boundary plane, are displaced from their initial positions (broken circles) to new ones (circles) by the distance of $b = |a+2c|/15$.

After the passage of the DSC dislocation, the same boundary configuration as before is produced again at the distance of one base DSC vector, $h = |7a-c|/15$, from the original position of the boundary. Thus the grain boundary sliding is accompanied by grain boundary migration. The ratio of grain boundary migration to grain boundary sliding is given by eq. (2).

$$R = M/S = h/b = |(7a-c)/15| / |(a+2c)/15| = c/a = 1.856. \quad (2)$$

As shown in Fig. 4, the direction of the grain boundary migration is pointing from lower right to upper left, and this results in the lower grain growing at the expense of the upper grain.

IV. Experimental Results

Figure 5 shows a series of optical micrographs taken at a fixed position. The testing temperature was 573 K, and the applied shear stress on the grain boundary plane was 0.1 MPa. The tensile axis is horizontal on the micrographs. The solid lines show the (0001) traces of both grains. Coupling of sliding and migration on a $\{1\bar{2}11\}$ coincidence boundary in Zn is clearly revealed. The horizontal fiducial lines make sharp bends by an angle of 0.2 rad at the initial and final positions of the grain boundary. The direction of the grain boundary migration, as indicated by the arrow in the figure, is pointing to the upper left, which is consistent with the geometrical prediction as shown in Fig. 4. From the microscopic examination of both surfaces and of both sides of the specimen after the test, it is ascertained that the coupling of sliding and migration occurred uniformly over the whole grain boundary.

Fig. 4 Coupling of sliding and migration to be produced by the glide motion of a DSC dislocation whose Burgers vector is $(a+2c)/15$.

Fig. 5 Micrographs showing a coupling of sliding and migration on a 0.52 rad $\langle 10\bar{1}0 \rangle$ symmetric tilt boundary in Zn. The arrow indicates the direction of the grain boundary migration. The solid lines show (0001) traces.

Fig. 6 Relationship between the amount of grain boundary sliding (S) and the amount of grain boundary migration (M) of a 0.52 rad $\langle 10\bar{1}0 \rangle$ symmetric tilt boundary in Zn. The experimental results (solid circles) and the theoretical prediction (solid line).

The amount of grain boundary sliding (S) and that of grain boundary migration (M) were measured on the micrographs, and plotted in a S vs M diagram in Fig. 6. The solid line shows the theoretical prediction, $M/S = c/a = 1.856$. A good agreement between the experimental results and the theoretical prediction is revealed.

When the tensile stress or testing temperature was changed during the test, the rate of grain boundary sliding changed accordingly, but the M/S ratio stayed constant.

V. Discussion

1. Atomic configuration of a $\{1\bar{2}11\}$ boundary in Zn

In this section, geometric consideration is made on the 3-dimensional atomic configuration of a $\{1\bar{2}11\}$ boundary in Zn. It is assumed that the 2-dimensional atomic arrangement on the boundary plane is the same as that of the $\{1\bar{2}11\}$ plane in an ideal crystal, and that the atoms on the boundary are common to both crystals abutting on the boundary. So, all the atoms on the boundary are coincidence sites. Then two types of grain boundary structure, type I and type II, are possible.

type I: Such a grain boundary atomic configuration that both crystals take an ABCD stacking sequence of $\{10\bar{1}0\}$ planes. (This type of the grain boundary can be constructed by a simple tilt rotation of 0.526 rad about the $\langle 10\bar{1}0 \rangle$ direction.)

type II: Such a grain boundary atomic configuration that one crystal takes an ABCD stacking sequence and the other crystal takes an AB'CD' stacking sequence of $\{10\bar{1}0\}$ planes. (This type of the grain boundary can be produced by a simple twist rotation of π about the normal of the $\{1\bar{2}11\}$ plane.)

Definition of A, B, B', C, D and D' $\{10\bar{1}0\}$ planes is given in Fig. 7.

The 2-dimensional atomic configurations on A and C $\{10\bar{1}0\}$ planes are common to both types of grain boundary structure. Figure 8(a) shows the atomic configuration on A $\{10\bar{1}0\}$ plane viewed parallel to $\langle 10\bar{1}0 \rangle$. On C $\{10\bar{1}0\}$ plane, the same configuration as this appears

Fig. 7 Definition of A, B, B', C, D and D' $\{10\bar{1}0\}$ planes in h. c. p. crystals.

Fig. 8 Atomic configuration on A and C $\{10\bar{1}0\}$ planes of both types of the grain boundary, (a) viewed parallel to $\langle 10\bar{1}0 \rangle$, and (b) viewed parallel to $(a+2c)$. Heavily shaded atoms are the coincidence sites on the grain boundary (G. B.).

translated by a distance of $|a+2c|/2$ along the boundary plane. As shown in the figure, all the atoms on the boundary plane are the coincidence sites on A and C $\{10\bar{1}0\}$ planes. Figure 8(b) shows the basal planes of both crystals viewed along the direction of $a+2c$. A good atomic matching is seen on the grain boundary plane (G.B.).

The grain boundary atomic configuration on B and D $\{10\bar{1}0\}$ planes which appears in type I grain boundary, as viewed along $\langle 10\bar{1}0 \rangle$ and $a+2c$, are shown in Fig. 9(a) and (b), respectively. No grain boundary coincidence sites appear on B and D $\{10\bar{1}0\}$ planes. A large overlapping of atoms and a wide gap are present on the boundary plane.

Fig. 9 Atomic configuration on B and D $\{10\bar{1}0\}$ planes of the type I grain boundary, (a) viewed parallel to $\langle 10\bar{1}0 \rangle$, and (b) viewed parallel to $(a+2c)$.

Fig. 10 Atomic configuration on B, B' and D, D' $\{10\bar{1}0\}$ planes of the type II grain boundary, (a) viewed parallel to $\langle 10\bar{1}0 \rangle$, and (b) viewed parallel to $(a+2c)$.

The type II grain boundary as shown in Fig. 10 is more realistic; atomic overlapping and opening are much reduced. In this type II boundary, the atomic configuration is not symmetric with respect to the grain boundary plane, since B and B' planes and D and D' planes are not coplanar. However, one might call this symmetric, seeing that the crystallographic orientation of the basal planes of both crystals are symmetric.

Although the exact relaxed boundary structure cannot be predicted based on the hard sphere model, a comparison between Fig. 9 and Fig. 10 may suggest that the type II boundary structure approximates the real boundary structure. Recently, Minonishi *et al.*⁽¹⁸⁾ have calculated the relaxed boundary configuration and its boundary energy of a $\{1\bar{2}11\}$ twin boundary, using a pair potential fitted to Ti. The calculated boundary configuration is what one obtains when small alternating translations along $\langle 10\bar{1}0 \rangle$ direction are imposed on the

Fig. 11 Hard sphere model of the type II grain boundary.

type II boundary structure. Their results on a $\{1\bar{2}11\}$ twin boundary in Ti might not be directly enlarged to a $\{1\bar{2}11\}$ boundary in Zn, since the axial ratio of Zn ($c/a=1.856$) is much larger than that of Ti ($c/a=1.587$). However, such a qualitative analogy might be made that the type II boundary configuration approximately represents the real boundary structure of a $\{1\bar{2}11\}$ boundary in both Ti and Zn. Figure 11 shows a 3-dimensional model of the type II boundary with its boundary plane parallel to $\{1\bar{2}11\}$ plane in h.c.p. crystals; it is seen that a good atomic matching is achieved.

2. Atomic shufflings involved in the glide motion of DSC dislocations

The experimental results reported in this paper have shown that the coupling of sliding and migration in $\{1\bar{2}11\}$ grain boundaries of Zn can be considered to be produced by the glide motion of DSC dislocations with Burgers vector of $(a+2c)/15$. In this section, geometrical consideration is made upon the atomic shufflings involved in the glide motion of a unit DSC dislocation in a $\{1\bar{2}11\}$ boundary of the type II structure. The atomic motion on A and C $\{10\bar{1}0\}$ planes has already been shown in Fig. 4; no shuffling is required in these planes. Figure 12(a) and (b) show the atomic positions before (broken circles) and after (circles) the passage of a unit DSC dislocation, as viewed parallel to $\langle 10\bar{1}0 \rangle$ and $a+2c$,

Fig. 12 Atomic shuffling required for the preservation of the type II grain boundary structure, (a) viewed parallel to $\langle 10\bar{1}0 \rangle$, and (b) viewed parallel to $a+2c$. After the passage of a $(a+2c)/15$ DSC dislocation, the atoms below the grain boundary (dashed line) move from their initial positions (dashed circles) to final ones (shaded circles), so that the grain boundary migrates to its new position (G. B.').

respectively; here the lower half-crystal is translated by a unit DSC vector parallel to the grain boundary with respect to the upper one. A local atomic configuration at α' after the passage of a DSC dislocation is the same as that at β in Fig. 10(a). On the other hand, a local atomic configuration at β' after the passage of a DSC dislocation requires atomic shuffling in order to be the same as that at α in Fig. 10(a). In order that the boundary configuration may be preserved, atoms represented by double broken circles which have belonged to the upper half-crystal before the passage of a DSC dislocation, must shuffle onto their new sites belonging to the lower half-crystal. Such atomic shufflings enable the same boundary structure as before to be reconstructed on the new boundary position (G.B.').

Figure 12(b) shows the atomic shufflings as viewed parallel to $a+2c$; in this figure only the atomic shufflings from D' planes of the upper to D planes of the lower are shown; however, on the adjacent basal planes, atomic shufflings from B' planes of the upper to B planes of the lower are required.

As seen from Fig. 12, these atomic shufflings consist of two components; a component with a half magnitude of the Burgers vector of a gliding DSC dislocation, and a component with a magnitude of $|\langle 10\bar{1}0 \rangle|/6$. As mentioned earlier, atomic motions on A and C planes

need no shuffling, when a unit DSC dislocation is gliding on the boundary plane. On the other hand, atomic motions comprising the coupling of sliding and migration necessitate shuffling of atoms on B, B', D and D' planes. Consequently, two atoms out of every four atoms, which are swept by the boundary plane when a unit DSC dislocation sweeps the boundary area of $|\langle 10\bar{1}0 \rangle| \cdot |a+2c|$, require shuffling to accomplish the coupling of sliding and migration. This proportion is relatively small, and so the atomic shuffling might not impose a very large resistance on the DSC dislocation glide⁽¹⁹⁾.

3. Some consideration on extrinsic DSC dislocations

The $(a+2c)/15$ DSC dislocations which give rise to the coupling of sliding and migration are considered to be dissociated from basal slip dislocations activated by the externally applied stress⁽²⁾⁽³⁾⁽⁹⁾⁽¹⁰⁾⁽¹²⁾. Besides this source of extrinsic DSC dislocations, it is conceivable that the $\{1\bar{2}11\}$ grain boundary itself contains intrinsically a multiplication mechanism for DSC dislocations; however, the details of this mechanism have not been made clear so far.

VI. Conclusion

In order to demonstrate that a specific coupling of sliding and migration as predicted by the DSC dislocation model actually occurs on a macroscopic scale, a $\{1\bar{2}11\}$ coincidence boundary of Zn was selected, and a shear stress was applied on the boundary plane at an elevated temperature to produce grain boundary sliding.

The amount of grain boundary migration was measured to be about twice as large as that of grain boundary sliding, in good agreement with the theoretically predicted ratio of $(c/a) = 1.856$, and the direction of grain boundary migration coincided with the prediction. Thus

the grain boundary dislocation theory which explained the grain boundary sliding by the glide motion of DSC dislocations was clearly demonstrated to hold.

Geometrical consideration is made on the grain boundary structure of this boundary and on the atomic shuffling involved in the coupling of sliding and migration.

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