Transactions of the Materials Research Society of Japan 33[2] 253-256 (2008)

Dislocation Models for Coupled Sliding and Migration of Coincidence Boundaries in Zinc Bi-crystals

Tohru TAKAHASHI[1]
[1]Department of Mechanical Systems Engineering, Faculty of Technology,
Tokyo University of Agriculture and Technology,
Naka-cho 2-24-16, Koganei, Tokyo 184-8588, JAPAN, takahas@cc.tuat.ac.jp

In the present study the grain boundary sliding behavior was investigated on zinc bi-crystal specimens containing some coincidence boundaries. Zinc bi-crystals whose orientations were controlled with seed crystals were grown from the melt by a modified Bridgman method. The $(1\bar{2}11)$, $(1\bar{2}16)$ and $(10\bar{1}2)$ coincidence boundaries in zinc were selected as typical cases. Bi-crystal test pieces where the grain boundary plane is inclined by 45 degrees to the tensile axis had dimensions of about 5mm × 4mm × 50mm. A tensile load was applied to the specimen at elevated temperatures. For the selected coincidence boundaries, the grain boundary dislocation modeling predicts a characteristic behavior of grain boundary sliding, based on the geometric framework of CSLs and DSC lattices. It is predicted that the grain boundary sliding should accompany grain boundary migration whose amount and direction is uniquely correlated to the grain boundary sliding. This theoretical prediction was proved to be true on the $(1\bar{2}11)$, $(1\bar{2}16)$ and $(10\bar{1}2)$ coincidence boundaries where the amount of the grain boundary migration was about 2, 8, and 7 times larger than that of grain boundary sliding, respectively. The experimental results gave a clear-cut evidence supporting the DSC dislocation modeling of grain boundary sliding in coincidence boundaries.

Key words: zinc, bi-crystal, coincidence boundary, sliding, migration

1. INTRODUCTION

Grain boundary sliding is a relative displacement between grains along the grain boundary plane, and it is considered as an independent deformation mode whose activity is enhanced at elevated temperatures. Beside its importance upon the high temperature deformation and strength of polycrystals, grain boundary sliding is involved in the nucleation of grain boundary cracks that brings intergranular fracture. Thus the grain boundary sliding should be focused on as an important issue with much relevance to materials strength and safety. The basic understanding of its mechanism, however, is not totally clear because of its complex dependence on diverse factors such as crystallography, morphology, etc. Grain boundaries can be categorized into 1) small angle boundaries and 2) large angle boundaries. Small angle boundaries with misorientation angles less than about 15 degrees can be composed of crystal lattice dislocations. When a set of edge dislocations in a small angle tilt boundary cooperatively move under an applied stress, the boundary shows stress induced boundary migration [1]. But such a behavior can rarely be seen because of the special situation for constituting small angle tilt grain boundaries. Large angle grain boundaries are largely considered to have random structure with somewhat relaxed atomic configuration on the grain boundary plane. Large angle boundaries generally show pure sliding displacement on the boundary plane, but the mechanism for this has not been satisfactorily clarified. An averaged behavior can experimentally be obtained, and hypothetical constitutive equation can be deduced for to apply to model calculation, however, some important aspect of grain boundary sliding has not been recognized. In late 1970s, grain boundary dislocation modeling was proposed where the structure and dynamic behavior of the coincidence boundaries were described in intrinsic and extrinsic grain boundary dislocations (GBDs)[2-5]. Such a modeling employed the geometric frameworks of coincidence site lattice (CSL) and its corresponding sub-lattice called DSC lattice (displacement of complete-pattern-shift lattice). Based on the GBD modeling, the grain boundary sliding (GBS) can be explained as the lateral motion of a DSC dislocation with its Burgers vector lying parallel to the grain boundary plane. At the same time the DSC vector displacement along the boundary plane brings the shift of the coincidence sites to newly formed coincidence sites. Then the energetically favored boundary configuration will be reconstructed at the next site in the wake of the gliding DSC dislocation. This will bring grain boundary migration (GBM) that is inevitably combined to grain boundary sliding. The DSC dislocation model puts out a very interesting insight into structure-behavior relationship concerning the coupling of GBS and GBM in coincidence boundaries. The amount of shift in coincidence sites that is produced by the DSC vector displacement along the grain boundary can be derived by a geometric construction on the DSC lattice. The GBM to be produced by the motion of DSC dislocation can be illustrated as the propagation of the grain boundary step that is combined with the DSC dislocation core. Figure 1 shows the schematic.

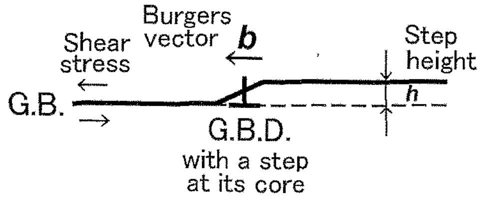

Figure 1 Schematic of a grain boundary dislocation configuration bringing coupled sliding and migration of the boundary

2. EXPERIMENTAL PROCEDURE

2.1 Selection of typical coincidence boundaries

For the purpose of the present study, typical coincidence boundaries have been selected based on the following intuitive criteria; A) a good atomic matching at the grain boundary , B) a short periodicity along the grain boundary, and C) a high planar density of boundary coincidence. By referring to a hypothetical model of grain boundary structures using hard spheres, a $[10\bar{1}0]$ symmetric tilt boundary with $(1\bar{2}11)$ boundary plane, a $[10\bar{1}0]$ symmetric tilt boundary with $(1\bar{2}16)$ boundary plane, and $[1\bar{2}10]$ symmetric tilt boundary with $(10\bar{1}2)$ boundary plane were selected.

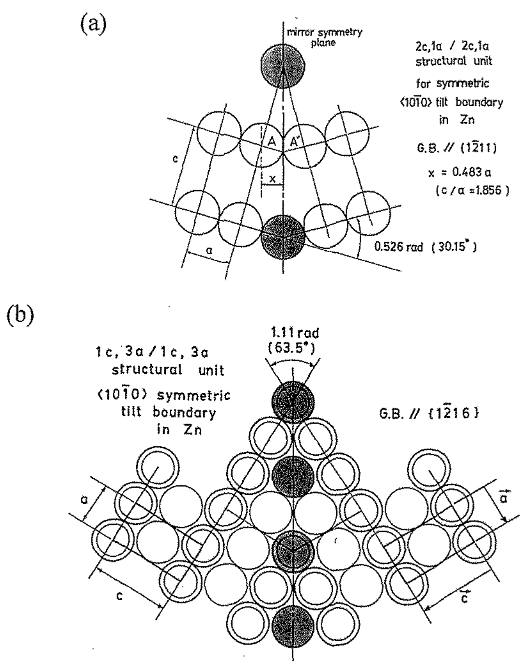

Figure 2 Hard sphere models of (a) $(1\bar{2}11)$ and (b) $(1\bar{2}16)$ boundary in zinc

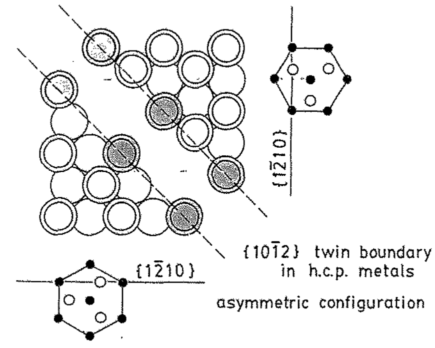

Figure 3 Assumed atomic configuration of $(10\bar{1}2)$ boundary in zinc

2.2 Specimen preparation

High Purity Zinc (99.999%) was used as material. Single and bi-crystal plates were grown from the melt by a modified Bridgman method using well-defined seed crystals. Crystallographic orientations of the component crystals were analyzed by X-ray diffraction patterns under back reflection Laue method, and the experimental error was measured to be within 2 degrees. Bar shaped specimens with the size of 4mm × 5mm × 50mm were spark cut and finished by electrolytic polishing. The boundary plane was oriented to make 45 degrees angle with the longitudinal axis. Fiducial lines were inscribed on the specimen surface using a diamond stylus tip. Shear stress of about 0.1MPa was applied to the grain boundary plane at elevated temperatures around 600K. The specimen surface was continuously observed in an optical microscope.

3. THEORETICAL PREDICTIONS BASED ON THE GRAIN BOUNDARY DISCLOCATION MODEL

3.1 Definition of CSLs and DSC Lattices

CSL (coincidence site lattice) is defined as a kind of superlattice that is formed by the "coincidence sites" where lattice sites coincide if two crystal lattices are superposed after a specific rotation around a common origin. The reciprocal of the relative fraction of coincidence sites as compared with the original lattice sites is a characteristic number, Σ value, of the CSL. The smaller value of Σ means shorter periodicity in grain boundary structure and lower boundary energy. DSC lattice is a sublattice of the CSL divided by Σ, and the DSC lattice vector characterizes the smallest possible displacements that can conserve the boundary structure of its corresponding coincidence boundary. So the DSC lattice vectors define possible relative displacements that preserve the low energy atomic configuration of the coincidence boundary. The energetically favored boundary structure will be reconstructed not on the original position of the boundary but at the new position that was shifted by multiples of DSC vector that is normal to the boundary plane. Such geometric consideration portrays that the DSC vector displacement along the boundary will be coupled with the motion of the boundary to its normal direction. The sliding to migration ratio and the direction of the grain boundary migration can be uniquely predicted. This can be described by the glide motion of a DSC dislocation that is combined by a boundary step at its core along the grain boundary plane.

3.2 DSC dislocation model predicting GBS-GBM in $(1\bar{2}11)$ coincidence boundary in zinc

Figure 4 shows the CSL and DSC lattice that can be applied to the $(1\bar{2}11)$ coincidence boundary in zinc. When a shear stress is applied to the grain boundary plane G.B. in the direction that the left half is moved downward with respect to the right half, the open circle in the left half that stands next to the original grain boundary plane will be brought into new coincidence site. Geometric calculations lead to a prediction that the amount of the grain boundary migration (M) is (c / a) times the amount of the grain boundary sliding (S), where c / a is the axial ratio of zinc crystal, namely 1.86.

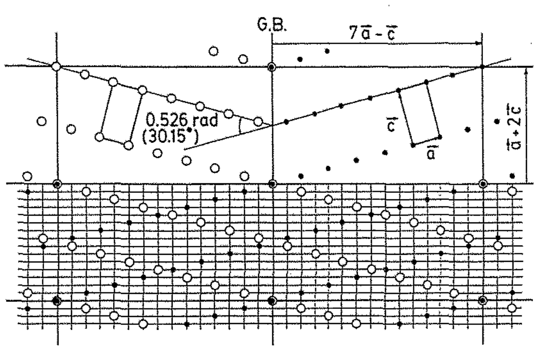

Figure 4 CSL and DSC lattice for $(1\bar{2}11)$ coincidence boundary in zinc

Figure 5 shows one possible way of measuring the M to S ratio of the coupled GBS-GBM. If the coupled GBS-GBM occurs uniformly and continuously, fiducial lines inscribed on the specimen surface will kink by a certain angle ϕ at the initial and final positions of the boundary plane (G.B.i and G.B.f) . The angle ϕ is dependent upon the M to S ratio.

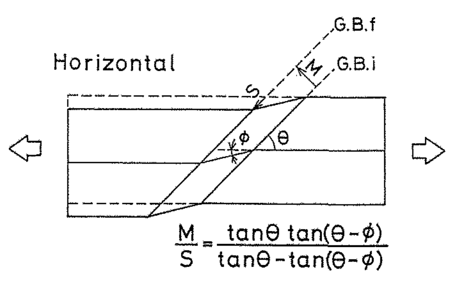

Figure 5 M / S ratio determination from angle ϕ

3.3 DSC dislocation model predicting GBS-GBM in $(1\bar{2}16)$ coincidence boundary in zinc

Figure 6 shows the CSL and DSC lattice that can be applied to the $(1\bar{2}16)$ coincidence boundary in zinc. When a shear stress is applied to the grain boundary plane G.B. in the direction that the top half is moved left with respect to the bottom half, the open circle O_1 in the top half will be brought into new coincidence site. Geometric calculations lead to a prediction that the amount of the grain boundary migration (M) is 8.33 times the amount of the grain boundary sliding (S). The value of 8.33 was derived from geometric consideration as $2 (c / a) / ((c / a)^2 - 3)$.

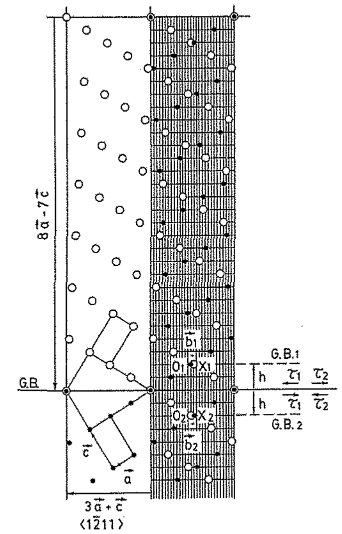

Figure 6 CSL and DSC lattice for $(1\bar{2}16)$ coincidence boundary in zinc

3.4 DSC dislocation model predicting GBS-GBM in $(10\bar{1}2)$ coincidence boundary in zinc

Figure 7 shows the CSL and DSC lattice that can be applied to the $(10\bar{1}2)$ coincidence boundary in zinc. Geometric calculations lead to a prediction that the amount of the grain boundary migration (M) is 7.21 times the amount of the grain boundary sliding (S). The value of 7.21 was derived from geometric consideration as $\sqrt{3}\ (c / a) / ((c / a)^2 - 3) = 7.21$.

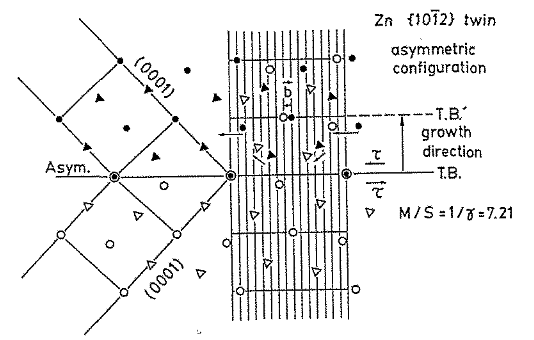

Figure 7 Grain boundary dislocation model for $(10\bar{1}2)$ coincidence boundary in zinc

4. RESULT AND DISCUSSION

4.1 Experimental observation of coupled GBS-GBM

Figure 8 shows the experimentally observed behavior of coupled GBS-GBM in (a) $(1\bar{2}11)$, (b) $(1\bar{2}16)$, and (c) $(10\bar{1}2)$ coincidence boundaries in zinc . The ratios of M / S were measured to be about 1.9, 8, and 7, in (a) $(1\bar{2}11)$, (b) $(1\bar{2}16)$, and (c) $(10\bar{1}2)$ coincidence boundaries, respectively. These ratios and the directions of grain boundary migration were all in good agreement with the geometric predictions.

(a)
(b)
(c)

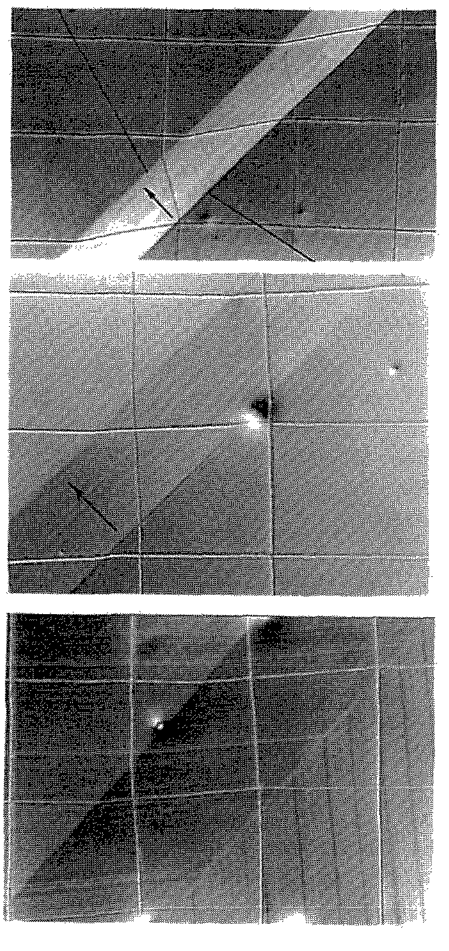

Figure 8 Observation of coupled GBS-GBM in (a) $(1\bar{2}11)$, (b) $(1\bar{2}16)$, and (c) $(10\bar{1}2)$ coincidence boundaries in zinc

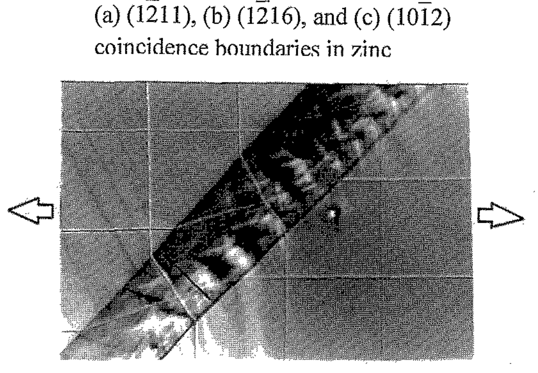

Figure 9 Coupled GBS-GBM of the $\Sigma 9$ (221) coincidence boundary in aluminum

4.2 Analogical extension to coincidence boundary in fcc metals

Figure 9 shows the coupled GBS-GBM on the $\Sigma 9$ (221) coincidence boundary in aluminum; this boundary has atomic configuration that is quite similar to the zinc $(1\bar{2}11)$ coincidence boundary. This behavior was also in good agreement with the DSC dislocation modeling.

4.3 Extension of the GBD modeling for GBS

The present study has mainly concentrated on experimental observation of a characteristic behavior of coupled GBS-GBM on (a) $(1\bar{2}11)$, (b) $(1\bar{2}16)$, and (c) $(10\bar{1}2)$ coincidence boundaries in zinc . There are many aspects of grain boundary sliding that remain not clarified. It is necessary to extend the applicability of the DSC dislocation modeling and to define the limitation of the model. Subjects to be investigated include the problems as follows.

1) effect of deviation from the exact CSL orientation
2) effect of boundary inclination into asymmetry
3) possibility in generalization of the model
4) analogy to twin growth
5) kinetics of grain boundary sliding rate
6) multiplication of GBDs in grain boundaries
7) characterization of necessary shuffling of atoms
8) stress reversal effect on boundary sliding rate, etc.

Some experimental effort was made to extend the applicability of the DSC dislocation model, but the details of that can not be contained in this paper.

5. CONCLUSION

Experimental evidence was obtained supporting the GBD Modeling of grain boundary sliding in some selected coincidence boundaries of zinc. The M / S ratio and the migration direction were just as predicted by the DSC dislocation theory based on the geometrical framework of CSL. Coupled GBS-GBM of coincidence boundaries are similar to the growth of twins in the plane normal direction. The nucleation of CSL boundary might be much more difficult than the ordinary deformation twins.

REFERENCES

[1] H. Fukutomi and R. Horiuchi: Transactions of the Japan Institute of Metals, 22 (1981), 633.
[2] R. C. Pond, D. A. Smith and P.W. J Southerden: Philosophical Magazine, A37 (1978), 27.
[3] D. A. Smith: "Dislocation Modeling of Physical Systems", Proceedings of the Acta-Scripta Metallurgica International Conference, Pergamon Press (1981), p569.
[4] R.W. Balluffi: Metallurgical Transactions, 13A (1982), 2069.
[5] W. Bollmann: "Crystal Defects and Crystalline Interfaces", Springer Verlag, (1970).

(Recieved September 8, 2007 ; Accepted December 30, 2007)