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Systematic Study of Al [001] Symmetric Tilt Grain Boundaries by First Principles Calculation

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Recently, severe plastic deformation such as Accumulative Roll Bonding [1], Equal Channel Angular Extrusion or High Pressure Torsion [2] have enabled to fabricate ultra-fine grained (UFG) materials which have fine microstructure where the average grain size is less than 1 μm. For example, it is reported that mechanical properties of UFG samples deviates from Hall-Petch law. The mechanism of grain refinement has been explained in terms of the so-called grain subdivision. It should be noted that the division of grains can be also regarded as introduction of a grain boundary (GB). Experimental studies using HREM and EBSD techniques have revealed that the of the grain subdivision resulted in the increase of GB number density as well as the increase of misorientation between adjoining two grains. However, it is still unclear which of these phenomena occurred first inducing the other phenomenon. In addition, in experimental approach, we can only observe the microstructure in the unit of working cycle and the observation is limited to two dimensions: Our knowledge as to what is happening to the sample during a cycle in three dimensional matter is limited, thus far. These difficulties impede further control of unique properties of UFG materials. Therefore, in order to reveal the detailed mechanism of the grain subdivision, the investigation for GB formation process is needed. Thus, by using atomistic simulation technique, various kinds of GBs generated from grain refinement have to be evaluated quantitatively and systematically.

In the present study, we have studied Al [001] symmetric tilt grain boundary, which has relatively simple structure and smaller periodicity along an axis parallel to GB plane makes it possible to deal with lower tilt angle GB with limited computational resources. GB formation process mainly consists of the movement, accumulation and alignment of dislocations. In the present study, three GB models, Glide model, Mirror model, CSL model, were employed. Figure 1 shows the three models with misorientation of 28.1 deg. In Glide model, dislocations are aligned along GB planes in alternative manner. CSL model has kite-like structural unit on GB planes, which are often observed by HREM [3]. The Mirror model was intermediate between Glide and CSL model and dislocations were placed in mirror symmetry configuration. Using these three models, we have systematically studied GBs with various misorientations.
The cell size, or the distance between GBs, was determined as 15 Å, such that the supercell contains sufficiently large grain interior region. Plane wave cutoff energy, the number of k-points, and FFT mesh size were determined so that total energy was converged within a several meV per atom.

For energetical evaluation, GB energy was calculated from total energy, which is obtained from first principle calculations, by

$$\gamma = \frac{E_{GB} - E_{perfect}}{2A}$$

where γ is GB energy, and E_{GB} or E_{perfect} are total energies of supercells with or without GB, respectively, after full relaxation of atomic configuration. A is the area of GB plane. Since three dimensional periodic boundary conditions are imposed for models, each GB models have 2 GBs so that the total energy was divided by $2A$.

By comparing GB energies of each models, Mirror model exhibited approximately twice as high GB energy as the other two models while GB energy of Glide model was very close to that of CSL model. Figure 2 compares the relaxed structures of Glide and CSL models with misorientation of 28.1 deg. As shown in the figure, both structures have kite structural units in atomic configuration and look very similar to each other. Similar trend is found for other misorientations. In general, low angle tilt GB, in which dislocations are relatively easily accommodated or released, is depicted by Glide model. On the other hand, high angle tilt GB, where dislocations have already rearranged and are difficult to decompose into individual dislocations, is depicted by CSL model. However, present study showed that these distinct models exhibited almost the same relaxed structures, which explains the fact that GB energies of both models were very close. Upon relaxation of the structure in first principles calculations, it searches for local energy minimum and cannot overcome energy barrier if present. The above fact, therefore, indicates that there is no noticeable energy barrier between Glide and CSL models and one transforms into the other by slight rotation and translation. For further investigation for GB structure, we focused on the distribution of inter-atomic distance in the vicinity of GB. We evaluated the correlation between GB energy and variance of inter-atomic distance of atoms within 10 Å from GB plane. If atomic interactions in the present models followed the theory of elasticity and bond length distribution is uniform over the GB region, there must be a proportional correlation. However, the present result showed far from the proportional correlation, which indicate that the theory of elasticity is no longer valid in these case and bond length distribution varies from place to place.

By systematic and quantitative evaluation for various GB models, it is found that Glide and CSL models were very close to each other in structural and energetical points of view. In addition, GBs where distance between dislocations is as short as dislocation core radius no longer follow the theory of elasticity. Further studies including stress field analysis in the vicinity of GB is needed for clarification of the GB formation through accumulation of dislocations, which leads to the understanding for the detailed mechanism of Grain Subdivision.

References
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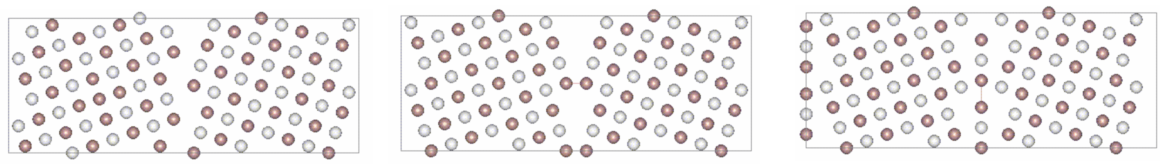
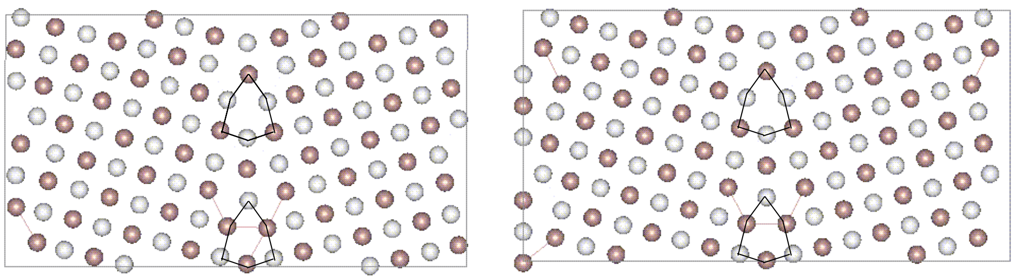


(a) Glide (b) Mirror (c) CSL

Fig. 1 Three GB models of [001] symmetric tilt GB with misorientation of 28.1 deg. before structural relaxation: (a) Glide model, (b)Mirror model, and (c) CSL model.



(a) Glide Model (b) CSL Model

Fig. 2 (a) Glide and (b) CSL models of [001] symmetric tilt GB with misorientation of 28.1 deg.