Energy of small angle tilt boundary in Al

Shigeto R. Nishitani

Department of Informatics, Kwansei Gakuin Univ.

Abstract

The critical inconsistency on the small angle boundary energy between the theoretical prediction of Read-Shockley model and the experimental results was discussed. The plots of the ratio between boundary energy E and the tilt angle θ against $\log\theta$ show different tendency between the EAM simulated and the experimental results. The first principles calculations on the small angle tilt boundary energy on Al $\langle 100\rangle$ direction were performed. Still the calculation sizes of the model are limited, the obtained values are located between the EAM simulated and the experimetal results.

1 Introduction

Small angle boundary energy is easily predicted by Read–Shockley model[1], which is a typical example of the reliability of the dislocation theory. The angle θ dependency of the small angle boundary energy E is given by,

$$E = \frac{1}{2}\tau_0 b\theta(A - \log\theta)\,, \tag{1}$$

where b is the size of Burger's vector, and τ_0 is determined by the mechanical properties of the target material, and A is related to the core energy of dislocation and is expected constant.

The left panel of Fig.1 shows the experimental [2], and calculated[3] θ dependency of symmetric tilt grain boundary energy of Al $\langle 100\rangle$ direction. The calculated curve shows the different angles of the tangents at both ends of $\theta \sim 0^\circ$ and $\sim 90^\circ$ due to the size difference of Burger's vectors, which are illustrated inside the plot. Those are so called geometrically necessary dislocations, whose sizes are a and $a/\sqrt{2}$, respectively, where a is the lattice constant. The experimental curve, however, shows an identical angle. Two

figures on the right panel are $E/\theta - \log\theta$ plots, which are derived by a slight modification of the previous equation,

$$\frac{E}{\theta} = \frac{1}{2}\tau_0 b(A - \log\theta)\,, \tag{2}$$

which tells that the ratio E/θ is linear to $\log\theta$. When we plot it, this linear dependency of the curves is observed even in the middle range of the angle as shown in Fig.1. Noticing that taking the logarithm of θ, the middle angles appear near zero, and both low angle ends locate at the negatively large region. The calculated result shows that the slope of the curve at near 90° is obviously smaller than that at near 0°, as expected from Burger's vectors of Read-Shockley model. On the other hand, the experimental results show almost identical slope, which inidicates obvious inconsistency against the calculated results or theoretical prediction.

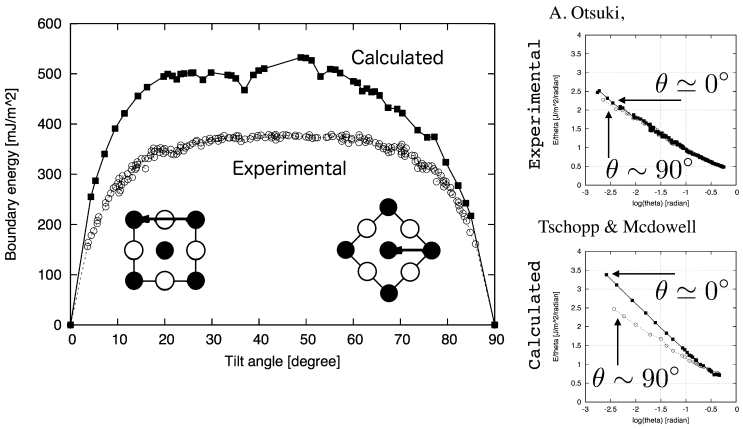

Figure 1: Experimental and calculated θ dependency of symmetric tilt grain boundary energy of Al. See text for details.

One expected reason of this inconsistency is that the calculated result was obtained using an empirical potentials of the embedding atom method. For getting more reliable calculated results, we have performed the first principles calculations of the symmetrical tilt boundary of Al.

2 Method

We used VASP (Vienna ab initio simulation package)[4] for the first principles calculations. We used PAW[5] and GGA[6] for the pseudo potentials.

Energy cut off for the plane wave was set 300 eV. k-points were automatically generated by VASP, because the cell sizes are depending on the anlges of the boundary. The length parameter for this automatic determination was set to be 50 due to no d electron for Al. The unit cells of grain boundary model were constructed for the anlges of $\theta = \arctan(1/n) \times 2$ for 0° side, and $90^\circ - \arctan(1/n) \times 2$ for 90° side, where $n = 3$, 5, 7 and 9. An example of the top view of the boundary model is shown in Fig.2 (a) for $\theta = 12.26^\circ, n = 7$. The rectangle drawn by the dotted line indicates the unit cell, and two grain boundaries are located at the center and the ends of the cell for keeping the periodic boundary condition. The depth (z-direction) of the unit cell is two layers, which are indicated by open and closed marks. This model includes 186 atoms of Al, and the atoms located near boundaries are deleted due to small interatomic distances for the init model. The atomic relaxations were performed by the automatic relaxation packaged in VASP. The outer dimensions of the cell are manually changed in order to avoid unintentional shape changes of the rectangle, and the minimum energies were determined by the energy surface fitting.

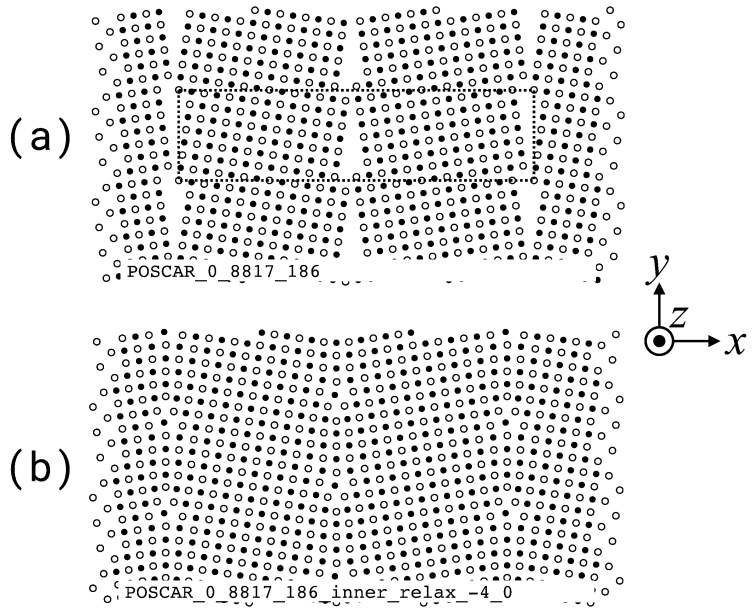

Figure 2: Top views of the boundary model for the misorientation angle of 12.26°, (a) before and (b) after relaxations.

3 Results

Fig.2 (b) shows an example of the relaxed atomic configuration. By the atomic relaxation, the atoms near boundaries move so as to fill the empty space of boundaries. The outer dimensions of the unit cell are estimated by the energy surface fitting of data. As shown in Fig.3 for this case, it gave the minimum energy of 440 mJ/m^2 at x = -5.26%, y = 0.36%, which is marked by a large ball near center of the surface.

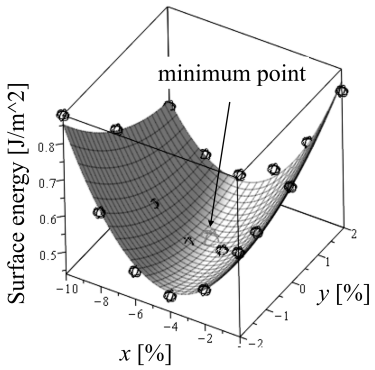

Figure 3: Energy surface of unit cell dimension changes.

Fig.4 shows the size dependency of boundary energy for each tilt angle. Roughly speaking, the larger the sizes of unit cell are, the lower the energies are. The saturated behavior, which is expected for usual size dependency of these models, however, is not appeared in the size ranges calculated in this study. Larger size models are necessary for getting the most stable energy.

Results obtained so far by the first principles (FP) calculations are shown with the experimental and previously reported EAM results on the left hand panel of Fig.5. Because we performed the calculations on multiple unit cells with small to large sizes for a specific tilt angle, multiple values are marked on a specific angle. The lines are connected along the minimum energies on tilt angles. These minimum values are located between experimental and EAM calculated values. The $E/\theta - \log\theta$ plot is shown in the right hand panel of Fig.5. Although two lines of $\theta \sim 0^\circ$ and $\sim 90^\circ$ are still separated, the split of two lines are not so clear comparing with the EAM results as shown on the right-bottom of Fig.1.

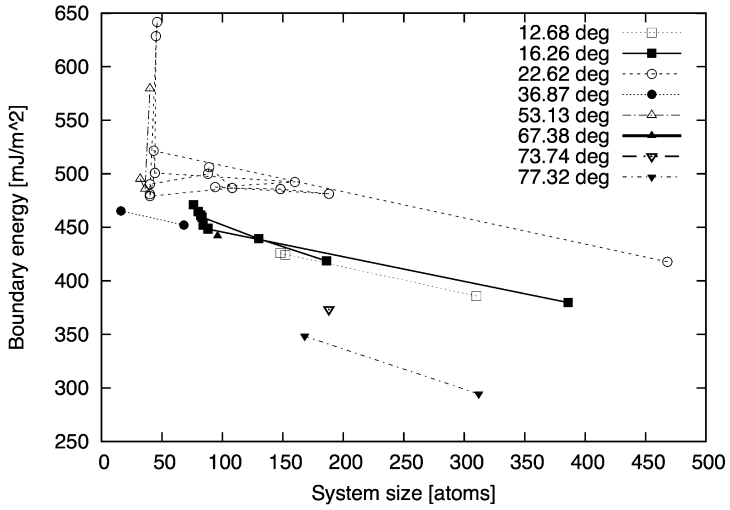

Figure 4: Size dependency of boundary energy for each tilt angle.

4 Summary

We have performed the first principles calculations on the tilt angle dependency of boundary energy of Al $\langle 100 \rangle$ direction. The calculated minimum energy of a specific angle is located between EAM calculations and experimental results. The inconsistency between the theoretical prediction and experiments on the small angle boundary enery has not yet been clarified by our calculations. The theoretical prediction of the linear relation between E/θ and $\log \theta$ is confirmed, but the slopes of two sides of $\theta \sim 0^\circ$ and $\sim 90^\circ$ are not clearly judged. The split of two lines obtained by our calculations is not so clear comparing with that of EAM calculations.

References

[1] W. T. Read and W. Shockley, "Dislocation models of crystal grain boundaries," *Phys. Rev.*, vol. 78, pp. 275–89, 1950.

[2] O. Akira, "Energies of [001] small angle grain boundaries in aluminum," *J. of Mater. Sci.*, vol. 40, pp. 3219–23, 2005.

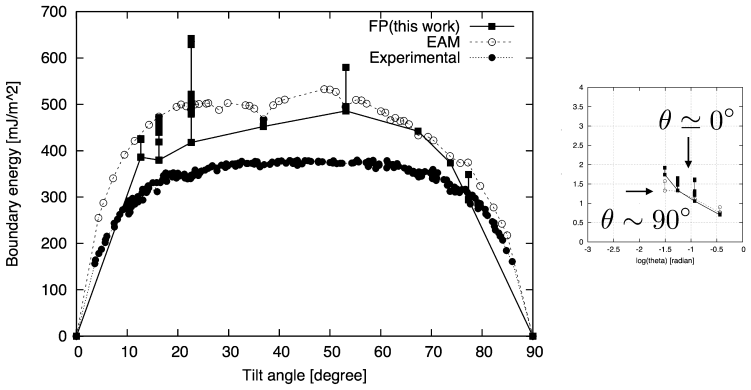

Figure 5: Tilt angle dependency of the boundary energy on Al ⟨100⟩ direction obtained by the first principles calculations. Experimental and EAM calculated results are also plotted. The right hand panel shows the $E/\theta - \log\theta$ plot. See text for details.

[3] M. A. Tschopp and D. L. Mcdowell, "Asymmetric tilt grain boundary structure and energy in copper and aluminium," *Phil. Mag.*, vol. 87, pp. 3871–92, 2007.

[4] G. Kresse and J. Hafner, "Ab initio molecular dynamics for liquid metals," *Phys. Rev. B*, vol. 47, pp. 558–61, 1993.

[5] G. Kresse and D. Joubert, "From ultrasoft pseudopotentials to the projector augmented-wave method," *Phys. Rev. B*, vol. 59, pp. 1758–75, 1999.

[6] J. P. Perdew and Y. Wang, "Accurate and simple analytic representation of the electron-gas correlation energy," *Phys. Rev. B*, vol. 45, pp. 13244–9, 1992.