Symmetric tilt boundary energy of Cu

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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,

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

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 bottom panel of Fig.1 shows the experimental[2], and calculated θ dependency of symmetric tilt grain boundary energy of Cu <100> direction. The calculated curve using EAM[3] shows the different angles of the tangents at both ends of θ~0° and ~90° 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. Figures on the top side panel are E/θ-log θ plots, which are derived from the previous equation

$$E/\theta = 1/2\ \tau_0\ b(A - \log\theta),$$

which tells that the ratio E/θ is linear to log θ. 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. The EAM 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 indicates obvious inconsistency against the calculated results or theoretical prediction.

For revealing this discrepancy, we are performing the first principles calculation.

2 Method

We used VASP(Vienna ab initio simulation package) for the first principles calculation[4]. The boundary models are constructed for Σ 3, 5, and 7 near 0° and 90° for Cu (100) symmetric tilt boundary. The ionic relaxations are performed by the routine provided in VASP under the hand-controlled outer shapes.

The pseudopotential for Cu is PAW PBE with the energy cutoff of 273.214 eV, which is the default value of POTCAR. The energy are obtained by tetrahedron method with Blöchl corrections. The energy convergences are checked by mainly k-point meshes and system sizes.

3 Results

The preliminary results are also plotted in Fig.1. The calculated time for Cu is much longer than Al, the calculated points are few. The models calculated angles are still high, however, shows similar values with the EAM results. We will report the E/θ-log θ plots with the lower angle results.

References

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Biographical Note

Ms. Yamada is a graduate student of Department of Quantum and Radiation Engineering, Osaka Prefecture University. She is now working on the experimental researches of point defects in glassy materials using positron annihilation method.

Prof. Nishitani is still struggling on VASP calculations.

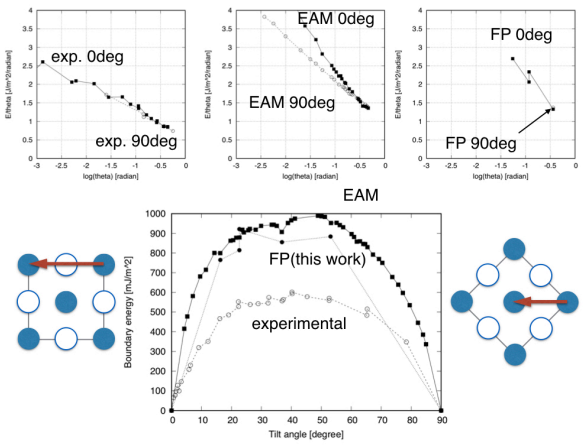

Figure 1. Experimental and calculated θ dependency of symmetric tilt grain boundary energy of Cu. See text for details.