[O14] Finite temperature boundary energy of Al

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We have an inconsistency on the symmetric tilt grain boundary energy of Al <100> boundaries between the experimental results and the first principles calculations. The experiments have been performed by the contact angle measurement between liquid metal and the boundary at thermal equilibrium condition [1]. On the other hand, the first principles calculations show the ground state energy difference between the defect and the perfect lattices. The aim of this research is the bridging this gap of the boundary energy by Einstein model [2].

The Einstein model of solid describes thermal vibrations as a 3D harmonic oscillator. Helmholtz free energy $\boldsymbol{F_i}$ of an atom at site $\boldsymbol{i}$ is expressed by the following equation;

$$F_i = E_i^0 - k_B T \ln Z_i = E_i^0 - k_B T \sum_{j=x,y,z} \ln\left(\frac{\exp(-\hbar\omega_j/2k_BT)}{1-\exp(-\hbar\omega_j/k_BT)}\right)$$

where, $\boldsymbol{E_i^0}$ are the on-site ground state energies, and $\boldsymbol{\varpi_j}$ are the vibration frequencies obtained by the spring constants of *x, y* and *z* directions. The $\hbar$ and $\boldsymbol{k_B}$ are Planck and Boltzmann constants. The spring constants were obtained by the energy calculations of VASP, after applying small deviations from the stable sites.

The symmetric tilt and twist boundary models of Al <100> are shown in Fig. 1. The grain boundaries are located at the middle and both ends for the periodic boundary condition. As shown in Fig. 2, the temperature dependency of the tilt boundary with the smaller angle (22.62deg) shows slightly different from the others. This finite temperature effect contributes the angle dependency of the tilt boundary and shows consistent results with the experiments.

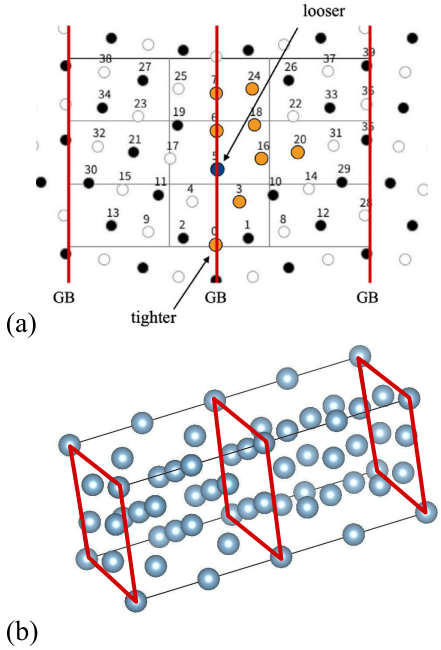

Figure 1. Atomistic models for (a) tilt and (b) twist boundaries.

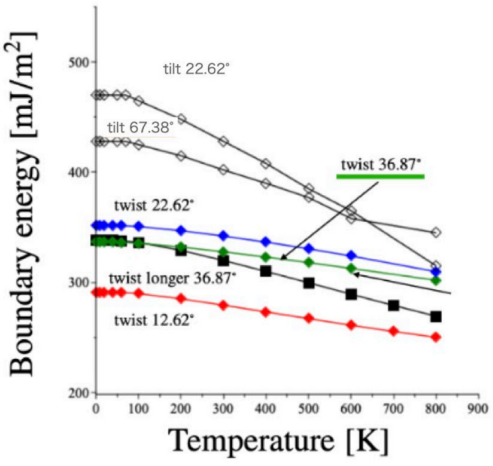

Figure 2. Temperature dependency of boundary energy of Al.

References

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Biographical Note

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He graduated from Dept. Materials, Kyoto Univ. Since 2004, he has been working in Dept. Informatics of Kwansei Gakuin Univ. His major is the Computational Materials Science and has studied the precipitation of Fe-Cu, metastable solvent epitaxy of SiC, and the formation of Mg- LPSO. He also contributes on Ruby gems.