# Shift and delete effect on aluminum twist grain boundary energy

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A widely accepted model for low-angle grain boundary is the Read-Shockley dislocation model [1]. For understanding high-angle grain boundaries, however, there is no unified model. The high degree of freedom in high-angle grain boundaries, in-plane translations and atom deletion at the grain boundary, makes it computationally expensive to explore the entire configuration space. In this study, we employed first-principles calculations to investigate these effects on low sigma symmetric twist boundaries in aluminum.

We employed both VASP and QMAS [2] for first-principles calculations. While VASP is widely used in materials science, QMAS has a routine implemented to calculate the individual atomic energies. To select high-energy atoms for deletion, we compared an empirical potential of EAM (embedded atom method) and QMAS. Although EAM involves arbitrariness due to the parametrized interactions, QMAS provides a theoretically predicted energy based on electronic theory. The results showed that while the absolute values differed, the order of energies was consistent. The energy of the (011) Σ3 model, which was applied the deletion process following this procedure, reproduced the experimentally obtained results [3]. The structure and the energy of this orientation can be interpreted as having collapsed from an ideal structure with energy extrapolated from the low-angle region of the Read-Shockley plot. As schematically drawn on Fig.1, while conventional high-angle models involve adding extra energy to a low-energy state, the collapse model suggests that the experimentally observed energy is obtained by relaxation from a higher-energy state.

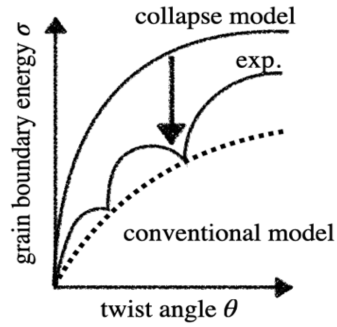


Fig. 1 Schematic comparison between conventional and collapse models.

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*References:*

[1] W. Shockley and W. T. Read, *Phys. Rev.,* **75** (1949), p. 692.
[2] S. Ishibashi, T. Tamura, S. Tanaka, M. Kohyama, and K. Terakura, Phys. Rev. B **76** (2007), 153310
[3] A. Otsuki, *Research on boundary energy of Al*, Ph.D. diss., (Kyoto Univ. 1990), pp.99-120.