Molecular static simulations for small angle tilt grain boundaries

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Read and Shockley derived the equation of the energy for the small angle tilt grain boundary, where the edge dislocations are located periodically[1]. The expressions are the following:

$$\left. \begin{aligned} E &= E_0\theta(A - \log\theta) \\ E_0 &= \frac{\mu b}{4\pi(1-\nu)} \end{aligned} \right\} \quad (1)$$

where A is the energy term from the higher order elastic and dislocation core contributions, μ and ν are shear modulus and Poisson ration, b is the magnitude of Burgers vector, and θ is the tilt angle of crystals.

Hasson *et al*. have simulated Al[100] symmetric tilt grain boundary using Morse potential and showed the results as in Fig.1 [2]. The tangent angles of the energy curve near 0 deg and 90 deg show different. This difference is interpreted from the magnitudes of the Burgers vectors of a[001] for 90 deg and $a/2$[011] for 0 deg. Otsuki, however, has reported the experimental results of the force balance measurement at the triple junction of grain boundaries for Al bi-crystals, as shown in Fig.2 [3]. The result shows that the tangnet angles for 0 deg and 90 deg are identical. For revealing this inconsistence, we are retrying the molecular static simulations for the small angle grain boundaries.

In this research, we use the interatomic potentials of Lennard-Jones type and EAM type. Static relaxations are performed for relatively large systems for describing small angle grain boundaries. The logarithmic plots of the grain boundary energies show different behavior for the potentials. Lennard-Jones potential shows the different tangent angles for the energy curve, where EAM potential shows identical. We are investigating the reason of this discrepancy in detail.

[1] W.T.Read and W.Shockley, "Imperfections in Nearly Perfect Crystals", ed by W.Shockley, (Wiley, New York, 1952), pp.352-376.
[2] G.C.Hasson, J.B.Guillot and B.Barou,Phys. Stat. Sol.(a), 2(1970),551.
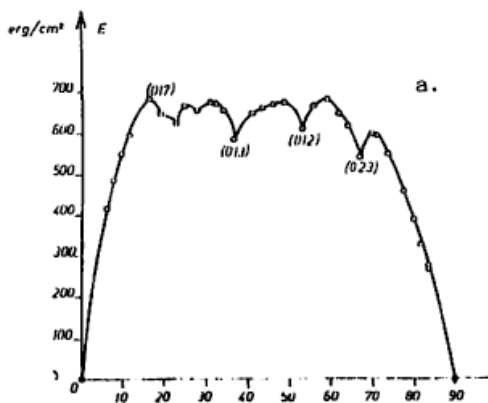[3] A.Otsuki, J.Material Science, 40(2005), 3219.

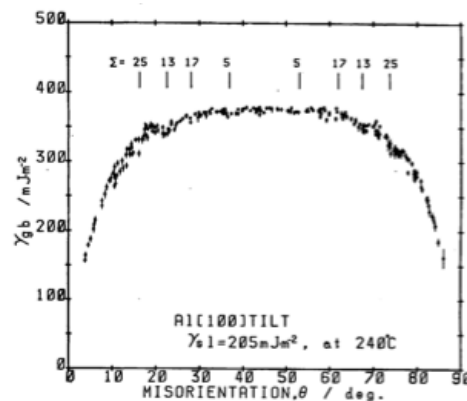Fig.1 Angle dependence of grain boundary energy simulated with Morse potential by Hasson *et al*.

Fig.2 Experimental results obtained by Otsuki.