Interface energy at limit radius in metallic system

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At the previous Calphad meeting held at Awaji, Prof. Kaptay gave a stimulating talk on the interface energy[1,2]. At the very beginning of his talk, I felt an unstability. After a while, I noticed that the contradiction is rooted in the different point of views on the interface energies. His is continuum, but mine is discrete. On this talk, I will show you the reason of the strangeness by discussing extreme behaviors of interface energies at the two limits of the radius, $r \to 0$ and ∞.

The starting point is the parabolic radius dependency of interface energy, where ∞ at $r \to 0$, and 0 at $r \to \infty$. In the discrete atomic systems, those are slightly different.

At first, we will see the limit as $r \to 0$. As the similarity with the other physics treatments, we have to avoid the infinity divergence. In case of the heterogeneous metallic alloy system, the typical interface are observed in the particles precipitated in matrix. When we change the number of the atoms in precipitate clusters, we can calculate the size dependency of the interface energy. The limit of the small size should be not zero but one, which means that the dilution limit is the answer for the maximum limit of interface energy in the precipitation process.

The second limit we will see is at $r \to \infty$. For this case, we will explore in the homogeneous system, where the energy of small angle symmetrical tilt interface is the target. Although the energy approaches to zero, the problem is on the angle dependency of it.

The classical theory of the small angle tilt boundary energy was derived by Read and Shockley[3], and is described by the equi-spaced dislocations aligning on the interface. The important derivation of this theory is that the tangents of (100) tilt boundary near 0 and 90 degrees are different due to the difference of Burger's vectors, as shown in Fig.2. This is confirmed by the computer simulations with the interatomic potentials[4].

The experimental results, however, show different tendency, where the tangent lines at 0 and 90 degree limits show the same slope[5]. We will report the first principles calculation results and discuss where this inconsistency comes from.

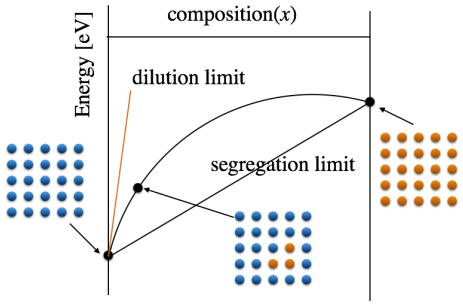

Figure 1: Schematic illustration between dilution limit and interface energy at small radius limit.

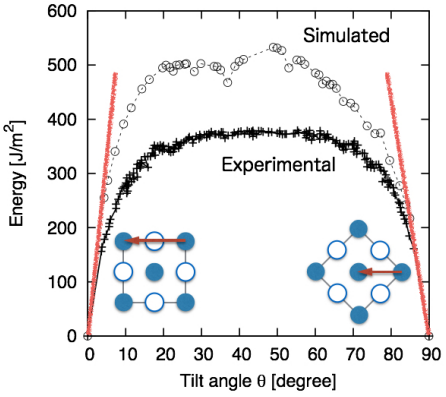

Figure 2: Simulated and experimental angular dependence of tilt boundary of Al (100) direction and related Burger's vectors. Experimental results are taken from [4] and simulated results calculated by EAM potential are taken from [5].

References

[1] G. Kaptay, Calphad XLV, (2016), p.65.

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[4] A. Otuki, J. Material Science, **40** (2005), 3219.

[5] M. A. Tschopp and D. L. Mcdowell, Phil. Mag., **87** (2007), 3871.