Interface energy at the 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]. At the very beginning of his talk, I felt an unstability. After a while, I noticed that the discomfort 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 behaviours of interface energies at the two limits of the radius, r =0 and ∞.

The starting point is the parabolic dependency of interface energy on radius, where ∞ at r =0, and 0 at r =∞. In the discrete atomistic systems, those are different. At first, we will see the limit of r =0. As the similarity with the other physics problems, we have to avoid the infinity divergence. In case of the heterogeneous metallic alloy system, the typical interface is 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 metallic systems.

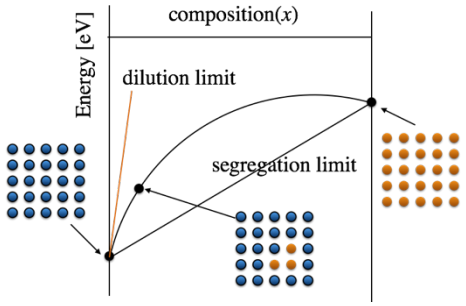

Fig.1 Schematic illustration between dilution limit and interface energy at small radius limit.

For the other limit of r =∞ , we will explore in the homogeneous system, the energy of small angle symmetrical tilt interface. Although the energy approaches to zero, the problem is the angle dependencies of it. The classical theory of the small angle tilt boundary energy was derived by Read and Shockley, 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. This is confirmed by the computer simulations with the interatomic potentials, but the experimental results show different tendency, where the tangent lines at 0 and 90 degree limits show the same slope[5]. We will report the first principles results and discuss where this inconsistency comes from.

[1] G. Kaptay, Calphad XLV, (2016), p.65, J. Nanoscience Nanotechnology, 12(2012), 2625.

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