[P66] Finite temperature first principles calculations on Mg added Al boundary energy

Y. Yuri, S. R. Nishitani and K. Horikawa

[1] Prog. of Computer Science, Kwansei Gakuin Univ., Sanda, 669-1330, Japan

e-mail address of corresponding author: get58857@kwansei.ac.jp

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Duralumin is the one of the widely used structural alloys, and is obtained by the age-hardening proceeded at the high temperatures. The grain-boundary segregation also occurs at the same time, and is thought to cause the embrittlement [1]. The total system energies is different with the added atom locating at the grain-boundary or inside the grain. This is the first step of the grain-boundary segregation. We have examined the energy differences of the Mg addition around the Al grain-boundary by the finite temperature first-principle calculations[2].

We have used the Einstein model for the harmonic oscillation approximation, and VASP for the first principles calculations. The finite temperature free energies of the system were calculated on the atomistic model of the Al <100> tilt boundary with the angle θ = 22.6° as shown in Fig. 1. For the z-axis, two layers are stacked, thus the atoms are one Mg and 79 Al. The boundaries are located at the center (site no: 0-5-6-7) and both ends (28-35-36-39) of the model. The free energy was calculated after the Mg atom was substituted on each site, with the approximation of the isotropic thermal expansion.

Since the site-20 is located at the center of the grain, which should be a good reference value, the total system energy of each site substituted model is measured from the energy of this site model. The 0K and 500K energies of each substitutional model are shown in Fig. 2. At the grain boundary, there are characteristic sites of number 0 and 5, we call them the looser and tighter sites respectively. The substitutional energy of the (tighter) site 0 at 0K shows +0.4 eV, and this site energy at 500K shows the identical value of +0.4 eV. On the other hand, the (looser) site 5 at 0K shows -0.44eV, but this site energy at 500K shows slightly small -0.36eV. The other site energies are scattered between them. The tighter site and looser site show positive and negative energies respectively, which are consistent with the atomic radius difference between Mg and Al, $(r_{\mathrm{Mg}} > r_{\mathrm{Al}})$. The boundary segregation is mainly controlled by this looser site, which is the center of the pentagonal bi-pyramid of the dislocation core.

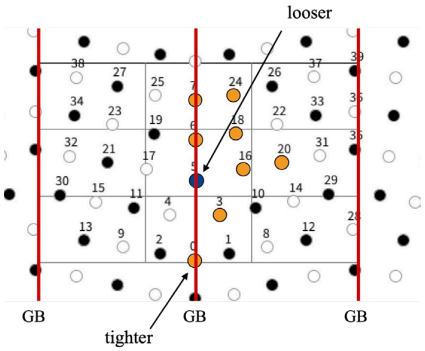

Figure 1. Al ⟨100⟩ tilt boundary model with the tilt angle θ = 22.6°.

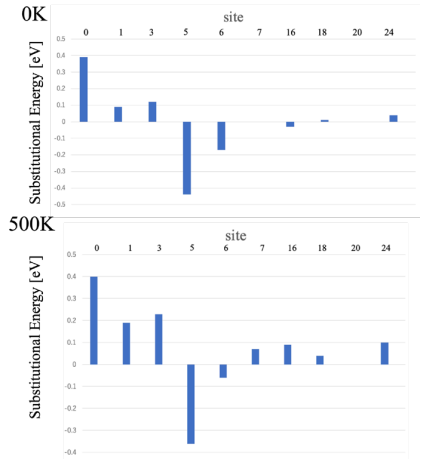

Figure 2. Substitutional energy of each site measured from the in-grain site 20 model at 0 and 500K.

References

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Yoshimasa Yuri

He is a graduate student of Department of Informatics, Kwansei Gakuin Univ. He is studying the Al grain-boundary, revealing from an energetic point of view with VASP. He also possesses practical skills on Ruby programming and CLI application by Thor.