Proceedings of the 12th International Conference on
Aluminium Alloys, September 5-9, 2010, Yokohama, Japan

pp. 1421-1425

Modeling Solid Solution Strengthening Using First-Principles Results of Misfit Strain with Friedel Model in Al-Based Alloys

Tokuteru Uesugi[1] and Kenji Higashi[1]
[1]Department of Materials Science, Graduate School of Engineering, Osaka Prefecture University,
1-1 Gakuen-cho, Naka-ku, Sakai, Osaka, 599-8531, Japan

The solid solution strengthening is an important strengthening way as well as the work hardening, precipitation hardening and grain refinement in aluminum alloys. In this work, we modeled the solid solution strengthening in aluminum-based binary alloys using Cottrell's procedure concerning the interaction between a solute atom and a dislocation and Friedel's equation. Then contributions to the yield strength due to the solid solution strengthening were estimated from the calculated values of the misfit strain. The misfit strains of Si, Zn, Sn and Pb in the Al-based binary alloys were calculated from the first principles. The size mismatch between the solute and solvent atom gives rise to a distortion of the surrounding lattice, which is called the misfit strain. The calculated values of amounts of solid solution strengthening were in good agreements with the available experimental values in Al-Zn alloys. This agreement provides confidence in the current computational approach. If the supersaturated solid solution could be formed during the non-equilibrium processing such as a melt-spinning process, new additional elements of Pb would be effective for the purpose of the solid solution strengthening.

Keywords: First-principles calculation, *Ab-initio* calculation, Solid solution strengthening, Misfit Strain

1. Introduction

Aluminum alloys are important materials due to their high technological value and their wide application such as the aerospace field, motorized vehicles and domestic industry. The solid solution strengthening (hardening) is an important strengthening way as well as the work hardening, dispersion/precipitation hardening and grain refinement in aluminum alloys. The additional elements for the purpose of the solid solution strengthening are Mg and Mn in commercial aluminum alloys. The yield strength depends on the effect of the work hardening and solid solution strengthening in non-heat-treatable aluminum alloys which include the 1xxx (pure Al), 3xxx, (Al-Mn) and 5xxx (Al-Mg) series alloys. The effect of Cu [1], Mg [2, 3], Zn [4], and for the solid solution strengthening in aluminum alloys has been well investigated. However, it is interesting to establish the presence or absence of other elements that is more effective for the solid solution strengthening than Mg and Mn. Our final goal is to predict the yield strength of the aluminum alloys strengthened by the solid solution hardening and design the composition of the new aluminum alloys.

The size mismatch between the solute and solvent atom gives rise to a distortion of the surrounding lattice, which is called the misfit strain. We have investigated the misfit strain of Fe solute atom in aluminum [5]. In this work, the misfit strains of Si, Zn, Sn and Pb solutes in aluminum were calculated from the first principles. We modeled the solid solution strengthening in aluminum-based binary alloys using Cottrell's procedure concerning the interaction between a solute atom and a dislocation and Friedel's equation. Then contributions to the yield strength due to the solid solution strengthening were estimated from the calculated values of the misfit strain in Al-based alloys.

2. Calculation procedure

The calculations of the misfit strain was performed using the Cambridge Serial Total-Energy Package (CASTEP) [6]. CASTEP is an *ab initio* pseudopotential method code for the solution of the electronic ground state of periodic systems with the wave functions expanded in plane-wave basis using a technique based on the density functional theory (DFT) [7, 8]. The electronic exchange-correlation energy is given by the generalized gradient approximation (GGA) (PW91) of Perdew *et al*. [9] in the DFT. Troullier-Martins pseudopotentials [10] was used for Al. Ultra-soft pseudopotentials [11] were used for the other elements. A Gaussian smearing [12] of 0.1 eV is applied to the occupation numbers. The cut-off energy of 350 eV for plane-wave basis was used.

For studying the misfit strain in the Al-based solid solution, a supercell containing 125 atoms as shown in Fig. 1, which is periodic in all three directions, was employed. The supercell contains a substituted solute atom per cell and corresponds to 0.8 at% dilute solid solution. The energy integration over a Brillouin zone was made with *k*-point grids according to the Monkhorst-Pack [13] sets of 2x2x2 *k*-points. The stable atomic configurations are obtained through relaxation according to the Hellmann-Feynman forces. The lattice constants at zero pressure were optimized using a Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization algorithm [14]. The misfit strain ε was derived from a fractional distance,

$$\varepsilon = \frac{r(a') - r_o(a')}{r_o(a')}, \tag{1}$$

where r and r_o is the distance between a solute atom and a solvent Al atom at the first nearest neighbor site. The distance r is measured in the cell which lattice constant was optimized to a' at zero pressure and atomic position are also relaxed. The distance r_o was measured in the cell which lattice constants were fixed to a', and atomic positions were fixed to ideal fcc lattice position.

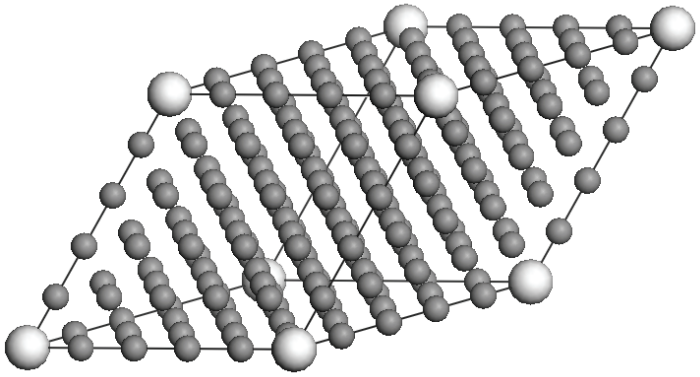

Fig. 1 Depiction of supercell containing 124 Al atoms and one solute atom for the calculations of misfit strains in Al-based solid solutions. Gray balls indicate Al atoms and white balls indicate solute atoms.

3. Results and discussion

The calculated misfit strains of Si, Zn, Sn and Pb solutes in the Al-based binary alloys are summarized in Table 1. The value of Fe solute, which have been calculated previously from first principles [5], is also shown in this table.

According to the dislocation theory, a solute atom interacts with a dislocation. The most important contribution to the interaction between a solute atom and a dislocation is usually that due to the distortion a solute atom produces in the surrounding solvent atoms. In Cottrell's procedure [15, 16] the maximum interaction force F_m between a solute atom and an edge dislocation is

$$F_m = \frac{\sqrt{3}}{2}\mu b^2 \varepsilon \frac{(1+\nu)}{(1-\nu)} \tag{2}$$

where μ is the shear modulus, b is the magnitude of the Burgers vector, ε is the misfit strain, and ν is the Poisson's ratio. In Friedel's theory [17, 18], the increasing critical shear stress $\Delta\tau_s$ for low concentration is

$$\Delta\tau_s = \frac{\sqrt{2}F_m^{3/2}}{b^3}\sqrt{\frac{c}{\mu}} \tag{3}$$

where c is the solute concentration. When F_m in Eq. (2) is substituted to Eq. (3), the increasing yield stress due to the solid solution strengthening in a polycristalline alloy $\Delta\sigma_s$ is obtained using the Taylor factor M as follows

$$\Delta\sigma_s = M\frac{3^{3/4}}{2}\left(\frac{1+\nu}{1-\nu}\right)^{3/2}\mu|\varepsilon|^{3/2}\sqrt{c}\,. \tag{4}$$

Eq. (4) indicates the yield stress increases as the square root of the concentration and the absolute value of misfit strain. In the case of the Al based solid solution, taking M = 3.06, μ = 26.5 GPa [19], ν = 0.347 [19], and the value of the misfit strain calculated from the first principles, Eq. (4) gives the contribution to the yield stress due to the solid solution strengthening.

Table 1 The calculated misfit strain ε and the maximum solubility limit c_{maxs} in the Al-based binary alloys.

Solute	ε (%)	c_{max} (at.%) [20]
Si	-0.61	1.59
Zn	-0.38	66.41
Sn	2.6	0.002
Pb	4.8	0.02
Fe	-3.9 [5]	0.025

Using the values of misfit strain shown in Table 1, the contribution to the yield stress due to the solid solution strengthening was obtained through the Eq. (4). The dependence of the contribution to the yield stress due to the solid solution strengthening as a function of the solute content is shown in Fig. 2. The experimental results in Al-Zn are also shown in this figure [4]. The calculated values of the amounts of solid solution strengthening were in good agreements with the available experimental values in Al-Zn alloys. This agreement provides confidence in our computational approach.

The amount of the solid solution strengthening depends on the absolute value of misfit strain and the solute content following Eq. (4). It is noted that the solute atoms only contribute to the solid solution strengthening. So, not only the misfit strain, but also the solubility limit is the important factor in order to design the aluminum alloys fabricated by the equilibrium processing such as ingot metallurgy. If the supersaturated solid solution could be formed during the non-equilibrium processing such as a melt-spinning process, new additional elements such as Pb and Fe would be effective for the purpose of the solid solution strengthening.

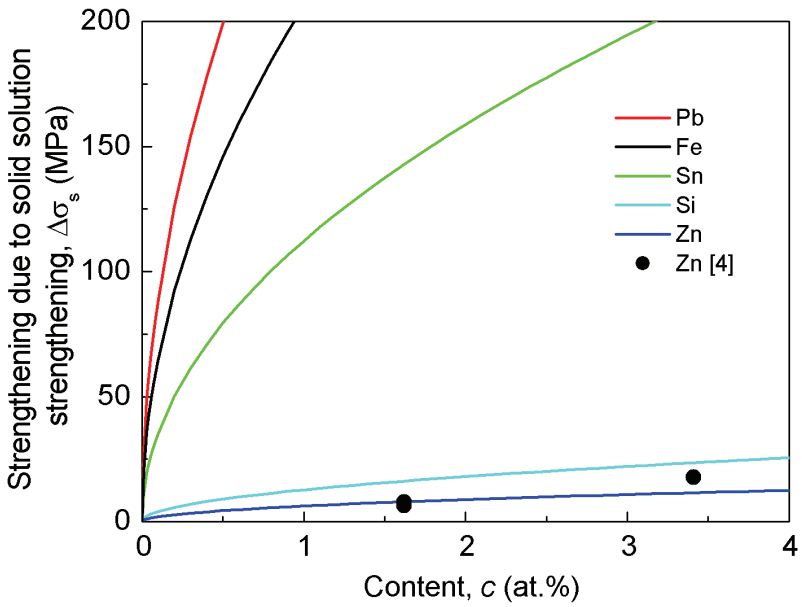

Fig. 2 The dependence of the contribution to the yield stress due to the solid solution strengthening as a function of the solute content in Al-Si, Al-Zn, Al-Sn, Al-Pb and Al-Fe alloys. Filled circles are the experimental results of Al-Zn alloys [4].

4. Summary

From the first-principles calculation, the misfit strain due to Si, Zn, Sn and Pb atom in aluminum was –0.61, -0.38, +2.6 and +4.8 %, respectively. The calculated values of the amounts of solid solution strengthening were in good agreements with the available experimental values in Al-Zn alloy. This agreement provides confidence in our computational approach. If the supersaturated solid solution could be formed during the non-equilibrium processing such as a melt-spinning process, new additional elements of Pb would be effective for the purpose of the solid solution strengthening.

Acknowledgment

This study was supported in part by a Grant-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan on Priority Areas "Giant Straining Process for Advanced Materials Containing Ultra-High Density Lattice Defects". The authors thank to Shimano Corp. and Sumitomo Electric Industries, Ltd. for their financial supports.

References

[1] D. Dew-Hughes and W. D. Robertson: Acta Metall. **8** (1960) 156-167.
[2] H. M. Tensi, P. Dropmann, and H. Z. Borchers: Z. Metallk. **61** (1970) 518-524.

[3] O. Ryen, O. Nijs, E. Sjolander, B. Holmedal, H. E. Ekstrom, and E. Nes: Metall. Mater. Trans. A **37A** (2006) 1999-2006.
[4] J. Dash and M. E. Fine: Acta Metall. **9** (1961) 149-154.
[5] T. Uesugi, Y. Takigawa, and K. Higashi: Mater. Sci. Forum **503-504** (2006) 209-214.
[6] M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias, and J. D. Joannopoulos: Rev. Mod. Phys. **64** (1992) 1045-1097.
[7] P. Hohenberg and W. Kohn: Phys. Rev. **136** (1964) B864-B871.
[8] W. Kohn and L. J. Sham: Phys. Rev. **140** (1965) A1133-A1138.
[9] J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh, and C. Fiolhais: Phys. Rev. B **46** (1992) 6671-6687.
[10] N. Troullier and J. L. Martins: Phys. Rev. B **43** (1991) 1993-2006.
[11] D. Vanderbilt: Phys. Rev. B **41** (1990) 7892-7895.
[12] C. L. Fu and K. M. Ho: Phys. Rev. B **28** (1983) 5480-5486.
[13] H. J. Monkhorst and J. D. Pack: Phys. Rev. B **13** (1976) 5188-5192.
[14] T. H. Fischer and J. Almlof: J. Phys. Chem. **96** (1992) 9768-9774.
[15] A. H. Cottrell: *Strength of Solids* (Phys. Soc., London 1948) p. 30.
[16] D. Hull and D. J. Bacon: *Introduction to dislocations*, fourth edition (Butterworth-Heinemann, Oxford, 2001) p. 202.
[17] J. Friedel: *Dislocations* (Pergamon Press, New York, 1964) p. 205.
[18] D. Hull and D. J. Bacon: *Introduction to dislocations*, fourth edition (Butterworth-Heinemann, Oxford, 2001) p. 220.
[19] J. P. Hirth and J. Lothe: *Theory of Dislocations*, second edition (Wiley, New York, 1982) p. 839.
[20] J. E. Hatch: *Aluminium: Properties and Physical Metallurgy*, (American Society for Metals, Ohio, 1984) p.29.