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Lattice mismatch modeling of aluminum alloys ☆

Dongwon Shin [a,*], Shibayan Roy [a,b], Thomas R. Watkins [a], Amit Shyam [a]

[a] Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
[b] Materials Science Centre, Indian Institute of Technology, IIT Kharagpur, 721302, India

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ABSTRACT

We present a theoretical framework to accurately predict the lattice mismatch between the fcc matrix and precipitates in the multi-component aluminum alloys as a function of temperature and composition. We use a computational thermodynamic approach to model the lattice parameters of the multi-component fcc solid solution and θ'-Al_2Cu precipitate phase. Better agreement between the predicted lattice parameters of fcc aluminum in five commercial alloys (206, 319, 356, A356, and A356 + 0.5Cu) and experimental data from the synchrotron X-ray diffraction (SXD) has been obtained when simulating supersaturated rather than equilibrium solid solutions. We use the thermal expansion coefficient of thermodynamically stable θ-Al_2Cu to describe temperature-dependent lattice parameters of meta-stable θ' and to show good agreement with the SXD data. Both coherent and semi-coherent interface mismatches between the fcc aluminum matrix and θ' in Al-Cu alloys are presented as a function of temperature. Our calculation results show that the concentration of solute atoms, particularly Cu, in the matrix greatly affects the lattice mismatch.

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1. Introduction

The control of the size, dispersion, and shape of precipitates (e.g., γ'-Ni_3Al in Ni alloys and θ'-Al_2Cu in Al alloys) *via* solution treatment and aging, which enhance certain mechanical properties (e.g., high temperature strength), has been a central theme of structural alloy design for decades [1–4]. While the coherency between the parent matrix and precipitate phases governs the morphology of the precipitate during aging of alloys, controlling the lattice coherency solely from an experimental trial-and-error approach in order to achieve desired alloy properties is cost prohibitive. Hence, developing a predictive capability for the lattice parameters of the matrix and precipitate as functions of elemental composition and temperature is of practical importance to alloy design.

The composition-dependent lattice parameters of solid solution phases have often been described with a linear relationship (i.e., Vegard's law [5]) at a given temperature. However, the varied electronic environment that the atoms in the multi-component solid solution experience frequently results in lattice parameters that exhibit non-negligible deviations from Vegards's law. In addition, thermal expansion of the lattice needs to be taken into account to describe the thermal effect on the lattice parameter as well as the compositional effect. Although there have been numerous studies that focused on accurately predicting lattice parameters from theoretical, experimental and empirical approaches [6–8], none of them simultaneously captured chemical and thermal influences on the lattice parameters of the multi-component solid solution phases.

In this regard, the CALPHAD (CALculation of PHAse Diagram) approach [9,10] offers a comprehensive and robust framework to model lattice parameters of complex solid solution phases in metallic alloy systems as a function of composition and temperature. Recently, phase-based properties other than Gibbs free energy have been successfully modeled *via* the CALPHAD approach (e.g., molar volume [11], thermal expansion [12], bulk modulus [12], density [13], and thermal conductivity [14]).

In the present work, we adopt the CALPHAD approach to model the lattice parameters of the aluminum matrix and precipitates in commercial aluminum alloys and to calculate their mismatch for the first time. We model the lattice parameters of the

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* Corresponding author.
E-mail address: shind@ornl.gov (D. Shin).

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multi-component fcc solid solution phase as functions of temperature and composition within the CALPHAD framework, whose model parameters are evaluated with experimental measurements and theoretical calculations. The predicted lattice parameters of commercial aluminum alloys are compared with the synchrotron X-ray diffraction (SXD) data, and calculated lattice mismatches between the aluminum matrix and θ'-Al_2Cu for both coherent and semi-coherent interfaces.

2. Modeling approach

2.1. Commercial aluminum alloys

In the present work, five commercial aluminum alloys (356, A356, A356 + 0.5Cu, 319, and 206) were selected (Table 1) to predict the lattice parameter of fcc aluminum matrices. The solubilities of six important alloying elements (Cu, Si, Mg, Zn, Mn, and Ni) are considered as they exhibit notable solubility in the fcc aluminum matrix as shown in Fig. 1. We exclude Fe and Ti in the present work as they commonly have very little solubility in the fcc aluminum matrix, and their nominal content in all alloys considered is low.

2.2. Lattice parameter modeling

Here, we use the CALPHAD framework to model the lattice parameters of multi-component fcc solid solutions. We start by modeling the lattice parameters of fcc aluminum with six alloying elements to reproduce available experimental and theoretical data. Temperature dependency of pure elements (including hypothetical fcc phases for Si, Mg, Zn, and Mn) has been modeled with polynomials to describe thermal expansion.

The thermal-expansion coefficient (α_L) of metals is often modeled as being linear with temperature, as shown in Eq. (1), where a is the lattice parameter of cubic pure element, and A and B are empirical parameters that can be derived from available information.

$$\alpha_L = \frac{1}{a} \times \frac{da}{dT} = A + BT \tag{1}$$

The lattice parameter of a cubic pure element can be obtained by integrating α_L based on the definition, and the integration constant can be determined using the lattice parameter (a_0) at a given temperature (T_0):

$$a = a_0 \exp\left(A(T - T_0) + \frac{B}{2}\left(T^2 - T_0^2\right)\right) \tag{2}$$

For most metals, the value of α_L is very small ($\sim 10^{-5}$/K). Therefore, the lattice parameter of cubic elements can be further simplified with the following polynomial:

$$a = a_0\left(A(T - T_0) + \frac{B}{2}\left(T^2 - T_0^2\right) + 1\right) \tag{3}$$

Next, we introduce interaction parameters between aluminum and alloying elements to describe non-ideal mixing behavior in the fcc solid solution, which does not follow Vegard's law. The Redlich-Kister polynomials [15], which are generally used to represent a deviation from ideal behavior in solid solutions in the conventional CALPHAD approach, were used to describe the nonlinear deviation in the fcc lattice parameter between aluminum and alloying elements as presented in Eq. (4):

$$a = \sum_i x_i{}^o a_i + {}^{ex}a \tag{4}$$

Table 1
Elemental compositions (in wt%) of commercial aluminum alloys considered in the present work. (Only the major alloying elements are listed.)

Alloy	Al	Si	Cu	Mg	Zn	Fe	Ni	Mn	Ti
356	Bal.	7.21	0.14	0.37	0.17	0.39	0.01	0.25	0.18
A356	Bal.	7.32	0.01	0.40	0.01	0.18	0.00	0.06	0.16
A356 + 0.5Cu	Bal.	7.46	0.44	0.34	0.01	0.14	0.00	0.08	0.16
319	Bal.	8.29	3.17	0.34	0.31	0.68	0.03	0.39	0.17
206	Bal.	0.14	5.18	0.37	0.01	0.15	0.00	0.25	0.02

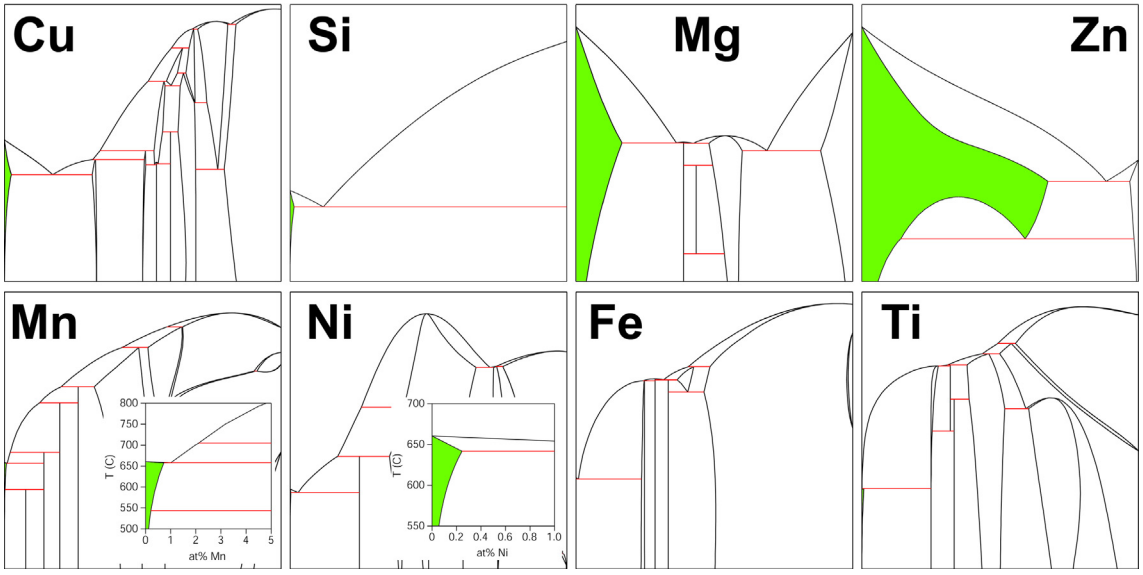

Fig. 1. Aluminum binary phase diagrams with major alloying elements in commercial alloys. Shaded areas represent the fcc solid solution phase in the Al-rich region in each binary.

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