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Assessment of the atomic mobilities for binary Al–Ag fcc alloys

Cuiping Wang, Cuiping Zhuang, Jiajia Han, Xingjun Liu*

Department of Materials Science and Engineering, College of Materials, and Research Center of Materials Design and Applications, Xiamen University, Xiamen 361005, PR China

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ABSTRACT

Diffusion in Al-based alloys is a practical topic that is essential to guide the design of materials. Based on various kinds of experimental diffusivities and thermodynamic parameters, the atomic mobilities in fcc Al–Ag alloys have been assessed as a function of temperature and composition using the DICTRA software package in this work. The calculated results are in good agreement with the experimental data. In addition, the obtained mobility parameters can reasonably predict the concentration profiles for a variety of diffusion couples in fcc Al–Ag alloys.

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1. Introduction

Diffusion plays a very important role in designing and understanding many important phenomena, such as precipitation, homogenization of alloys, recrystallization, grain boundary migration, creep, solidification and protective coatings [1,2]. It is generally accepted that estimating the kinetics of diffusive phase transformation from the rate of volume diffusion of different components is a well-established procedure if this is the rate determining process. Although the experimental method is significant for assessing mobility parameters, there are still many limitations. Recently, computer simulation has become an important and effective tool to gain insight into complex material processes [3–5].

The DICTRA (Diffusion Controlled TRAnsformation) software package is an effective tool, which is an extension of the CALPHAD method and operates under the CALPHAD framework [6–10]. Based on the thermodynamic and mobility parameters, the DICTRA software package can assess the atomic mobilities as a function of temperature and composition. In the past few years, the atomic mobilities for several Al-based binary systems have been investigated using DICTRA. These binary systems include Al–Cu [11], Al–Mg [12], Al–Zn [13], Al–Fe [14], Al–Ni [14], Al–Cr [15], Al–Ti [16], Al–V [16]. However, the atomic mobilities for the fcc phase in the Al–Ag binary system has not been assessed. Thus, the present work is to assess the atomic mobilities in face-centered cubic Al–Ag alloys through the DICTRA software package.

2. Experimental information

Great efforts have been made on the measurements of the diffusion coefficients in the Al–Ag binary system. The experimental data of impurity diffusion coefficients, tracer diffusion coefficients, intrinsic diffusion coefficients and inter-diffusion coefficients [17–23] are considered in the present work [17–23]. The experimental data referenced in this work is listed in Table 1.

Alexander [17] and Peterson [18] have measured the impurity diffusion coefficients of Ag in pure Al by the lathe sectioning method at the temperature range of 600–900 K. The impurity diffusion coefficients of Al in pure Ag have also been investigated by Fogelson [19], who obtained the impurity diffusion coefficients of Al in Ag at about 800–1300 K by using the X-ray diffraction method. Several authors [19] have made contribution to the measurement of tracer diffusion coefficients. Using the lathe sectioning technique, Alexander [17] employed the radioactive ^{110}Ag to measure the tracer diffusion coefficients of Ag in pure Al and Al-1 at.% Ag alloy at about 600–1000 K and 600–900 K, respectively. Intrinsic diffusion coefficients and inter-diffusion coefficients in various Al–Ag alloys also have been investigated by several authors [20–23]. Heumann [20,21] measured the intrinsic diffusion of the Al-rich solid solution in the composition range of 0 to 10 at.% Ag from 600 to 900 K with the aid of the microprobe analysis technique. Furthermore, Abbott and Haworth [22] measured the intrinsic diffusion coefficients between 600 and 800 K in square diffusion couples consisting of low concentration Al–Ag alloys and pure Al by the electron probe microanalysis. The concentration profiles were also obtained by Abbott and Haworth [22] via the electron probe microanalysis (EPMA). Chryssoulakis et al. [23] measured the inter-diffusion coefficients in the composition range

* Corresponding author. Tel.: +86 592 2187888; fax: +86 592 2187966.
E-mail address: lxj@xmu.edu.cn (C. Wang).

Table 1
Experimental diffusion data selected in the present optimization.

Type of data	Temperature (K)	Method	Refs.
Impurity diffusion coefficient	600–900	Lathe sectioning technique	Alexander and Slifkin [17]
	600–900	Lathe sectioning technique	Peterson and Rothman [18]
Tracer diffusion coefficient	800–1300	X-ray diffraction method	Fogelson et al. [19]
	600–1000	Lathe sectioning technique	Alexander and Slifkin [17]
Intrinsic diffusion coefficient	600–900	Lathe sectioning technique	Alexander and Slifkin [17]
	700–900	Microprobe analysis	Heumann and Dittrich [20]
	600–900	Microprobe analysis	Heumann and Bghmer [21]
Inter-diffusion coefficient	600–800	Electron probe microanalysis	Abbott and Haworth [22]
	600–800	Transient technique	Chrysoulakis et al. [23]

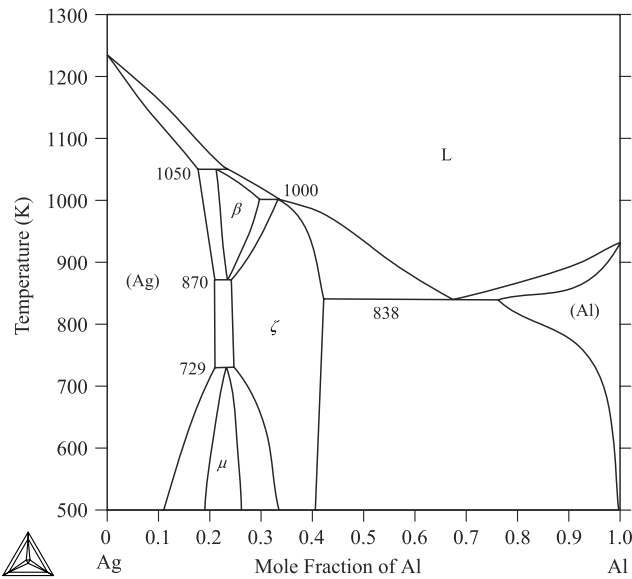


Fig. 1. Calculated phase diagram of the Al–Ag binary system from [29].

of 0 to 20 at.% Ag in the temperature range of 600–800 K using the transient technique method. All these data mentioned above are employed for the present optimization in view of their mutual consistency.

3. Modeling of atomic mobility

The temporal profile of the diffusing species k is given by Fick's law in the mass conservation form as follows:

$$\frac{\partial C_k}{\partial t} = -\text{div}(\bar{J}_k). \quad (1)$$

where C_k is the concentration in moles per volume, and div denotes the divergence operator. The diffusional flux of the species, \bar{J}_k , in a multicomponent system is given in the volume-fixed frame of reference by Fick's law as:

$$\bar{J}_k = -\sum_{j=1}^{n-1} \tilde{D}_{kj}^n \nabla C_j. \quad (2)$$

\tilde{D}_{kj}^n is the chemical diffusion coefficient. The summation is performed over $(n - 1)$ independent concentrations as the dependent n component may be taken as the solvent. \tilde{D}_{kj}^n in a

substitutional solution phase which is given by the following expression [9,24]:

$$\tilde{D}_{kj}^n = \sum_i (\delta_{ik} - x_k) x_i M_i \left(\frac{\partial \mu_i}{\partial x_j} - \frac{\partial \mu_i}{\partial x_n} \right) \quad (3)$$

where δ_{ik} is the Kronecker delta ($\delta_{ik} = 1$ if $i = k$, otherwise $\delta_{ik} = 0$), x_i the mole fraction, μ_i the chemical potential of element i and M_i the composition dependent atomic mobilities.

From the absolute-rate theory arguments, the mobility parameters M_i for the element i , can be divided into a frequency factor M_i^0 and an activation enthalpy Q_i . According to the suggestion by Jönsson [24,25], the M_i can be pressed as:

$$M_i = \exp\left(\frac{RT \ln M_i^0}{RT}\right) \exp\left(\frac{-Q_i}{RT}\right) \frac{1}{RT} {}^{mg}\Omega \quad (4)$$

where R is the gas constant, T is the temperature, and ${}^{mg}\Omega$ is a factor taking into account a ferromagnetic contribution to the diffusion. Both M_i^0 and Q_i are temperature, composition and pressure dependent factors. Because the ferromagnetic effect for fcc phase can be ignored [26], combining $RT \ln M_i^0$ and Q_i into one parameter $\Delta G_i^* = RT \ln M_i^0 - Q_i$, Eq. (4) can be simplified to as:

$$M_i = \exp\left(\frac{\Delta G_i^*}{RT}\right) \frac{1}{RT}. \quad (5)$$

Similar to the phenomenological CALPHAD approach, Andersson and Ågren [9] suggested that the parameter ΔG_i^* should be assumed as a function of composition, which can be expressed by a Redlich–Kister polynomial [27]. For the fcc Al–Ag alloys, ΔG_i^* is given as follows:

$$\Delta G_i^* = x_{Al} \Delta G_i^{Al} + x_{Ag} \Delta G_i^{Ag} + x_{Al} x_{Ag} \sum_{j=0}^n \Delta^{(j)} G_i^{Al,Ag} (x_{Al} - x_{Ag})^j \quad (6)$$

where $\Delta^{(j)} G_i^{Al,Ag}$ is the interaction term for diffusion between Ag and Al. It is seen that M_i can be obtained through the available ΔG_i^* .

Assuming the mono-vacancy atomic exchange as the main diffusion mechanism, the tracer diffusivity D_i^* can be related to the atomic mobility M_i by the Einstein's relation:

$$D_i^* = RT M_i. \quad (7)$$

In a binary system, the tracer diffusivity D_i^* can be applied to calculate chemical diffusion coefficient \tilde{D} by Darken's equation [28]:

$$\tilde{D} = (x_B D_A^* + x_A D_B^*) \phi \quad (8)$$

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