



## Interdiffusion and atomic mobility studies in Ni-rich fcc Ni–Al–Mn alloys



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### ABSTRACT

By employing nine groups of bulk diffusion couples together with electron probe microanalysis technique, the composition dependence of ternary interdiffusion coefficients in Ni-rich fcc Ni–Al–Mn alloys at 1373 K was determined via the Matano–Kirkaldy method. The experimental interdiffusion coefficients were critically assessed to obtain the atomic mobilities of Ni, Al and Mn in fcc Ni–Al–Mn alloys by using the DICTRA (Diffusion-Controlled TRAnsfOrmations) software package. The reliability of these mobilities was validated by comprehensive comparison between the model-predicted diffusion properties and the experimental data. The obtained atomic mobilities could be used to describe various diffusion phenomena in fcc Ni–Al–Mn alloys, such as the concentration profiles, interdiffusion flux and diffusion paths.

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### 1. Introduction

Nickel-based superalloys are an unusual class of metallic materials with an exceptional combination of high-temperature strength, toughness and resistance to degradation in corrosive or oxidizing environment. These materials have been widely used in aircraft and power-generation turbines, rocket engines, and other challenging environments, including nuclear power and chemical processing plants [1]. The Ni–Al system is the binary basis for superalloy compositions. As the level of Al added to  $\gamma$ -nickel (fcc-Ni) increases, a second precipitate phase  $\text{Ni}_3\text{Al}$  ( $L1_2$ ) appears and the basic structure of superalloys is formed. In the design of new superalloys, refractory alloying elements with large differences in electronic structure and atomic radii compared to Ni are often added for solid-solution strengthening of the  $\gamma$  phase. A major concern in this process is the avoidance of a class of phases known as topologically closed-packed phases (TCPs) [2]. Mn is one of the alloying elements that may cause the existence of TCPs in Ni–Al system [3], and its diffusion behavior is thus chosen to study in this work.

Moreover, Al–Mn–Ni based alloy is one of the aluminum casting alloys successfully applied in the aerospace and automotive industry [4], but the upgrading of products is in a relatively low speed because of long experimental and detection period. Recently, new alloy-design tools based on the phase-field approach coupled

with CALPHAD (CALculation of PHase Diagrams) method [5–9] have been increasingly used in designing new alloys and simulating candidate alloys to seek more practical light alloy with a high strength in the microstructure scale. Its ability to predict phase transformation and structure evolution is sensitively dependent on the quality of the thermodynamic and kinetic databases [10,11]. Many experimental studies on ternary diffusion have been performed in the fcc solid solutions, such as Cu–Al–Fe [12], Cu–Al–Mn [13–15] and Cu–Al–Ni [16–18]. Up to now, the general composition dependence of diffusivities in fcc Ni–Al–Mn system is still unknown, which is also within our ongoing work in developing the kinetic database for multi-component Al alloys [12,15,19–21]. Consequently, there is an urgent need to obtain the accurate diffusivities in fcc Ni–Al–Mn alloys.

As is shown in Fig. 1, Fcc<sub>A1</sub> phase has a large homogeneity range in Ni-rich corner of the Ni–Al–Mn system at 1373 K [22]. Since the composition range of fcc phase region in Al-rich corner is very small, the binary diffusivity (self- and impurity diffusivity) could sufficiently describe the interdiffusion in this ternary region. Therefore, the diffusion couple experiment, as a traditional but effective way to obtain diffusivities among various experimental techniques, is used in the present work to investigate the interdiffusion coefficients in Ni-rich fcc Ni–Al–Mn alloys at 1373 K. The atomic mobilities of Al, Mn and Ni in fcc Ni–Al–Mn alloys are then evaluated via DICTRA (Diffusion-Controlled TRAnsfOrmations) software package [23] based on the experimental diffusivities. Subsequently, the reliability of the obtained atomic mobilities is validated by comparing various calculated diffusion properties

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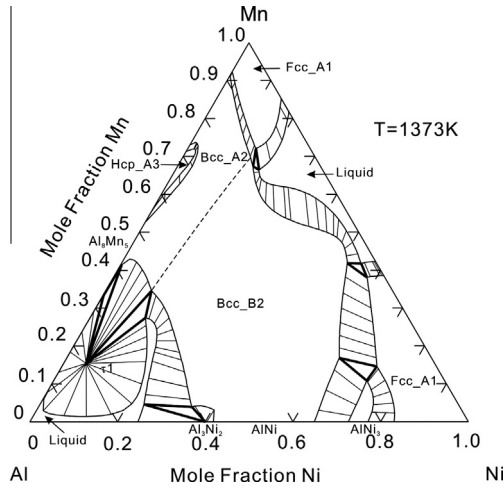


Fig. 1. Calculated isothermal section of the Ni–Al–Mn system at 1373 K according to [17].

with the corresponding experimental data, including ternary interdiffusion coefficients, concentration profiles, diffusion flux and diffusion paths.

## 2. Experimental procedures

Al (purity: 99.9 wt.%), Mn (purity: 99.9 wt.%) and Ni (purity: 99.99 wt.%) were used as starting materials. Nine diffusion couples, as shown in Table 1, were prepared in the following steps. First, terminal Ni–Al, Ni–Mn and fcc Ni–Al–Mn alloys with different compositions were melted by using arc melting and casted into the buttons under an argon atmosphere using a non-consumable W electrode (WKDHL-1, Opto-electronics Co. Ltd., Beijing, China). The buttons were re-melted five times to improve their homogeneities. In spite of the high volatility of Mn, no chemical analysis for the alloys was conducted since the weight losses of alloys were all less than 1 wt.% during arc-melting.

The buttons were cut into suitably sized blocks of  $6 \times 6 \times 16 \text{ mm}^3$  via electrical discharge machining after mechanically removing the surface material, and then sealed into an evacuated quartz tube ( $4 \times 10^{-4}$  bar), homogenized in an L4514-type diffusion furnace (Qingdao Instrument & Equipment Co. Ltd., China) at  $1373 \pm 5 \text{ K}$  for 30 days. After that, all the samples were grounded on SiC papers to remove surface contamination. The diffusion surface of each sample was polished on diamond impregnated cloth to a finish of  $0.5 \mu\text{m}$ . Subsequently, diffusion couples were prepared by binding the polished surfaces of two samples together with Mo wire.

The diffusion assemblies were sealed into evacuated quartz tubes, and annealed at 1373 K for 86.4 ks (1 day), followed by water quenching. The annealed couples were metallographically polished along the planes parallel to diffusion direction. Solute concentration profiles in these diffusion couples were measured by electronic-probe microanalysis (EPMA, JXA-8800R, Electron Optics. Ltd., Tokyo, Japan) under the operation condition of 20 kV voltage, 20 mA current and a  $40^\circ$  take-off angle.

Table 1

List of terminal compositions of the nine diffusion couples in the present work.

Couple name	Composition (at.%)	Temperature (K)	Diffusion time (ks)
A1	Ni/Ni–10.1Mn–10.2Al	1373	86.4
A2	Ni/Ni–15.2Mn–10.2Al	1373	86.4
A3	Ni/Ni–25.0Mn–5.0Al	1373	86.4
B1	Ni–5.6Al/Ni–10.3Mn	1373	86.4
B2	Ni–5.2Al/Ni–20.3Mn	1373	86.4
B3	Ni–5.1Al/Ni–28.7Mn	1373	86.4
B4	Ni–10.1Al/Ni–10.2Mn	1373	86.4
B5	Ni–10.1Al/Ni–20.5Mn	1373	86.4
B6	Ni–10.3Al/Ni–29.8Mn	1373	86.4

## 3. Evaluation and modeling of ternary diffusivities

### 3.1. Evaluation of ternary interdiffusion coefficients

The concentration profiles for diffusion couples are analyzed by means of the Matano–Kirkaldy method [24,25] to get the ternary interdiffusion coefficients in the fcc Ni–Al–Mn alloys. On the basis of Onsager's formalism [26], the interdiffusion in a ternary alloy 1–2–3 is described by an extended Fick's second law on the basis of Matano coordinates:

$$\frac{\partial C_1}{\partial t} = \frac{\partial}{\partial x} \left( \tilde{D}_{11}^3 \frac{\partial C_1}{\partial x} \right) + \frac{\partial}{\partial x} \left( \tilde{D}_{12}^3 \frac{\partial C_2}{\partial x} \right) \quad (1)$$

and

$$\frac{\partial C_2}{\partial t} = \frac{\partial}{\partial x} \left( \tilde{D}_{21}^3 \frac{\partial C_1}{\partial x} \right) + \frac{\partial}{\partial x} \left( \tilde{D}_{22}^3 \frac{\partial C_2}{\partial x} \right) \quad (2)$$

where component 3 is taken as the dependent solvent,  $C_1$  and  $C_2$  are the concentrations of solutes 1 and 2,  $t$  is the diffusion time and  $x$  is the diffusion distance from Matano interface.  $\tilde{D}_{11}^3$  and  $\tilde{D}_{22}^3$  are the main interdiffusion coefficients, while  $\tilde{D}_{12}^3$  and  $\tilde{D}_{21}^3$  are the cross interdiffusion coefficients. In this study, the solvent is Ni, and solutes are Al and Mn, respectively.

Kirkaldy et al. [25] have shown that Eqs. (1) and (2) can be solved by an extension of the Boltzman–Matano method into a ternary one:

$$\int_{C_1^-}^{C_1^+} x \cdot dC_1 = -2t \left( \tilde{D}_{11}^3 \frac{\partial C_1}{\partial x} + \tilde{D}_{12}^3 \frac{\partial C_2}{\partial x} \right) \quad (3)$$

and

$$\int_{C_2^-}^{C_2^+} x \cdot dC_2 = -2t \left( \tilde{D}_{21}^3 \frac{\partial C_1}{\partial x} + \tilde{D}_{22}^3 \frac{\partial C_2}{\partial x} \right) \quad (4)$$

and the origin for  $x$  is chosen in such a way that

$$\int_{C_i^-}^{C_i^+} x \cdot dC_i = 0 \quad \text{for } i = 1, 2 \quad (5)$$

where  $C_i^-$  and  $C_i^+$  ( $i = 1, 2$ ) are the terminal compositions at the end of the diffusion couples. The four interdiffusion coefficients in Eqs. (3) and (4) are evaluated at the intersection compositions ( $C_1$  and  $C_2$ ) of every two diffusion paths.

### 3.2. Atomic mobility and diffusivity

According to the absolute-reaction rate theory, the atomic mobility of element  $k$ ,  $M_k$ , may be divided into a frequency factor  $M_k^0$  and an activation enthalpy  $Q_k$  [27]. According to Andersson and Ågren [28],  $M_k$  can be expressed as

$$M_k = \exp \left( \frac{RT \ln M_k^0}{RT} \right) \exp \left( \frac{-Q_k}{RT} \right) \frac{1}{RT} \text{mg}\Omega \quad (6)$$

where  $R$  is the gas constant and  $T$  is the absolute temperature.  $\text{mg}\Omega$  is a factor taking into account a ferromagnetic contribution to the diffusion coefficient. For fcc phase the ferromagnetic contribution to diffusion is negligible [29], and thus the corresponding atomic mobility parameters in the DICTRA notation,  $Q_k$  and  $RT \ln M_k^0$ , can be merged into one parameter, i.e.  $\Phi_k = -Q_k + RT \ln M_k^0$ . In the spirit of CALPHAD approach, the composition dependency of  $\Phi_k$  can be represented with the Redlich–Kister polynomial [30]:

$$\Phi_k = \sum_i x_i \Phi_k^i + \sum_i \sum_{j>i} x_i x_j \left[ \sum_r \Phi_k^{ij,r} (x_i - x_j)^r \right] + \sum_i \sum_{j>i} \sum_{k>j} x_i x_j x_k \left[ \sum_s \nu_{ijk}^s \Phi_k^{i,j,k} \right] \quad (s = i, j \text{ or } k) \quad (7)$$

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