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Assessment of the diffusional mobilities in fcc Ni–Nb and fcc Ni–Mo alloys

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ABSTRACT

The atomic mobilities of the fcc Ni–Nb and Ni–Mo binary system have been assessed on the basis of the available kinetic information and given as functions of temperatures and composition in the CALPHAD format using the DICTRA software package in this work. Good agreement between the calculated and reported experimental diffusion coefficients is obtained. By using optimized mobility parameters, the concentration profiles of the diffusion zone in the binary Ni–Nb and Ni–Mo diffusion couples can be predicted. The assessed atomic mobility parameters are an important part of the construction of mobility database in Ni based alloys, and are also useful in designing high-temperature Ni-based alloy.
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1. Introduction

Due to the attractive combination of unique mechanical and physical properties, such as extraordinary good corrosion resistance [1], high strength under high temperature [2], and good weldability [3], Ni based alloy is one of the most useful high-temperature alloys, which can provide ideal engineering properties in many industrial areas [4]. Ni based alloy containing Nb and Mo is desired to increase strength and corrosion resistance, which plays an important role in nuclear reactors, high temperature energy conversion device components [5,6]. It is generally accepted that estimating the rate of a phase transformation and the diffusion information of different components is a well-established procedure. Diffusion plays a very important role in optimizing material microstructures and understanding the mechanical and physical properties of Ni–Nb and Ni–Mo alloys. Thus, in order to determine alloys stability and even maintain adequate processing designs, it is of great importance to study kinetic characteristics of Ni–Mo and Ni–Nb alloys.

The DICTRA (Diffusion Controlled TRAnsformation) program has been developed to simulate and predict microstructure evolution, which is an extension of the CALPHAD (CALculation of PHAse Diagram) approach and operates under the CALPHAD framework [7–11]. It makes it possible to simulate diffusion-limited phenomena for multi-component alloys with the thermodynamic and kinetic data. In this software, lots of diffusivities used in the simulation can be easily calculated from the combination of thermodynamic and mobility parameters.

It is evident that the diffusion controlled growth of the tcp phases (topological close packed phases) play an important part in the diffusion process of Ni–Nb and Ni–Mo alloys, but it is difficult to assess the diffusional mobilities of tcp phase. The aim of this present work is to assess the atomic mobilities of fcc Ni–Nb and fcc Ni–Mo alloys as a function of temperature and composition through the DICTRA software package. The prediction for diffusion characteristics of diffusion profiles is also presented by applying the assessed mobility parameters.

2. Model description

For a substitutional solution containing n components, referred to the volume-fixed frame of reference, the diffusion flux of species k is given by the Fick–Onsager law as:

$$J_k = -\sum_{j=1}^{n-1} D_{kj}^{n} \nabla C_j \tag{1}$$

where D_{kj}^{n} is the inter-diffusion coefficient, ∇C_j is the concentration gradient of species j, the summation is performed over $(n-1)$ independent concentrations with the dependent n elements taken as the solvent. The temporal profile of the species k is governed by the mass conservation law, can be described as follows:

$$\frac{\partial C_k}{\partial t} = -\nabla \times J_k \tag{2}$$

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Referring to the volume-fixed frame of reference, the inter-diffusion coefficient D_{kj}^{n} is given by:

$$D_{kj}^{n}=\sum_{i=1}^{n}(\delta_{ik}-x_k)x_iM_i\left(\frac{\partial\mu_i}{\partial x_j}-\frac{\partial\mu_i}{\partial x_n}\right) \tag{3}$$

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 and M_i the atomic mobility of element i.

Let us take a general binary substitutional phase containing elements A and B into consideration, in the spirit of CALPHAD method, the mobility M_i for the elements i ($i=A$ or B) can be divided into a frequency factor M_i^0 and an activation enthalpy Q_i. From the absolute-rate theory arguments, the M_i can be given by the following expression:

$$M_i=\exp\left(\frac{RT\ln(M_i^0)}{RT}\right)\exp\left(\frac{-Q}{RT}\right)\frac{1}{RT}=\frac{1}{RT}\exp\left(\frac{\Phi_i}{RT}\right) \tag{4}$$

where Φ_i is a composition-dependent property. In the CALPHAD treatment, Φ_i is expanded with a Redlick–Kister polynomial as:

$$\Phi_i=x_A\Phi_i^A+x_B\Phi_i^B+x_Ax_B\sum_r{}^r\Phi_i^{A,B}(x_A-x_B)^r \tag{5}$$

where Φ_i^A, Φ_i^B and $\Phi_i^{A,B}$ are the model parameters to be evaluated from experimental data in this work; x_A and x_B are the molar fractions of A and B, respectively.

The tracer diffusion coefficients for A and B can be related to the mobility by the Einstein's relation:

$$D_A^*=RTM_A \tag{6}$$

$$D_B^*=RTM_B \tag{7}$$

Also, the intrinsic diffusion coefficients for A and B that characterize the diffusion rates of elements on the lattice reference frame, can be expressed by:

$$D_A^I=D_A^*F \tag{8}$$

$$D_B^I=D_B^*F \tag{9}$$

where the superscript I denotes the intrinsic reference frame or the lattice reference frame. F is the thermodynamic factor defined by:

$$F=\frac{x_Ax_B}{RT}\left(\frac{\partial^2G_m}{\partial^2x_A}+\frac{\partial^2G_m}{\partial^2x_B}-2\frac{\partial^2G_m}{\partial x_A\partial x_B}\right) \tag{10}$$

where G_m is the molar Gibbs free energy of a substitutional phase.

In the binary system, we can calculate inter-diffusion coefficient $\tilde{D}$ by Darken's equation by applying the tracer diffusion coefficients:

$$\tilde{D}=(x_AD_A^I+x_BD_B^I)=(x_AD_A^*+x_BD_B^*)F \tag{11}$$

3. Experimental information

3.1. The Ni–Nb system

Some researchers measured the impurity diffusion coefficients for the fcc phase in the Ni–Nb system. Karunaratne et al. [12] have measured the impurity diffusion coefficients of Nb in pure Ni over the temperature range from 1173 to 1573 K by sectioning method. Using the same technique, Bergner et al. [13] also measured the impurity diffusion coefficients of Nb in pure Ni from 1116 to1527 K. The data of these two groups are consistent with each other. Patil et al. [14] studied the impurity diffusion coefficients of Nb in Ni in the temperature range of 1473–1773 K by diffusion bonding. However, there is a discrepancy between the data reported by Karunaratne et al. [12] and those reported by Patil et al. [14], the overall agreement is poor especially at lower temperature. The activation energy and the pre-exponential factors reported by Patil et al. [14] are substantially low compared to those of other impurities of Ni based alloy. Take the accordance of most experimental data and experimental error into consideration, only the data in Refs. [12,13] have been employed in the present work.

Karunaratne et al. [12] also investigated inter-diffusion coefficients in fcc Ni–Nb alloys by the diffusion couple technique. The diffusion couples were prepared and annealing at various temperature ranging from 1173 to 1573 K, the concentration distribution in the diffusion zones was measured, and the inter-diffusion coefficients were presented. Karunaratne et al. [12] also carried out chemical diffusion experiments in Ni–Nb alloys. Then the samples are annealed under helium atmosphere (1 atm pressure) at the temperature of 1431 K for 24 and 48 h, respectively. The concentration profiles of Ni–Ni 4 wt% Nb couples were established by using a CAMEBAX electron probe microanalyser in the wavelength dispersive mode.

Patil et al. [14] measured the concentration–distance profile of Ni–Ni 4.6 at% Nb couples on the electron probe microanalyser by investigating characteristic X-ray radiation and counting the rates of the X-ray signals. The elemental distribution of Nb and Ni across the diffusion zone is established by using a CAMEBAX electron probe microanalyser.

Sprengel et al. [15,16] investigated inter-diffusion coefficients in Ni_3Nb and NiNb at the temperature ranging from 1186 to 1398 K by the diffusion couple technique. Balam et al. [17] carried out chemical diffusion experiments of μ phase (Ni_7Nb_6) in the Ni–Nb alloys. The diffusion couples were prepared and annealing at various temperature ranging from 1273 to 1473 K, the concentration distribution in the diffusion zones was measured, and the inter-diffusion coefficients, instrict diffusion coefficients and tracer diffusion coefficients were presented.

3.2. The Ni–Mo system

Karunaratne et al. [12] reported the impurity diffusion coefficients of Mo in fcc Ni using sectioning method at the temperature ranged from 1173 to 1573 K. The diffusion coefficients studied by Minamino et al. [18] are in remarkable agreement with Karunaratne's et al. [12]. Also, the data of Heijwegen et al. [19] are in good agreement with those reported by Minamino et al. [18] and Karunaratne et al. [12]. These three groups of data have all been adopted in the present work. Karunaratne et al. [12] also investigated inter-diffusion coefficients in fcc Ni–Mo alloys by the diffusion couple technique. The samples were prepared and annealing at various temperatures ranging from 1173 to 1573 K and the inter-diffusion coefficients were presented. The samples were annealed under helium atmosphere (1 atm pressure) at 1473 K for 48 and 120 h respectively, the concentration distribution in the diffusion zones was measured. The concentration profiles of Ni–Ni 10 wt% Mo couples were established by using a CAMEBAX electron probe microanalyser in the wavelength dispersive mode.

Ugaste et al. [20] explored the inter-diffusion coefficients in the temperature range from 1443 to 1563 K with Ni/Mo diffusion couples and the Matano method. The specimens were homogenized for 10 h at 1523 K and annealed for 8 h at 1473 K. The concentration profile of Ni–Ni 9 at% Mo couples was taken by local crystallographic analysis on the MS-46 micro X-ray analyzer.

Lanam et al. [21] investigated the inter-diffusion coefficients at 1473 K with Ni-30 wt% Mo diffusion couples. The specimens were homogenized at 1473 K with an applied pressure of 6.89×10^6 Pa.

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