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Diffusion behavior and atomic mobilities for fcc Cu–Cr–Ni alloys

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ABSTRACT

In this work, diffusion couples of fcc Cu–Cr–Ni alloys annealed at 1373 K for 80 h are investigated. The interdiffusion coefficients are retrieved from common compositions of two diffusion couples, which are then combined with thermodynamic descriptions to explore atomic mobilities of Cu, Cr and Ni in fcc Cu–Cr–Ni alloys within the CALPHAD framework. In order to confirm the quality of such kinetic characteristics, a comparison between calculated and experimentally measured concentration profiles of diffusion couples and diffusion paths in Gibbs triangle is made, where the agreement is excellent. The results of this study contribute to the establishment of a general Ni-based mobility database for alloy design.

1. Introduction

Cu–Cr–Ni alloys feature good corrosion resistance and superior mechanical properties, which leads to their wide applications in shipbuilding industry [1]. In addition, such alloys can also be applied in electronic industry as corrosion-resistant conductor materials [2]. In order to further optimize the properties of Cu–Cr–Ni alloys, which thus promote further applications in industry, it is inevitable to explore the diffusion behaviors, as kinetic information plays a decisive role in alloy microstructure evolution [3].

Nowadays, CALPHAD-based kinetic technology has been well developed for materials scientists in alloy design. Within the framework of CALPHAD, atomic mobilities can be combined with thermodynamic parameters to gain further insights into diffusion characteristics, thereby facilitating investigation of composition and phase evolution in multi-component alloys. However, accurate atomic mobilities for multi-component alloys are still in shortage. The atomic mobilities for fcc Cu–Ni and Cr–Ni alloys have been reported by Wang et al. [4] and Engstrom and Agren [5], respectively. However, the temperature effect for interaction parameters of Cr and Ni was not included. The atomic mobilities for fcc Cu–Cr–Ni alloys are still absent in the literature. Thus, the aim of this work is to investigate diffusion characteristics and related atomic mobilities for fcc Cu–Cr–Ni alloys with the aid of CALPHAD technology. 1373 K is an important annealing temperature for casted Ni-based alloys. Thus, kinetic study at this temperature can help to gain more insights on how the inhomogeneity can be reduced. It is noted that the service temperature for Ni-based alloys is usually below 1000 K, at which grain boundary diffusion is significant. In view of such situation, diffusion characteristics for only 1373 K are explored in this work, and the atomic mobilities presented can be used for alloy design around 1373 K. In the future, much work is still needed to assess the temperature dependence of the atomic mobilities for Cr–Ni binary system, after which the temperature-dependence of atomic mobilities for Cu–Cr–Ni ternary system can be well established.

2. Diffusion methodology

2.1. Establishment of diffusion modeling

For Cu, Cr and Ni elements in fcc Cu–Cr–Ni ternary alloys, the inter-diffusion fluxes defined in the number-fixed frame of reference, can be expressed as [6]:

$$\vec{J}^{N}_{Cu} = -\tilde{D}^{Ni}_{CuCu}\nabla C_{Cu} - \tilde{D}^{Ni}_{CuCr}\nabla C_{Cr} \quad (1)$$

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Table 1
Alloy concentrations for the diffusion couples used in this work.

Alloy designation	Molar fractions		
	Cu	Cr	Ni
1	0	0.3	0.7
2	0	0.2	0.8
3	0	0.1	0.9
4	0.1	0	0.9
5	0.2	0	0.8
6	0.3	0	0.7

$$\vec{J}^{N}_{Cr} = -\tilde{D}^{Ni}_{CrCu}\nabla C_{Cu} - \tilde{D}^{Ni}_{CrCr}\nabla C_{Cr} \quad (2)$$

$$\vec{J}^{N}_{Cu} + \vec{J}^{N}_{Cr} + \vec{J}^{N}_{Ni} = 0 \quad (3)$$

where $\vec{J}^{N}_{Cu}$, $\vec{J}^{N}_{Cr}$ and $\vec{J}^{N}_{Ni}$ indicate the inter-diffusion fluxes of Cu, Cr and Ni, respectively; the superscript N denotes the number-fixed frame of reference; C_{Cu} and C_{Cr} stand for the volume compositions of Cu and Cr, respectively; $\tilde{D}^{Ni}_{CuCu}$, $\tilde{D}^{Ni}_{CuCr}$ $\tilde{D}^{Ni}_{CrCu}$ and $\tilde{D}^{Ni}_{CrCr}$ are the inter-diffusion coefficients with Ni being the dependent element.

In consideration of the lattice-fixed frame reference, the intrinsic diffusion fluxes of Cu, Cr and Ni can be given by Ref. [6]:

$$\vec{J}^{I}_{Cu} = -{}^{I}D^{Ni}_{CuCu}\nabla C_{Cu} - {}^{I}D^{Ni}_{CuCr}\nabla C_{Cr} \quad (4)$$

$$\vec{J}^{I}_{Cr} = -{}^{I}D^{Ni}_{CrCu}\nabla C_{Cu} - {}^{I}D^{Ni}_{CrCr}\nabla C_{Cr} \quad (5)$$

$$\vec{J}^{I}_{Ni} = -{}^{I}D^{Ni}_{NiCu}\nabla C_{Cu} - {}^{I}D^{Ni}_{NiCr}\nabla C_{Cr} \quad (6)$$

where $\vec{J}^{I}_{Cu}$, $\vec{J}^{I}_{Cr}$ and $\vec{J}^{I}_{Ni}$ are the intrinsic diffusion fluxes of Cu, Cr and Ni, respectively; the superscript I denotes the lattice-fixed frame reference; ${}^{I}D^{Ni}_{CuCu}$, ${}^{I}D^{Ni}_{CuCr}$, ${}^{I}D^{Ni}_{CrCu}$, ${}^{I}D^{Ni}_{CrCr}$, ${}^{I}D^{Ni}_{NiCu}$ and ${}^{I}D^{Ni}_{NiCr}$ stand for the six intrinsic diffusion coefficients with Ni being the dependent element.

The relation between the inter-diffusion coefficients and the intrinsic coefficients can be given as follows [6]:

$$\tilde{D}^{Ni}_{ij} = {}^{I}D^{Ni}_{ij} - x_i\left({}^{I}D^{Ni}_{Cuj} + {}^{I}D^{Ni}_{Crj} + {}^{I}D^{Ni}_{Nij}\right) \quad (7)$$

where i and j stand for Cu, Cr or Ni.

The values of six intrinsic diffusion coefficients defined in Eqs. (4)–(6) can be calculated by Ref. [6]:

$${}^{I}D^{Ni}_{ij} = x_i M_i\left(\frac{\partial\mu_i}{\partial x_j} - \frac{\partial\mu_j}{\partial x_{Ni}}\right) \quad (8)$$

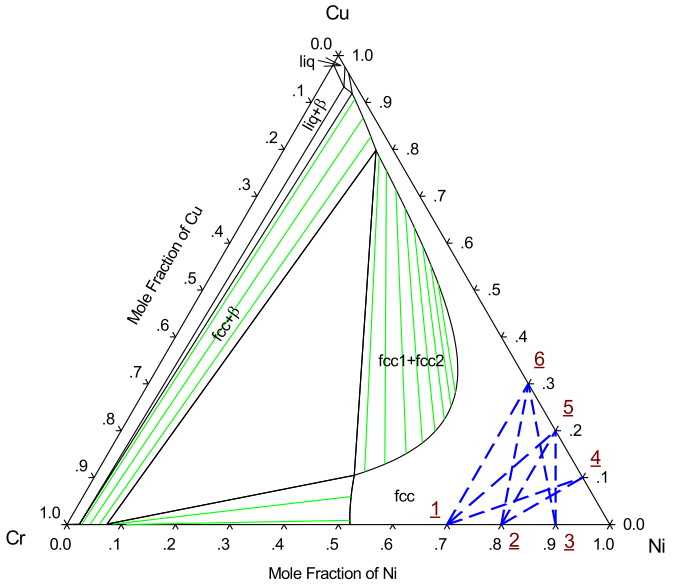

Fig. 1. Isothermal section of Cu–Cr–Ni phase diagram with the concentration scheme for diffusion couples superimposed (T = 1373 K).

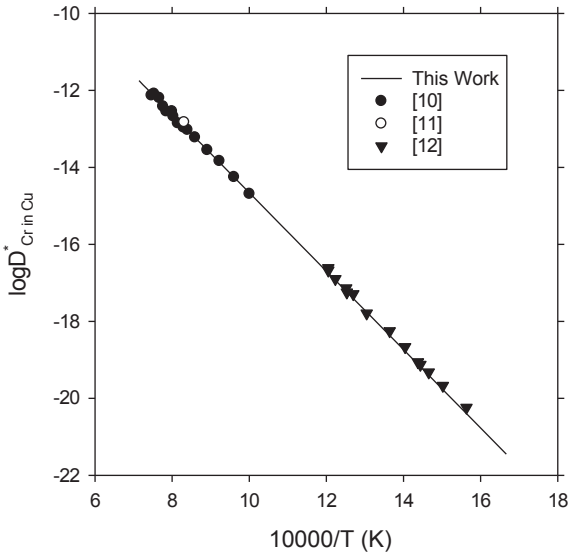

Fig. 2. Calculated and measured impurity diffusion coefficients of Cr in fcc Cu.

Table 2
Mobility parameters for Cu, Cr and Ni in fcc Cu–Cr–Ni alloys (all in SI units).

Phase	Model	Mobility	Parameters
fcc	$(Cu,Cr,Ni)_1(Va)_1$	Cu	$\Phi^{Cu:Va}_{Cu} = -205872 - 82.53T$ [4]
			$\Phi^{Ni:Va}_{Cu} = -250125 - 85.3T$ [4]
			$\Phi^{Cr:Va}_{Cu} = -235000 - 82T$
			${}^{0}\Phi^{Cu,Ni:Va}_{Cu} = 23887 - 17.7T$ [4]
			${}^{0}\Phi^{Cr,Ni:Va}_{Cu} = 18425.37$
			${}^{0}\Phi^{Cu,Cr,Ni:Va}_{Cu} = 75329.48$
			${}^{1}\Phi^{Cu,Cr,Ni:Va}_{Cu} = 82196.42$
			${}^{2}\Phi^{Cu,Cr,Ni:Va}_{Cu} = 73985.47$
		Cr	$\Phi^{Cr:Va}_{Cr} = -235000 - 82T$ [5]
			$\Phi^{Ni:Va}_{Cr} = -287000 - 64.4T$ [5]
			$\Phi^{Cu:Va}_{Cr} = -195000 - 85.62T$
			${}^{0}\Phi^{Cr,Ni:Va}_{Cr} = -68000$ [5]
			${}^{0}\Phi^{Cu,Ni:Va}_{Cr} = 24168.29$
			${}^{0}\Phi^{Cu,Cr,Ni:Va}_{Cr} = 86255.24$
			${}^{1}\Phi^{Cu,Cr,Ni:Va}_{Cr} = 73985.14$
			${}^{2}\Phi^{Cu,Cr,Ni:Va}_{Cr} = 96351.24$
		Ni	$\Phi^{Ni:Va}_{Ni} = -287000 - 69.8T$ [4]
			$\Phi^{Cu:Va}_{Ni} = -232788 - 71.1T$ [4]
			$\Phi^{Cr:Va}_{Ni} = -235000 - 82T$ [5]
			${}^{0}\Phi^{Cu,Ni:Va}_{Ni} = 106790 - 75.4T$ [4]
			${}^{0}\Phi^{Cr,Ni:Va}_{Ni} = -81000$ [5]
			${}^{0}\Phi^{Cu,Cr:Va}_{Ni} = 62172.36$
			${}^{0}\Phi^{Cu,Cr,Ni:Va}_{Ni} = 121345.85$
			${}^{1}\Phi^{Cu,Cr,Ni:Va}_{Ni} = 115432.96$
			${}^{2}\Phi^{Cu,Cr,Ni:Va}_{Ni} = 106122.52$