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Invited article

Experimental and computational study of interdiffusion for fcc Ni–Cu–Cr alloys

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ABSTRACT

The interdiffusion behavior of fcc Ni–Cu–Cr alloys has been studied by experiments and computational methods. The concentration profiles of binary fcc Ni–Cu diffusion couples annealed at 1123 and 1273 K and those of ternary fcc Ni–Cu–Cr diffusion couples annealed at 1173, 1273 and 1373 K have been measured by using electron probe microanalysis (EPMA). Then the interdiffusion coefficients were determined using the Sauer–Freise and Whittle–Green method based on the measured concentration profiles of binary and ternary diffusion couples, respectively. Based on the diffusion coefficients reported in the literature and those determined in the present work, the atomic mobilities for fcc Ni–Cu–Cr alloys have been assessed. To validate the present assessed mobilities, various diffusion coefficients (i.e., impurity, tracer and intrinsic diffusion coefficients), concentration profiles and diffusion paths of fcc Ni–Cu–Cr alloys were calculated and compared with the experimental data. Good agreements and predictions were obtained.

1. Introduction

Ni–Cu-based alloys are important corrosion resistance alloys and find wide applications in industry such as petrochemical engineering, electricity and electronic industry [1–3]. The practical processes, such as solidification, homogenization, precipitation, bonding and coating are largely affected by diffusion. Understanding diffusion behaviors is critical for both materials design and deployment.

The Ni–Cu–Cr system is a common ternary system in the Ni–Cu-based alloys. Cu can form infinite solid solution with Ni in a wide temperature range. Cr plays an important role in solid solution strengthening which improves the high-temperature strength. When the alloys are on service at high temperatures, the formation of Cr_2O_3 has the merit of improving the oxidation resistance. In spite of its importance, the interdiffusion behavior is not fully explored.

By using the CALPHAD approach [4,5] to study diffusion kinetics [6–8], Wang et al. [9] assessed the Ni–Cu binary system for the first time and Zhang et al. [10] reassessed this system adopting the Ni self-diffusion parameter from the work by Zhang et al. [8]. Later, Campbell and Rukhin [11] showed that the Ni self-diffusion parameter from Neumann and Tölle [12] agrees best with the experimental data. The interdiffusion coefficients adopted in the work by Wang et al. [9] and Zhang et al. [10] were measured at 1273 K. In the present work, the interdiffusion coefficients were determined at 1123 K and 1273 K before reassessing the Ni–Cu binary system. Jönsson [13] assessed the fcc Ni–Cr binary system by adopting the interdiffusion coefficients with Cr content below 5 at% from Davin et al. [14]. Zhu et al. [15] investigated this system with new experimental data on interdiffusion coefficients for the Cr content up to 21 at%. As the fcc single phase region is very narrow for the Cu–Cr system [16], it is difficult to obtain the interdiffusion coefficients for fcc Cu–Cr alloys. Xu et al. [17] investigated the diffusion couples of fcc Cu–Cr–Ni alloys annealed at 1373 K and obtained the atomic mobilities. In the present work, the interdiffusion coefficients in fcc Ni–Cu–Cr alloys were determined at a wide temperature range of 1173–1373 K.

The main objectives of this work are: (1) to obtain the concentration profiles of fcc Ni–Cu diffusion couples at 1123 K and 1273 K and those of fcc Ni–Cu–Cr diffusion couples at 1173 K, 1273 K and 1373 K by means of EPMA; (2) to determine the interdiffusion coefficients and obtain the atomic mobilities for fcc Ni–Cu and Ni–Cu–Cr alloys; (3) to validate the accuracy of atomic mobilities obtained in the present work by comparing with the experimental diffusion coefficients, concentration profiles and diffusion paths.

2. Experimental information

2.1. Experimental procedures

In the present work, totally 17 pairs of diffusion couples are measured as listed in Table 1, and schematically shown on the isothermal section of the ternary Ni–Cu–Cr system in Fig. 1.

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Pure Ni (purity 99.999 wt%), Cu (purity 99.999 wt%) and Cr (purity 99.95 wt%) foils were used as raw materials, which were melted by arc melting under an argon atmosphere. The arc melting was repeated five times to ensure homogeneity. Then all the ingots were hot-rolled at 1273 K to decrease the secondary dendrite arm spacing and facilitate homogenization. All the ingots were sealed in quartz capsules with argon pressure reaching 5000 Pa and homogenized at 1273 K for 240 h, followed by water quenching to avoid precipitation. Small bulk samples with the size of $6 \times 6 \times 6$ mm^3 were cut from the ingots. All surfaces were ground and one of them was polished. Two polished surfaces were put together and the well-contacted diffusion couple was fixed by a specially-made Mo clamp to form a diffusion-couple assembly, which was then put in quartz capsules with an argon pressure of 5000 Pa. After annealing treatments as listed in Table 1, all assemblies are quenched into cold water. The concentration profiles on the diffusion couples were measured using EPMA.

Table 1
Summary of the diffusion couples and experimental conditions in the present work.

No.	Nominal composition (at%)	Temperature (K)	Diffusion time (h)
A1	Ni/Ni–15Cu–20Cr	1173	120
A2	Ni–10Cr/Ni–10Cu–25Cr		
A3	Ni–15Cu/Ni–25Cu–10Cr		
A4	Ni–30Cr/Ni–30Cu		
A5	Ni–20Cr/Ni–20Cu		
B1	Ni/Ni–15Cu–20Cr	1273	48
B2	Ni–10Cr/Ni–10Cu–25Cr		
B3	Ni–15Cu/Ni–25Cu–10Cr		
B4	Ni–30Cr/Ni–30Cu		
B5	Ni–20Cr/Ni–20Cu		
C1	Ni/Ni–15Cu–20Cr	1373	24
C2	Ni–10Cr/Ni–10Cu–25Cr		
C3	Ni–15Cu/Ni–25Cu–10Cr		
C4	Ni–30Cr/Ni–30Cu		
C5	Ni–20Cr/Ni–20Cu		
D1	Ni/Cu	1273	185
D2	Ni/Cu	1123	114

2.2. Determination of the interdiffusion coefficients

The experimental concentration profiles of the diffusion couples were analyzed by the error function expansion (ERFEX) method as shown in the following equation [18,19],

$$X(z) = \sum_i a_i erf\left[(b_i - c_i)z + d_i\right] \quad (1)$$

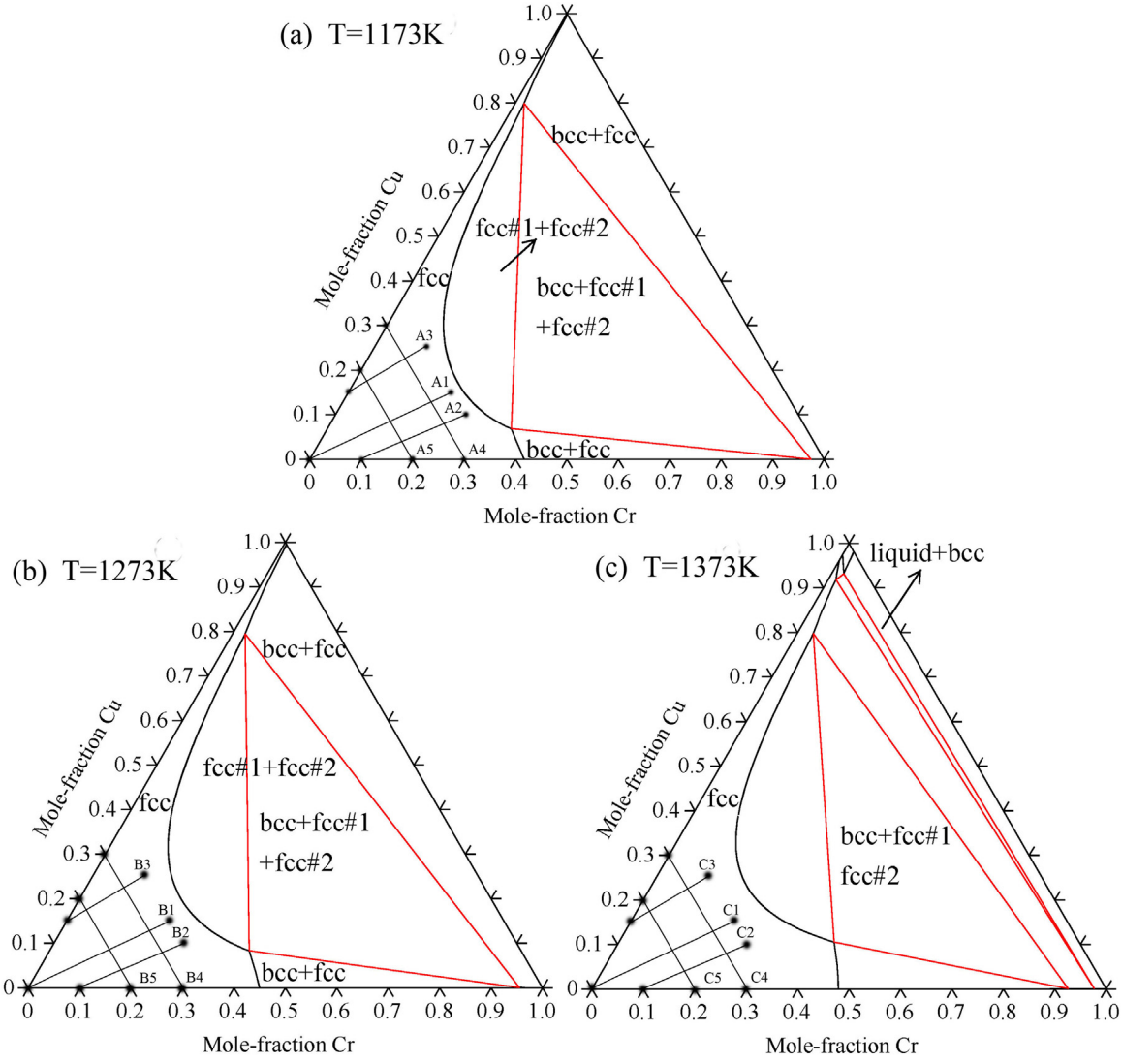

Fig. 1. Calculated Ni–Cu–Cr isothermal sections at (a) 1173 K, (b) 1273 K and (c) 1373 K. The diffusion couples (A1-5, B1-5 and C1-5) assembled in the present work are plotted.