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ARTICLE

Interdiffusion and Atomic Mobilities in Ni-rich fcc Ni-Cr-W Alloys

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Abstract: Six diffusion couples of Ni-Cr-W ternary alloys were prepared, annealed at 1473 K for 72 h and measured by the electron probe microanalysis combined with Whittle-Green method in order to determine the interdiffusion coefficients. The experimental interdiffusion coefficients were critically assessed to obtain the atomic mobilities by means of DICTRA software package. A good agreement has been obtained by comprehensive comparison between the experimental data and the model-predicted diffusion properties, which verifies the reliability of the atomic mobilities of Ni, Cr and W in Ni-Cr-W alloys. The diffusion phenomena, such as diffusion paths and the concentration-distance profiles in the Ni-Cr-W ternary system can be reasonably described by the presently obtained atomic mobilities.

Key words: Ni-Cr-W alloy; atomic mobility; diffusion couple; interdiffusion coefficients; DICTRA

Ni-based superalloys are one of the most ideal materials, which have high strength, good oxidation and corrosion resistance at high temperature. Based on these advantages, they have been widely used in engines, gas turbines, aircraft and many other industries[1,2]. It has been reported that, Cr and W, which are frequently added elements in superalloys, could improve the performance of Ni-based superalloys by solid-solution strengthening[3]. Therefore, the Ni-Cr-W ternary system is significant for the exploration of the Ni-based superalloys. To know the diffusion kinetics of Ni-Cr-W alloys is important which can help to determine the stability of alloys under long-term service conditions and deal with processing designs.

Based on CALPHAD (calculation of phase diagram) approach, DICTRA (diffusion controlled transformation) is a successful software for simulating and predicting microstructure evolution. DICTRA has thus been applied to investigate many different types of materials using different models, combining the atomic mobility and thermodynamic databases[4-8]. For the purpose of getting the knowledge of the diffusion kinetic about the Ni-Cr-W ternary system, the assessment of atomic mobilities is necessary. Until now, Ni-Cr and Ni-W binary system are established[9]. However, the ternary system of Ni-Cr-W alloys is still lacking. The major purposes of this work are: (1) to determine the interdiffusion coefficients of fcc Ni-Cr-W alloys by diffusion couples annealed at 1473 K for 72 h; (2) to verify the reliability of the obtained mobility parameters by comprehensive comparison between the model-predicted diffusion properties and the corresponding experimental data.

1 Experiment Procedure

1.1 Preparation of diffusion couples

Ni (purity: 99.9 wt%), Cr (purity: 99.9 wt%) and W (purity: 99.9 wt%) were used as starting materials. According to the experimental isothermal section of the Ni-Cr-W system at 1473 K, six diffusion couples were chosen in fcc single phase region to prepare in the present work which are listed in Table 1. The diffusion couples were prepared with following steps:

First, the samples were melted into alloy ingots by arc

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Table 1 Nominal compositions for the diffusion couples in this work

Couple name	Diffusion couple/at%	Annealing temperature/K	Annealing time/h
A1	Ni/Ni-10.9Cr-7.5W	1473	72
A2	Ni/Ni-5.5Cr-8.5W	1473	72
B1	Ni-10.8Cr/Ni-8W	1473	72
B2	Ni-21Cr/Ni-8W	1473	72
B3	Ni-10.5Cr/Ni-4.5W	1473	72
B4	Ni-21Cr/Ni-4.5W	1473	72

melting with argon atmosphere according to the composition shown in Table 1. Arc melting was repeated five times, in order to ensure each of the alloy ingots obtained homogeneously. Then, the alloy blocks were linearly cut into suitably sized bars of 4 mm×4 mm×7 mm. Then, all the samples were ground on the SiC papers to remove surface contamination. After that, these small bars were vacuum-packed in quartz tubes, which were placed at a temperature of 1473 K for solution treatment. After five days annealing, the samples were quenched into ice water, in order to cause grain growth and decrease the effect of grain boundary diffusion. Then, every surface used to diffuse which was polished. Afterwards, the diffusion couples were fixed by Mo wires according to Table 1. These diffusion couples were sealed into evacuated quartz tubes and annealed at 1473 K for 72 h, followed by ice water quenching. Then, the couples were cut longitudinally to expose the diffusion interface, and each of the interfaces was polished as before. After standard metallographic preparation, the diffusion couples shown in Table 1, were tested by EPMA (JXA-8100, JEOL, Japan, the accelerating voltage and probe current were 20 kV and 1.0×10^{-8} A, respectively). A local concentration-distance profile was obtained by selecting a straight line through the diffusion interface for line analysis.

1.2 Determination of interdiffusion coefficients

According to Kirkaldy's method[10], the diffusion for a component i of concentration C_i in a ternary system can be described by Fick's second law:

$$\frac{\partial C_i}{\partial t}=\sum_{j=1}^{2}\frac{\partial}{\partial x}\left(\tilde{D}_{ij}^{3}\frac{\partial C_j}{\partial x}\right)\quad i=1,2 \tag{1}$$

where C_i is the concentration of element i, t is the diffusion time, and x is the diffusion distance, $\tilde{D}_{ij}^{3}$ is the interdiffusion coefficient of the ternary system. When i and j take the same value, the diffusion coefficients, $\tilde{D}_{11}^{3}$ and $\tilde{D}_{22}^{3}$, are called the main interdiffusion coefficients. The main diffusion coefficients represent the influence of the concentration gradients of elements 1 and 2 on their own fluxes. When i and j take different values, $\tilde{D}_{12}^{3}$ and $\tilde{D}_{21}^{3}$ are called cross interdiffusion coefficients. The cross diffusion coefficients represent the influences of the concentration gradients of element 2 and element 1 on the fluxes of each other.

For semi-infinite diffusion couples, based on the commonest initial conditions and boundary conditions, we can obtain:

$$\begin{aligned}&C_i(-x,0)=C_i(-\infty,t)=C_i^-\\&C_i(x,0)=C_i(+\infty,t)=C_i^+\end{aligned}\quad i=1,2 \tag{2}$$

then the solutions of Eq. 1 are:

$$\int_{C_i^-}^{C_i^+}x\mathrm{d}C_i=-2t\sum_{j=1}^{2}\tilde{D}_{ij}^{3}\frac{\mathrm{d}C_j}{\mathrm{d}x} \tag{3}$$

In order to avoid Matano interface calculations, Whittle and Green[11] introduced the normalized concentration parameters $Y_i=(C_i-C_i^-)/(C_i^+-C_i^-)$ and then Eq.(3) can become:

$$\frac{1}{2t}\frac{\mathrm{d}x}{\mathrm{d}Y_1}\left[(1-Y_1)\int_{-\infty}^{x}Y_1\cdot\mathrm{d}x+Y_1\int_{x}^{+\infty}(1-Y_1)\cdot\mathrm{d}x\right]=\tilde{D}_{11}^{3}+\tilde{D}_{12}^{3}\frac{C_2^+-C_2^-}{C_1^+-C_1^-}\cdot\frac{\mathrm{d}Y_2}{\mathrm{d}Y_1} \tag{4}$$

$$\frac{1}{2t}\frac{\mathrm{d}x}{\mathrm{d}Y_2}\left[(1-Y_2)\int_{-\infty}^{x}Y_2\cdot\mathrm{d}x+Y_2\int_{x}^{+\infty}(1-Y_2)\cdot\mathrm{d}x\right]=\tilde{D}_{22}^{3}+\tilde{D}_{21}^{3}\frac{C_1^+-C_1^-}{C_2^+-C_2^-}\cdot\frac{\mathrm{d}Y_1}{\mathrm{d}Y_2} \tag{5}$$

In these two equations, there are four diffusion coefficients. In order to obtain the results, two diffusion couples whose diffusion paths cross at a common concentration were demanded.

2 Model Description

Based on the absolute reaction rate theory[12,13], M_w is the atomic mobility of element w, which may be divided into a frequency factor M_w^0 and an activation enthalpy Q_w[14,15]. M_w can be described as:

$$M_w=M_w^0\exp\left(-\frac{Q_w}{RT}\right)\frac{1}{RT}{}^{\mathrm{mg}}\Gamma \tag{6}$$

where R is the gas constant and T is the absolute temperature, ${}^{\mathrm{mg}}\Gamma$ is a magnetic-related transformation factor, which is taken into account of the effect of the ferromagnetic transition[16]. It has been suggested that one should expand the logarithm of the frequency factor, $\ln M_w^0$ rather than the value itself, which approach allows M_w to get another way for expression:

$$M_w=\exp\left(\frac{RT\ln M_w^0}{RT}\right)\exp\left(-\frac{Q_w}{RT}\right)\frac{1}{RT}{}^{\mathrm{mg}}\Gamma \tag{7}$$

For the fcc phase, the ferromagnetic contribution to diffusion is negligible, ${}^{\mathrm{mg}}\Gamma=1$. Then we can use kinetic parameters to combine M_w^0 and Q_w, which is called Φ_w: $\Phi_w=RT\ln M_w^0-Q_w$. $\Phi_w=RT\ln[RTM]$. Φ_w can be represented by the Redlich-Kister polynomia for binary terms[17]. For ternary system solid solution, the kinetic parameters can be expressed as[18]:

$$\Phi_w=\sum_i x_i\Phi_w^i+\sum_i\sum_{j>i}x_ix_j\left[\sum_{r=0}^{m}{}^{r}\Phi_w^{i,j}(x_i-x_j)^r\right]+\sum_i\sum_{j>i}\sum_{k>j}x_ix_jx_k\left[v_{ijk}^{s}\,{}^{s}\Phi_w^{i,j,k}\right]\quad(s=i,j\text{ or }k) \tag{8}$$

where x_i is the mole fraction of element i, Φ_w^i is the value of

Φ_w for pure i and thus represents one of the endpoint value in the composition space. ${}^{r}\Phi_w^{i,j}$ is the binary interaction parameter, ${}^{s}\Phi_w^{i,j,k}$ is for the ternary. For the parameter $v_{i,j,k}^{s}$, it is given by:

$$v_{i,j,k}^{s} = x_s + \left(1 - x_i - x_j - x_k\right)/3 \quad (9)$$

where x_i, x_j, x_k and x_s represent the mole fractions of the elements i, j, k and s, respectively.

Assuming the mono-vacancy atomic exchange mechanism, the tracer diffusivity D_w^* is related to the atomic mobility by the Einstein relation:

$$D_w^* = RTM_w \quad (10)$$

The interdiffusion coefficients with n as the dependent species are correlated to the atomic mobility by:

$$\tilde{D}_{kj}^{n} = \sum_i \left(\delta_{ik} - x_k\right) \cdot x_i \cdot M_i \cdot \left(\frac{\partial \mu_i}{\partial x_j} - \frac{\partial \mu_i}{\partial x_n}\right) \quad (11)$$

where the Kronecker delta δ_{ik}=1 when i=k; otherwise δ_{ik}=0. x_i, μ_i and M_i are the mole fraction, chemical potential and mobility of element i, respectively.

3 Results and Discussion

3.1 Interdiffusion coefficients

Based on the diffusion experiment in the fcc single phase, interdiffusion coefficients $\tilde{D}_{\mathrm{CrCr}}^{\mathrm{Ni}}$, $\tilde{D}_{\mathrm{CrW}}^{\mathrm{Ni}}$, $\tilde{D}_{\mathrm{WW}}^{\mathrm{Ni}}$, $\tilde{D}_{\mathrm{WCr}}^{\mathrm{Ni}}$ can be evaluated on the nine points which are obtained from the diffusion paths intersecting each other in the Gibbs triangle of Ni-rich Ni-Cr-W system via the Whittle and Green method. The experimentally measured main interdiffusion coefficients ($\tilde{D}_{\mathrm{CrCr}}^{\mathrm{Ni}}$, $\tilde{D}_{\mathrm{WW}}^{\mathrm{Ni}}$), the corresponding cross interdiffusion coefficients ($\tilde{D}_{\mathrm{CrW}}^{\mathrm{Ni}}$, $\tilde{D}_{\mathrm{WCr}}^{\mathrm{Ni}}$) and the DICTRA-extracted ones are listed in Table 2. From Table 2, it can be seen that, the main interdiffusion coefficients show all the positive values, while the cross interdiffusion coefficients are positive or negative. The most important information we get is that the values of $\tilde{D}_{\mathrm{CrCr}}^{\mathrm{Ni}}$ is much larger than $\tilde{D}_{\mathrm{WW}}^{\mathrm{Ni}}$. This phenomenon indicates Cr diffuses much faster than W, which is almost 3.7 times on average. So far, All the presently obtained interdiffusion coefficients are further validated by the following constraints[19].

$$\tilde{D}_{\mathrm{CrCr}}^{\mathrm{Ni}} + \tilde{D}_{\mathrm{WW}}^{\mathrm{Ni}} > 0 \quad (12)$$

$$\tilde{D}_{\mathrm{CrCr}}^{\mathrm{Ni}} \cdot \tilde{D}_{\mathrm{WW}}^{\mathrm{Ni}} - \tilde{D}_{\mathrm{CrW}}^{\mathrm{Ni}} \cdot \tilde{D}_{\mathrm{WCr}}^{\mathrm{Ni}} \geqslant 0 \quad (13)$$

$$\left(\tilde{D}_{\mathrm{CrCr}}^{\mathrm{Ni}} - \tilde{D}_{\mathrm{WW}}^{\mathrm{Ni}}\right)^2 + 4\tilde{D}_{\mathrm{CrW}}^{\mathrm{Ni}} \cdot \tilde{D}_{\mathrm{WCr}}^{\mathrm{Ni}} \geqslant 0 \quad (14)$$

Since the obtained interdiffusion coefficients satisfy these constraints which are illustrated in Eqs.(12~14), it can be proved that the obtained interdiffusion coefficients are reasonable.

3.2 Assessment of atomic mobility

The thermodynamic description for Ni-Cr-W system is obtained from the previous work of Gustafson[20]. The calculated isothermal section of the Ni-Cr-W system at 1473 K is presented in Fig.1. The atomic mobilities for the self-diffusion of Ni, W and Cr are taken from Zhang et al[21] and Campbell et al[9]. The atomic mobility parameters for Ni-Cr and Ni-W systems were assessed by Campbell[9]. Because the fcc phase of Cr-W system is metastable, the experimental data is unavailable. For simplification, the impurity diffusion coefficient of Cr in the hypothetical fcc-W is assumed to be equivalent to the self-diffusion coefficient of fcc-W, and the impurity diffusion coefficient of W in the hypothetical fcc-Cr is set to be equal to the self-diffusivity of Cr in the fcc-Cr in the present work. The similar assumption has been taken in a large amount of work[22,23].

The atomic mobilities from literatures are listed in Table3. Based on the existing binary atomic mobilities in Table 3 and the experimental interdiffusion coefficients in Table 2, the atomic mobilities for fcc ternary Ni-Cr-W alloys were assessed in the PARROT module of the DICTRA software. All of the atomic mobility parameters for Ni-Cr-W alloys are listed into Table 3.

Comparison between the calculated main interdiffusion coefficients (numbers in brackets) and the experimental measurements are shown in Fig.2a and Fig.2b. It can be seen that in most cases the agreement between the calculations and the experimental results is very good.

The calculated logarithmic values of the interdiffusion coefficients are compared with the experimental ones in Fig.3. The points located around the diagonal line are the logarithms of the main interdiffusion coefficients obtained in this work, while the dashed lines refer to the diffusion coefficients with a factor of 2 or 0.5 from the model-predicted main diffusion coefficients. Such factor is a generally accepted experimental error for measurement of diffusivities. It indicates that the calculated

Table 2 Experimental interdiffusion coefficients and DICTRA-extracted diffusivities in fcc Ni-Cr-W alloys annealed at 1473 K for 72 h

Intersection diffusion paths	Composition/at%		Interdiffusion coefficient/$\times10^{-15}$ $m^2 \cdot s^{-1}$				DICTRA-extracted diffusivity/$\times10^{-15}$ $m^2 \cdot s^{-1}$			
	Cr	W	$\tilde{D}_{\mathrm{CrCr}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{CrW}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{WW}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{WCr}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{CrCr}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{CrW}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{WW}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{WCr}}^{\mathrm{Ni}}$
A1-B1	4.95	5.03	13.5	6.1	2.8	0.4	11.8	1.4	2.5	0.9
A1-B2	7.31	6.74	13.8	15.3	3.8	1.0	15.6	6.8	8.1	7.9
A1-B3	4.31	3.15	15.8	5.5	3.0	0.3	15.0	0.1	1.9	0.7
A1-B4	4.75	4.60	13.5	6.2	3.1	0.1	12.4	0.6	2.3	1.2
A2-B1	2.98	7.08	8.0	2.7	4.8	3.2	8.6	0.7	2.4	0.5
A2-B2	3.57	7.89	6.8	4.0	3.0	0.5	7.9	1.4	2.9	0.9
A2-B3	2.12	4.30	11.6	2.3	3.2	0.4	13.0	0	2.0	0.2
A2-B4	2.22	4.64	11.8	2.0	3.2	–0.4	12.3	0	2.0	0.3
B1-B4	5.59	4.43	13.7	5.6	2.7	0	7.9	1.4	3.0	0.9

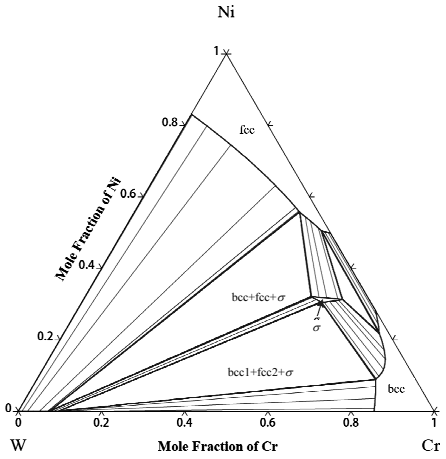

Fig.1 Calculated isothermal section at 1473 K in the Ni-Cr-W system using the thermodynamic parameters of Gustafson[20]

Table 3 Atomic mobility for fcc Ni-Cr-W alloys

Atom	Mobility	Reference
Ni	$Q_{Ni}^{Ni}=-271377.6-81.8T$	[21]
	$Q_{Ni}^{Cr}=-235000.0-82.0T$	[9]
	$Q_{Ni}^{W}=-628250.0-63.5T$	[9]
	$Q_{Ni}^{Ni,Cr}=-81000.0$	[9]
	$Q_{Ni}^{Ni,W}=175736.0$	[9]
	$Q_{Ni}^{Cr,W}=8792319.5$	This work
Cr	$Q_{Cr}^{Cr}=-235000.0-82.0T$	[9]
	$Q_{Cr}^{Ni}=-287000.0-64.4T$	[9]
	$Q_{Cr}^{W}=-311423.0-70.1T$	This work
	$Q_{Cr}^{Cr,Ni}=-68000.0$	[9]
	$Q_{Cr}^{Ni,W}=-237585.4$	This work
W	$Q_{W}^{W}=-311423.0-70.1T$	[9]
	$Q_{W}^{Ni}=-282130.0-87.2T$	[9]
	$Q_{W}^{Cr}=-235000.0-82.0T$	This work
	$Q_{W}^{W,Ni}=-97025.0$	[9]
	$Q_{W}^{Ni,Cr}=-344562.1$	This work

results are in good agreement with the experimental ones.

3.3 Validation of the present atomic mobility

In order to evaluate the reliability of the present mobility database, its application to predict the diffusion behaviors such as the concentration-distance profiles and the diffusion paths of ternary diffusion couples are performed. As shown in Fig.4, the calculated concentration-distance profiles for Cr and W in diffusion couples A1, A2, B1, B2, B3 and B4 annealed at 1473 K for 72 h have been contrasted with the experimentally measured data. It can be clearly seen that the experimental data fit the calculated curves well, which indicates that the atomic mobilities obtained from this experiment are reliable.

Take Fig.4e as an example, in the Ni-10.5Cr/Ni-4.5W diffusion couple, the diffusion distance of Cr is almost 500 μm and the diffusion distance of W in the same condition is almost 200 μm. The reason for this situation is that the diffusion rate

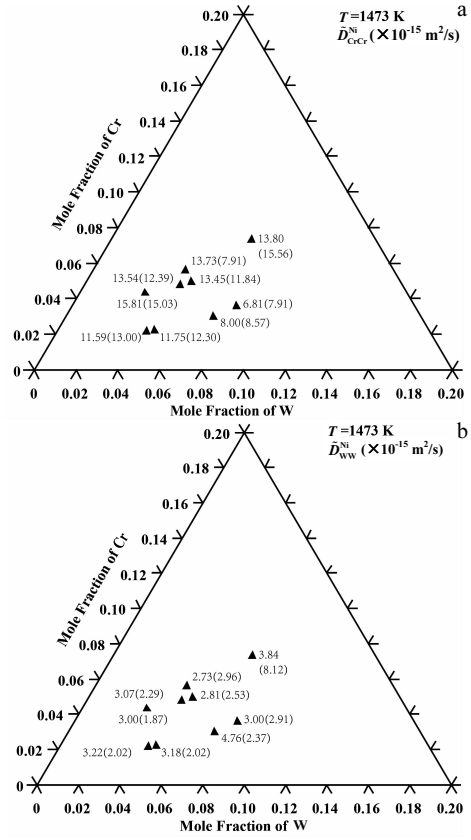

Fig.2 Comparison between the calculated main interdiffusion coefficients (numbers in brackets) and the experimental measurements: (a) $\tilde{D}_{CrCr}^{Ni}$ and (b) $\tilde{D}_{WW}^{Ni}$

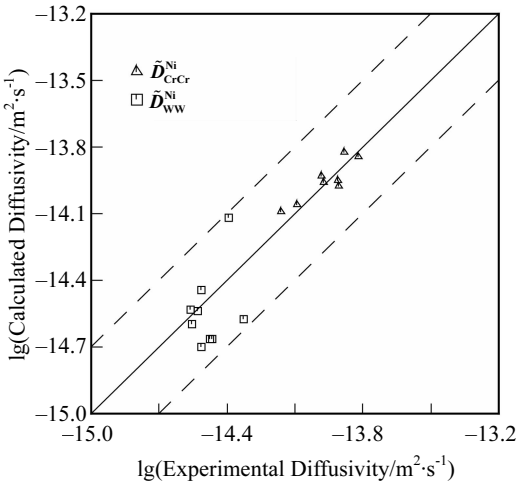

Fig.3 Comparison between the calculated main interdiffusion coefficients of the fcc Ni-Cr-W system at 1473 K and the experimental values

of Cr is much faster than that of W at 1473 K in fcc Ni-Cr-W ternary system. In other words, the interdiffusion coefficient of Cr is much larger than that of W. The comparison of the data

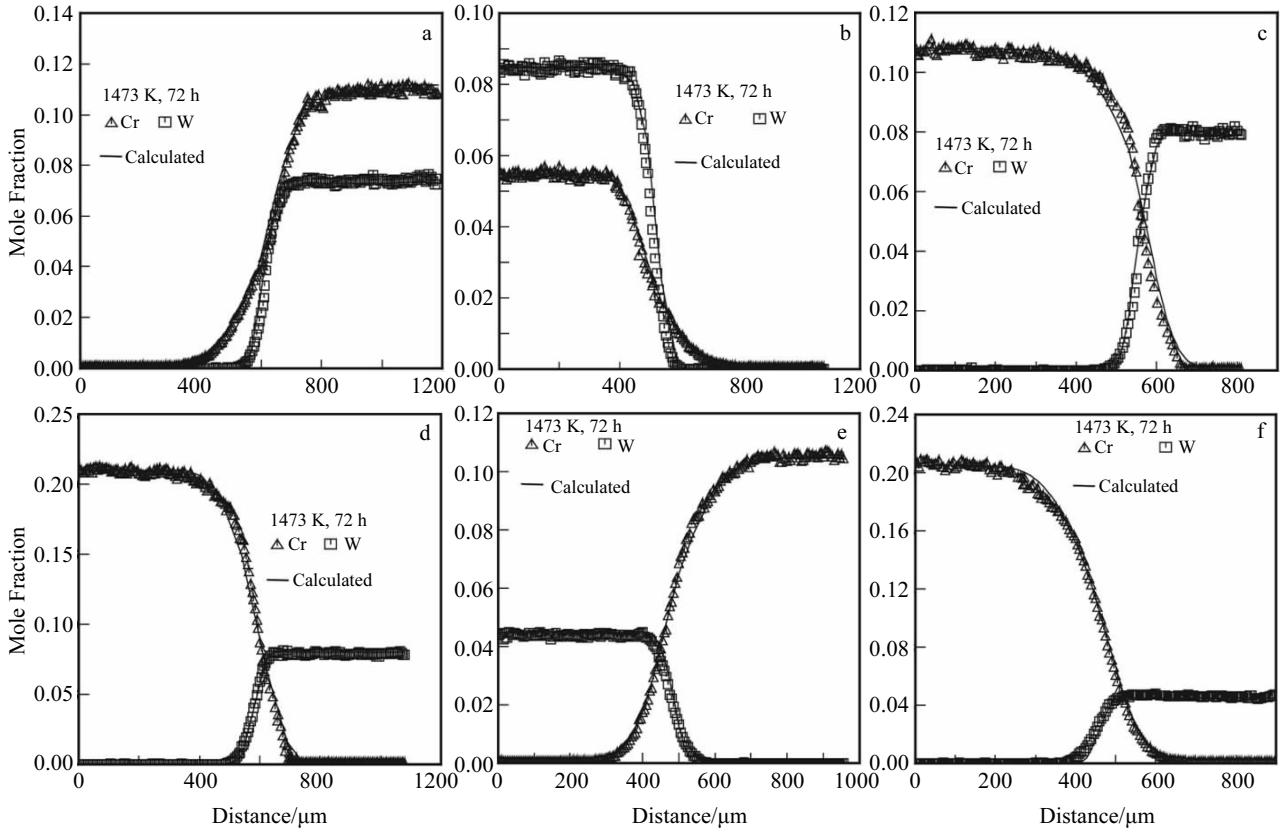

Fig.4 Model-predicted concentration profiles of six diffusion couples annealed at 1473 K for 72 h together with the corresponding experimental ones measured in the present work: (a) A1, (b) A2, (c) B1, (d) B2, (e) B3, and (f) B4

from other diffusion couples' concentration-distance profiles can verify this statement.

Fig.5 shows the diffusion paths for six diffusion couples (A1, A2, B1, B2, B3 and B4) of the Ni-rich corner in fcc Ni-Cr-W ternary system, which is annealed at 1473 K for 72 h. The S-shaped diffusion paths are observed, which is caused by the difference in diffusion coefficients and the mass balance of the diffusion species in solid-solid diffusion couples. As can be seen from this figure, the diffusion paths almost cover the whole region of the fcc phase in Ni-Cr-W alloys and the calculated results have a good agreement with the experimental data, which also proves the validity of the mobility parameters.

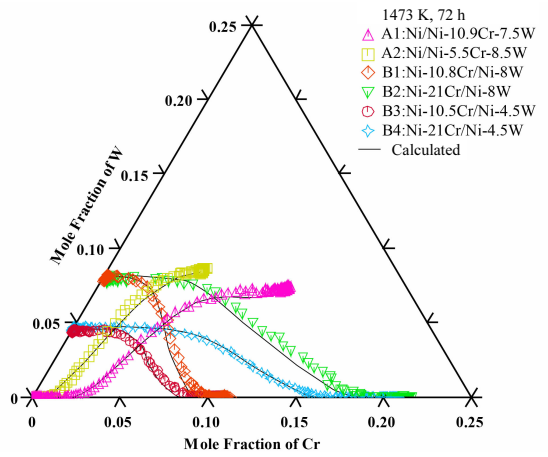

Fig.5 Comparison between the calculated and the measured diffusion paths for the six diffusion couples (A1, A2, B1, B2, B3 and B4) annealed at 1473 K for 72 h

4 Conclusions

1) The interdiffusion coefficients are obtained from six diffusion couples of fcc Ni-Cr-W alloys prepared at 1473 K for 72 h by EPMA and Whittle-Green method. Using DICTRA software package via the measured experimental data and thermodynamic description, the atomic mobilities of Ni, Cr and W in Ni-Cr-W ternary system can be assessed.

2) A good agreement is obtained from comprehensive comparison between calculated and the experimental results.

3) The diffusion phenomena such as concentration-distance profiles and diffusion paths can be reasonably described. In Ni-Cr-W ternary system, Cr diffuses much faster than W in the Ni-rich alloys.

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Ni-Cr-W 三元系富 Ni 侧 fcc 相的互扩散及原子迁移率研究

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摘　要：利用电子探针微量分析与 Whittle-Green 方法确定了在 1200 ℃下退火 72 h 的 Ni-Cr-W 三元合金体系的互扩散系数。通过 DICTRA 软件包对实验互扩散系数进行评估以确定原子迁移率。通过全面分析比较模型预测的扩散特性和实验数据的良好一致性验证了原子迁移率的合理性。 Ni-Cr-W 三元体系中的扩散现象，如扩散路径和浓度-距离曲线可以通过获得的原子迁移率合理地描述，进一步证明了本研究所获得的原子迁移率参数的可靠性。

关键词：Ni-Cr-W 合金；原子迁移率；扩散偶；互扩散系数；DICTRA

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