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ARTICLE

Interdiffusion and Atomic Mobilities in Ni-rich fcc Ni-Nb-Ti Alloys

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Abstract: Experimental diffusion data in Ni-rich fcc Ni-Nb-Ti alloys at 1273 K was measured by electronic-probe microanalysis and the interdiffusion coefficients have been determined using Whittle and Green method. The atomic mobilities of Ni, Nb and Ti in Ni-Nb-Ti alloys have been obtained through assessing the interdiffusion data critically with the DICTRA software. Comprehensive comparisons between calculated and experimental diffusion coefficients show that the atomic mobilities obtained in this work could well reproduce the experimental data. And the validity of the diffusion mobilities was tested by simulating the concentration-distance profiles and diffusion paths in diffusion couples.

Key words: Ni-Nb-Ti alloys; atomic mobility; interdiffusion coefficients; diffusion couples; DICTRA

The Ni-based superalloys are widely used in aerospace industry because of their excellent mechanical properties at temperature close to their melting points. The Ni-Ti binary system is a subsystem for Ni-based superalloys. Nb is also an important traditional alloying element in Ni-based superalloys. The addition of Nb in Ni-Ti system can improve its ductility and expand thermal hysteresis[1-3]. Therefore, the Ni-Nb-Ti ternary system is significant for the exploration of the Ni-based superalloys. Knowledge of the kinetic characteristics of Ni-Nb-Ti alloys is of extreme importance, as diffusion process plays a very important role in governing much of heat treatment processing of Ni-based alloys, and it has a key effect on the microstructures and performance of alloys. Such information is very helpful not only in estimating the life time of alloys under long-term service but also in dealing with processing designs.

It is realized that the DICTRA (DIffusion Controlled TRAnsformation) software program which is an extension of the CALPHAD (CALculation of PHAse Diagram) approach and operates under the CALPHAD framework[4-8], is very useful to evaluate the atomic mobilities to establish kinetic databases. Combining the atomic mobility databases and the thermodynamic databases, various kinds of diffusion information can be calculated and the calculated results are very important for the assessment of the atomic mobility parameters.

Up to now, while many experiments have been carried out to determine the atomic mobilities of Ni-based alloys, including the binary Ni-Ti,[9] Ni-Nb[10] systems, the atomic mobilities for Ni-Nb-Ti ternary system are still unavailable in the literature. The main purposes of this study are listed as follows: (i) to experimentally measure the inter-diffusivities of the fcc Ni-Nb-Ti alloys at the temperature of 1273 K with solid-solid diffusion couples; (ii) to assess the atomic mobilities of the fcc phase for Ni-Nb-Ti alloy system; (iii) to simulate the diffusion paths and concentration profiles with the obtained mobility parameters; (iv) to examine the consistency between the simulated results and the experimental data.

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1 Experiment Procedure

1.1 Preparation of diffusion couples

Ni (purity: 99.9 wt%), Nb (purity: 99.9 wt%) and Ti (purity: 99.98 wt%) were used as starting materials. In order to cover most of the concentration regime in fcc single phase region, six diffusion couples, as shown in Table 1, were prepared in the following steps:

Firstly, all the alloys with the nominal composition listed in Table 1 were prepared in the form of 30 g ingots by arc melting under an argon atmosphere. The ingots were melted for five times to make sure that the composition was homogeneous.

Secondly, these alloy ingots were cut into blocks in size of 4 mm×4 mm×7 mm by wire-electrode discharging machining. These small blocks were solid-solution treated under vacuum in quartz capsules at 1273 K for 4 d to promote homogenization and grain growth. Then the surfaces of the samples were polished through 0.05 μm alumina for good bonds.

Subsequently, the diffusion couples were bound by Mo wires and then encapsulated in evacuated quartz tubes. These couples were annealed at 1273 K for 5 d and quenched in the ice water. After standard metallographic preparation, these annealed diffusion couples were examined by EPMA (JXA-8100, JEOL, Japan, the accelerating voltage and probe current were 20 kV and 1.0×10^{-8} A, respectively) to measure the local concentration-distance profiles.

1.2 Determination of interdiffusion coefficients

According to Kirkaldy[11], in a ternary alloy where component 3 represents the solvent, and Fick's second law of diffusion for a component i of concentration C_i in a ternary system can be solved as

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

where x stands for the distance, t represents time, C_i is concentration of element i, and $\tilde{D}_{ij}^{3}$ are the interdiffusion coefficients. The main interdiffusion coefficients, $\tilde{D}_{11}^{3}$ and $\tilde{D}_{22}^{3}$, reflect how much the concentration gradients of elements 1 and 2 affect their own fluxes. And $\tilde{D}_{12}^{3}$ and $\tilde{D}_{21}^{3}$ are the cross interdiffusion coefficients which stand for the influences of the concentration gradients of element 2 and element 1 on the fluxes of each other, respectively.

Table 1 Nominal composition for the diffusion couples in this work

Diffusion couple	Composition/at%	Temperature/K	Diffusion time/s
A1	Ni-2.20Nb/Ni-1.80Ti	1273	432 000
A2	Ni-4.70Nb/Ni-3.31Ti	1273	432 000
A3	Ni-4.70Nb/Ni-5.35Ti	1273	432 000
A4	Ni-4.70Nb/Ni-8.56Ti	1273	432 000
B1	Ni/Ni-5.27Nb-2.08Ti	1273	432 000
B2	Ni/Ni-1.29Nb-6.99Ti	1273	432 000

In semi-infinite diffusion couples, based on usual initial and boundary conditions, we have

$$C_i(-x,0)=C_i(-\infty,t)=C_i^{-}$$
$$C_i(x,0)=C_i(+\infty,t)=C_i^{+} \quad \text{for } i=1, 2 \tag{2}$$

then the solutions of Eq.(1) are:

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

To avoid the calculating of Matano interface, Whittle and Green[12] introduced the normalized concentration parameter $Y_i=(C_i-C_i^{-})/(C_i^{+}-C_i^{-})$, and then the Eq.(3) becomes:

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

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

Then we need two diffusion couples of which diffusion paths have a common concentration point, to determine the four diffusion coefficients in Eqs.(4) and (5).

2 Model Description

According to absolute-reaction rate theory[13,14], the mobility coefficient for an element α, M_α, may be solved with a frequency factor M_α^0 and an activation enthalpy Q_α [4,15],

$$M_\alpha=M_\alpha^0\exp(-\frac{Q_\alpha}{RT})\frac{1}{RT}{}^{\mathrm{mg}}\Gamma \tag{6}$$

where R is the gas constant and T represents the absolute temperature, and ${}^{\mathrm{mg}}\Gamma$ is a factor considering the influence of the ferromagnetic transition[16], which is a function of the alloy composition. It has been suggested that one should expand the logarithm of the frequency factor, ln M_α^0 rather than the value itself. Thus the mobility, M_α can be transformed to:

$$M_\alpha=\exp(\frac{RT\ln M_\alpha^0}{RT})\exp(-\frac{Q_\alpha}{RT})\frac{1}{RT}{}^{\mathrm{mg}}\Gamma \tag{7}$$

for the fcc phase, the ferromagnetic contribution to diffusion can be ignored. Then M_α^0 and Q_α can be transformed to one parameter: $\Phi_\alpha=RT\ln M_\alpha^0-Q_\alpha$, and Φ_α can be expressed by the Red lich-Kister polynomial[17] for binary terms and a power series expansion for ternary terms[18]:

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

where x_i stands for the mole fraction of element i, Φ_α^i is the value of Φ_α for pure i and thus represents one of the endpoint value in the composition space, ${}^{r}\Phi_\alpha^{i,j}$ and ${}^{s}\Phi_\alpha^{i,j,k}$ represent binary and ternary interaction parameters. For the

parameter v_{ijk}^{s}, it can be solved as:

$$v_{ijk}^{s} = x_s + (1 - x_i - x_j - x_k)/3 \quad (9)$$

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

The diffusion mobility can be related to the diffusion coefficient, assuming a mono-vacancy mechanism coupled neglecting correlation factors, the tracer diffusion coefficient D_{α}^{*} is directly related to the mobility M_{α} by the Einstein relation as:

$$D_{\alpha}^{*} = RTM_{\alpha} \quad (10)$$

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

$$\tilde{D}_{ij}^{n} = \sum_{i}(\delta_{ik} - x_k) \cdot x_i \cdot M_i \cdot (\frac{\partial \mu_i}{\partial x_j} - \frac{\partial \mu_i}{\partial x_n}) \quad (11)$$

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

3 Results and Discussion

3.1 Interdiffusion coefficients

In this work, four interdiffusion coefficients $\tilde{D}_{\mathrm{TiTi}}^{\mathrm{Ni}}$, $\tilde{D}_{\mathrm{TiNb}}^{\mathrm{Ni}}$, $\tilde{D}_{\mathrm{NbNb}}^{\mathrm{Ni}}$, $\tilde{D}_{\mathrm{NbTi}}^{\mathrm{Ni}}$ were determined at the intersection composition of the diffusion paths based on the Whittle and Green method, using Eqs.(4) and (5). The experimentally measured major interdiffusion coefficients and the corresponding minor interdiffusion coefficients, as well as the DICTRA-extracted ones, are given in Table 2. It can be seen that the major interdiffusion coefficients and the minor interdiffusion coefficients are positive. Meanwhile, the value of $\tilde{D}_{\mathrm{TiTi}}^{\mathrm{Ni}}$ is larger than $\tilde{D}_{\mathrm{NbNb}}^{\mathrm{Ni}}$, on average, by 1.5 times. This indicates that Ti diffuses faster than Nb. All the presently obtained interdiffusion coefficients are further validated by the following constraints[19],

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

$$\tilde{D}_{\mathrm{TiTi}}^{\mathrm{Ni}} \cdot \tilde{D}_{\mathrm{NbNb}}^{\mathrm{Ni}} - \tilde{D}_{\mathrm{TiNb}}^{\mathrm{Ni}} \cdot \tilde{D}_{\mathrm{NbTi}}^{\mathrm{Ni}} \geq 0 \quad (13)$$

$$(\tilde{D}_{\mathrm{TiTi}}^{\mathrm{Ni}} - \tilde{D}_{\mathrm{NbNb}}^{\mathrm{Ni}})^2 + 4\tilde{D}_{\mathrm{TiNb}}^{\mathrm{Ni}} \cdot \tilde{D}_{\mathrm{NbTi}}^{\mathrm{Ni}} \geq 0 \quad (14)$$

Substituting the presently obtained interdiffusion coefficients into Eqs. (12~14), it is found that all the constraints can be satisfied. Therefore, the presently measured and calculated interdiffusion coefficients are considered to be reasonable.

3.2 Assessment of atomic mobility

The thermodynamic description for Ni-Nb-Ti system is obtained from the previous work of Matsumono et al[20]. The calculated isothermal section of the Ni-Nb-Ti system at 1273 K is presented in Fig.1. The atomic mobilities for the self-diffusion of fcc Ni are taken from Zhang et al.[21] And the atomic mobilities for Ni-Ti and Ni-Nb systems were assessed by Liu et al[9] and Liu et al[10], respectively. Since the fcc phase of Nb-Ti system is non-equilibrium steady states under common condition, its experimental data is unavailable. For simplification, the impurity diffusion coefficient of Ti in the hypothetical fcc-Nb is assumed to be equivalent to the self-diffusion coefficient of fcc-Nb, and the impurity diffusion coefficient of Nb in the hypothetical fcc-Ti is set to be equal to the self-diffusivity of Ti in the fcc-Ti in the present work. Similar assumption has been taken in the work of Zhou et al.[22] The atomic mobilities from literature are listed in Table 3. Based on the existing atomic mobilities in Table 3 and the experimental interdiffusion coefficients in Table 2, the atomic mobilities for fcc ternary Ni-Nb-Ti alloys were assessed in the PARROT module of the DICTRA software and the results are listed in Table 3 as well.

Fig.2 illustrates the comparison between the presently calculated main diffusion coefficients and the experimental values. As can be seen, there is a good match between the calculated interdiffusivities and the experimental ones. The calculated logarithmic values of main interdiffusion coefficients are equal to the experimental ones along the diagonal

Table 2 Experimental interdiffusion coefficients and DICTRA-extracted diffusivities in fcc Ni-Nb-Ti alloys annealed at 1273 K for 432000 s

Intersection diffusion paths	Composition/at%		Interdiffusion coefficient/$\times 10^{-15}$ m^2·s^{-1}				DICTRA-extracted diffusivity/$\times 10^{-15}$ m^2·s^{-1}			
	Ti	Nb	$\tilde{D}_{\mathrm{TiTi}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{TiNb}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{NbNb}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{NbTi}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{TiTi}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{TiNb}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{NbNb}}^{\mathrm{Ni}}$	$\tilde{D}_{\mathrm{NbTi}}^{\mathrm{Ni}}$
A1-B1	0.62	1.38	4.224	0.463	3.587	2.867	2.764	0.573	2.633	0.904
A1-B2	1.52	0.22	5.638	1.981	2.455	0.496	3.186	1.211	2.700	0.224
A2-B1	1.15	2.99	4.018	0.440	3.811	1.094	3.680	1.292	2.839	1.591
A2-B2	2.98	0.46	5.632	1.260	3.743	0.262	4.154	2.217	3.033	0.464
A3-B1	1.28	3.55	3.879	0.482	3.649	1.140	4.046	1.598	3.167	2.014
A3-B2	4.18	0.80	5.373	1.118	3.208	0.238	4.941	3.005	3.336	0.777
A4-B1	1.50	4.32	4.151	0.375	3.164	1.794	4.709	2.159	3.913	2.825
A4-B2	6.01	1.16	4.845	1.743	2.188	0.077	5.928	3.089	3.768	1.100

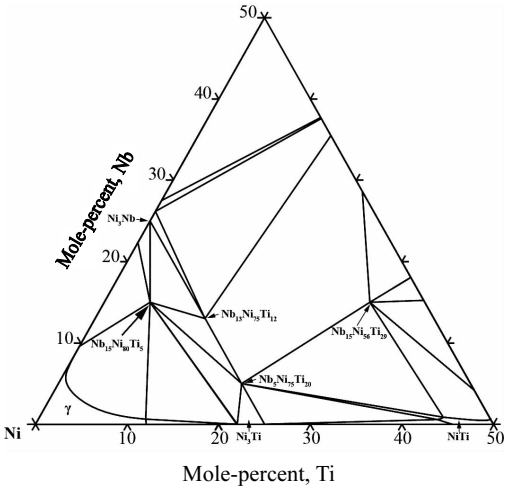

Fig.1 Calculated isothermal section at 1273 K in the Ni-Nb-Ti system using the thermodynamic parameters of Matsumoto et al[20]

Table 3 Assessed atomic mobilities for fcc Ni-Nb-Ti alloys

Atom	Mobility	Reference
Ni	$Q_{\mathrm{Ni}}^{\mathrm{Ni}}=-271377.6-81.79T$	[21]
	$Q_{\mathrm{Ni}}^{\mathrm{Ti}}=-132849.8-81.40T$	[9]
	$Q_{\mathrm{Ni}}^{\mathrm{Ni,Ti}}=351220.4$	[9]
	$Q_{\mathrm{Ni}}^{\mathrm{Nb}}=-217919.25-76.76T$	[10]
	$Q_{\mathrm{Ni}}^{\mathrm{Ni,Nb}}=1236140.21$	[10]
	$Q_{\mathrm{Ni}}^{\mathrm{Ti,Nb}}=-34192823.7$	This work
Ti	$Q_{\mathrm{Ti}}^{\mathrm{Ti}}=-132849.8-81.40T$	[9]
	$Q_{\mathrm{Ti}}^{\mathrm{Ni}}=-276771.3-63.82T$	[9]
	$Q_{\mathrm{Ti}}^{\mathrm{Nb}}=-217919.25-76.76T$	This work
	$Q_{\mathrm{Ti}}^{\mathrm{Ti,Ni}}=-176117.8$	[9]
	$Q_{\mathrm{Ti}}^{\mathrm{Ni,Nb}}=28720$	This work
Nb	$Q_{\mathrm{Nb}}^{\mathrm{Nb}}=-217919.25-76.76T$	[10]
	$Q_{\mathrm{Nb}}^{\mathrm{Ni}}=-253446-80.39T$	[10]
	$Q_{\mathrm{Nb}}^{\mathrm{Ti}}=-132849.8-81.40T$	This work
	$Q_{\mathrm{Nb}}^{\mathrm{Nb,Ni}}=-408725.27$	[10]
	$Q_{\mathrm{Nb}}^{\mathrm{Ni,Ti}}=-51776$	This work

line. The dashed lines with a factor of 2 or 0.5 from the diagonal line are shown as well. Such a factor is a generally accepted experimental error for measurement of diffusivities. It can be learned from the good agreement between the calculated results and the experimental ones in Fig.2.

3.3 Validation of the present atomic mobility

Comparison between the calculated diffusion coefficients and the experimental ones is far from enough to verify the reliability of the assessed diffusion mobility. In conjunction with the Ni-Nb-Ti thermodynamic data, the assessed atomic mobility can be used to predict much of the diffusion behavior during experiment. It is necessary to compare the simulated concentration profiles and diffusion paths with the experimental data from this work. Fig.3 presents the comparisons between the calculated and experimental concentration-distance profiles for Ti and Nb in the diffusion couples (A1, A2, A3, A4, B1, B2) annealed at 1273 K for 432 000 s. It is obvious that the calculated results are all in acceptable agreement with the experimental values, which confirms the reliability of the mobilities obtained in this work. As we can see from Fig.3f, Ti diffuses faster than Nb, due to the larger diffusion coefficient of Ti in fcc Ni-Nb-Ti solution.

For a diffusion couple, the degree of eccentricity will increase with increasing difference between the two major diffusion coefficients. If the two major coefficients are equal, the diffusion path curve will degenerate to a straight line. Fig.4 shows the calculated diffusion paths for various ternary diffusion couples (A1, A2, A3, A4, B1, B2) annealed at 1273 K for 432 000 s, compared with the corresponding experimental data. The almost straight diffusion paths are observed in this work, which is caused by the slight difference between the two major diffusion coefficients. As shown in the figure, there exists a good agreement between calculated results and experimental values, which also proves the validity of the mobilities obtained in the present work.

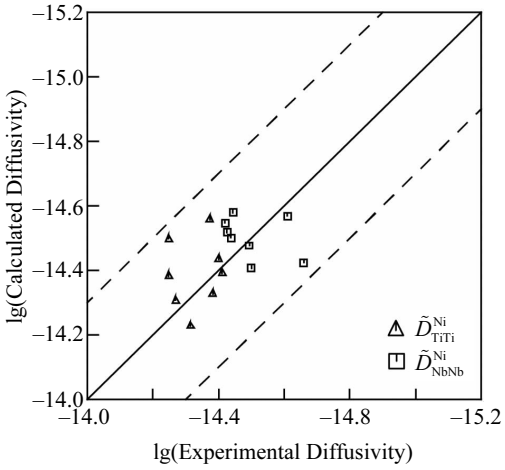

Fig.2 Comparison between the calculated major interdiffusion coefficients of the fcc Ni-Nb-Ti system at 1273 K and the experimental values (dashed lines refer to the diffusion coefficients with a factor of 2 or 0.5 from the model-predicted ones)

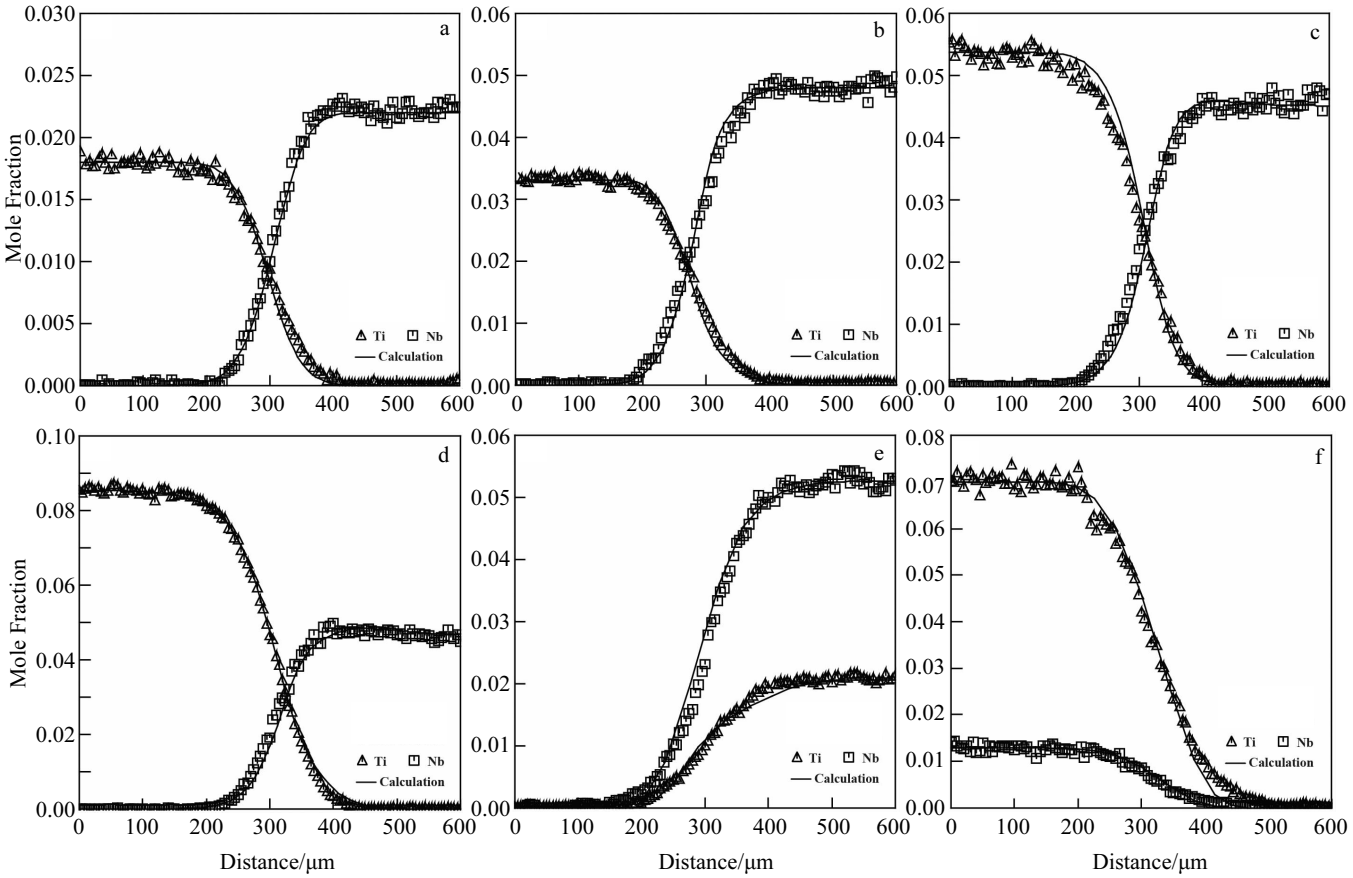

Fig.3 Comparison between the calculated and the measured concentration profiles for the six diffusion couples annealed at 1273 K for 432 000 s: (a) A1, (b) A2, (c) A3, (d) A4, (e) B1, and (f) B2

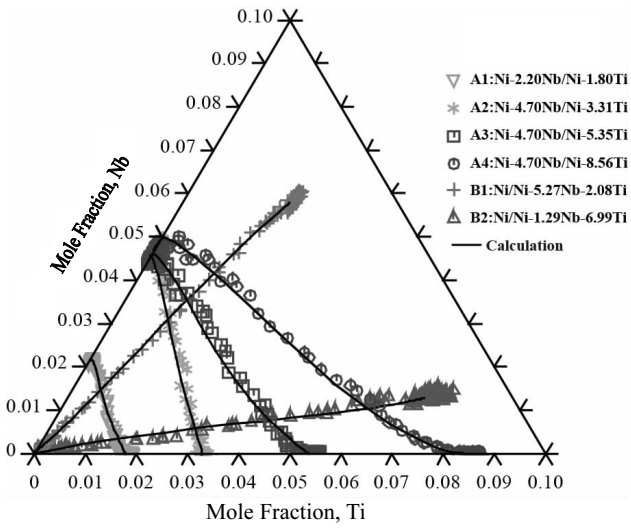

Fig.4 Calculated diffusion paths for various ternary Ni-Nb-Ti diffusion couples annealed at 1273 K for 432 000 s, compared with the experimental data measured in this work

4 Conclusions

1) Interdiffusion coefficients for fcc Ni-Nb-Ti ternary alloys can be determined by means of Whittle and Green method combined with EPMA technique. Based on the available thermodynamic and the experimental diffusivity data, the atomic mobilities in fcc Ni-Nb-Ti alloys can be assessed using the DICTRA software package.

2) There is a good match between calculated interdiffusivities and measured ones. The validation of the atomic mobilities obtained can be also made by successfully simulating the concentration profiles and diffusion paths in the prepared diffusion couples.

3) The atomic mobility obtained in this work can act as a supplement of nickel based alloy diffusion databases and are valuable for the superalloys designing.

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Ni-Nb-Ti 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 EPMA 技术测定了 Ni-Nb-Ti 三元系富 Ni 侧合金在 1273 K 下的扩散数据，并使用 Whittle 和 Green 方法计算了 Ni-Nb-Ti 三元系在 1273 K 下的互扩散系数。通过 DICTRA 软件优化得到 Ni-Nb-Ti 三元系的 fcc 相的原子迁移率，运用优化得到的的原子迁移率计算出的互扩散系数与实验数据具有较好的一致性，从而验证了所得的原子迁移率的可靠性。同时通过运用原子迁移率拟合各扩散偶的的浓度-距离曲线和扩散路径，进一步验证了原子迁移率的合理性。

关键词：Ni-Nb-Ti 合金；原子迁移率；互扩散系数；扩散偶；DICTRA

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