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ARTICLE

Interdiffusion and Atomic Mobilities in Co-rich fcc Co-Cr-V Alloys

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Abstract: Diffusion couples for Co-rich fcc Co-Cr-V alloys were prepared, all of which were annealed at 1473 K for 259200 s. The interdiffusion coefficients in fcc Co-Cr-V ternary systems were investigated by means of Whittle and Green method with the help of electronic-probe microanalysis (EPMA). On the basis of the thermodynamic parameters available in the literature, the interdiffusion data were critically assessed to develop the atomic mobilities of the fcc Co-Cr-V alloys via the DICTRA software. Comprehensive comparisons between the calculated and experimental diffusion coefficients show that the experimental data can be well reproduced by the atomic mobilities obtained in this work. And the validity of the diffusion mobilities was tested by simulating the concentration-distance profiles and diffusion paths in diffusion couples.

Key words: Co-Cr-V alloy; diffusion couple; interdiffusion coefficient; DICTRA; atomic mobility

Co-based superalloys with the γ/γ' microstructure were found to possess higher strength and compressibility than the conventional Ni-based superalloys and offer promise as candidates for the next-generation high temperature materials[1]. It was reported that the addition of V can improve the microstructure and high temperature properties of Co-based superalloys by stabilizing the γ'-phase[2]. Cr is also an important traditional alloying element in Co-based superalloys[3, 4]. The Co-Cr-V ternary system is essential for exploring Co-based superalloys. Because the diffusion process is expected to govern most of heat treatment processing of Co-based alloys and plays a very important role in optimizing material microstructures of Co-Cr-V alloys, it is of great importance to study the kinetic characteristics of Co-Cr-V alloys.

In the past few decades, the DICTRA (DIffusion Controlled TRAnsformation) software 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[5-9]. Based on the thermodynamic and mobility parameters, this software can be used to evaluate the atomic mobilities to establish a kinetic database. So far, only a few Co-based ternary systems have been assessed[10-16]. However, the atomic mobility for the Co-Cr-V ternary system has not been studied. The major purposes of this work are: (1) to experimentally measure the inter-diffusivities of the fcc Co-Cr-V alloys at the temperature of 1473 K; (2) to assess the atomic mobilities of Co-Cr-V systems based on the present experimental results as well as literatures through the DICTRA software package; (3) to verify the reliability of the obtained mobility parameters by comparing the calculated interdiffusion coefficients, concentration profiles and diffusion paths with the corresponding experimental data in the diffusion couples.

1 Experiment

1.1 Preparation of diffusion couples

Co (purity: 99.9 wt%), Cr (purity: 99.99 wt%) and V (purity: 99.95 wt%) were used as raw materials. Five diffusion couples, as shown in Table 1, were prepared in the following steps. Every alloy ingot with the nominal composition listed in Table 1, was prepared by arc melting under an argon atmosphere. The arc melting was repeated 5 times to attain a homogeneous

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composition. Then the alloy blocks were linearly cut into suitably sized bars of 4 mm×4 mm×4 mm. Next, these small bars were solid-solution treated under vacuum in quartz capsules at 1473 K for 5 d followed by ice water quenching to cause grain growth and decrease the effect of grain boundary diffusion. After that, the diffusion surface of each sample was polished to a mirror-like quality. Then the polished samples were bound together by Mo wires to form five diffusion couples with end-members, as shown in Table 1. These diffusion couples were sealed in evacuated quartz tubes and annealed at 1473 K for 259 200 s followed by ice water quenching. After the standard metallographic preparation, these annealed diffusion couples were examined by electronic-probe microanalysis (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[17], Fick's second law of diffusion for a component i of concentration C_i in a ternary system can be given as

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

where, x is distance, t represents time, C_i is concentration of element i, and $\tilde{D}_{ij}^{3}$ are the interdiffusivity in which component 3 represents the solvent. The main interdiffusion coefficients, $\tilde{D}_{11}^{3}$ and $\tilde{D}_{22}^{3}$, represent the influence of the concentration gradients of elements 1 and 2 on their own fluxes. While $\tilde{D}_{12}^{3}$ and $\tilde{D}_{21}^{3}$ are the cross interdiffusion coefficients which represent the influences of the concentration gradients of element 2 and element 1 on the fluxes of each other.

Under the usual initial and boundary conditions prevalent for semi-infinite diffusion couples, we have

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

Then the solutions of Eq.(1) is

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

To avoid calculating the Matano interface, Whittle and Green[18] introduce a normalized concentration parameter $Y_i=(C_i-C_i^-)/(C_i^+-C_i^-)$, then Eq.(3) can be transformed to:

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

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

To solve the four diffusion coefficients in Eq.(4) and Eq.(5), two diffusion couples are required whose diffusion paths intersect at a common concentration.

Table 1 List of nominal composition for the diffusion couples in this work

Couple	Composition/at%	Temperature/K	Time/s
A1	Co/Co-20Cr-10V	1473	259 200
A2	Co/Co-10.06Cr-19.4V	1473	259 200
B1	Co-5.2Cr/Co-15V	1473	259 200
B2	Co-10Cr/Co-14.9V	1473	259 200
B3	Co-14.7Cr/Co-10V	1473	259 200

2 Model

According to absolute-reaction rate theory[19, 20], the mobility coefficient M_{B} for an element B can be divided into a frequency factor M_B^0 and an activation enthalpy Q_B [5, 21]:

$$M_B=M_B^0\exp(-\frac{Q_B}{RT})\frac{1}{RT}{}^{\mathrm{mg}}\Gamma \tag{6}$$

where R is the gas constant and T is the absolute temperature, ${}^{\mathrm{mg}}\Gamma$ is a factor taking into account the effect of the ferromagnetic transition[22], which is a function of the alloy composition. It has been suggested that one should expand the logarithm of the frequency factor, $\ln M_B^0$, instead of the value itself. Thus the mobility M_{B} is expressed as:

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

for the fcc phase, the ferromagnetic contribution to diffusion is negligible, and then M_B^0 and Q_B can be merged into one parameter: $\varPhi_B=RT\ln M_B^0-Q_B$, $\varPhi_{\mathrm{B}}$ can be represented by the Redlich-Kister polynomial[23] for binary terms and a power series expansion for ternary terms[24]:

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

$$s=i,j\text{ or }k \tag{8}$$

where, x_i is the mole fraction of element i, $\varPhi_B^i$ is the value of $\varPhi_B$ for pure i which represents an endpoint value in the composition space, ${}^{r}\varPhi_B^{i,j}$ and ${}^{s}\varPhi_B^{i,j,k}$ represent binary and ternary interaction parameters, respectively. For the parameter v_{ijk}^{s}, it can be expressed as:

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

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

The diffusion mobility can be related to the diffusion coefficient. Assuming a coupled mono-vacancy mechanism neglecting correlation factors, the tracer diffusivity D_B^* is directly related to the mobility M_B by means of the Einstein relation:

$$D_B^*=RTM_B \tag{10}$$

The interdiffusion coefficient with n as a dependent species is correlated to the atomic mobility:

$$\tilde{D}_{kj}^{n}=\sum_i(\delta_{ik}-x_k)x_iM_i(\frac{\partial\mu_i}{\partial x_j}-\frac{\partial\mu_i}{\partial x_n}) \tag{11}$$

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

3 Results and Discussion

3.1 Interdiffusion coefficients

Using Eqs.(4) and (5), four interdiffusion coefficients $\tilde{D}^{\mathrm{Co}}_{\mathrm{CrCr}}$, $\tilde{D}^{\mathrm{Co}}_{\mathrm{CrV}}$, $\tilde{D}^{\mathrm{Co}}_{\mathrm{VV}}$, $\tilde{D}^{\mathrm{Co}}_{\mathrm{VCr}}$ were determined at the intersection composition of the diffusion paths based on the Whittle and Green method. Table 2 lists the main interdiffusion coefficients and corresponding cross interdiffusion coefficients measured experimentally, as well as the DICTRA-extracted ones. The main interdiffusion coefficients show the positive values, while the cross interdiffusion coefficients are positive or negative. The value of $\tilde{D}^{\mathrm{Co}}_{\mathrm{VV}}$ is larger by about a half-order of magnitude than that of $\tilde{D}^{\mathrm{Co}}_{\mathrm{CrCr}}$, indicating that V diffuse faster than Cr. Meanwhile, the main interdiffusivities $\tilde{D}^{\mathrm{Co}}_{\mathrm{CrCr}}$ and $\tilde{D}^{\mathrm{Co}}_{\mathrm{VV}}$ are generally larger than the absolute values of $\tilde{D}^{\mathrm{Co}}_{\mathrm{CrV}}$ and $\tilde{D}^{\mathrm{Co}}_{\mathrm{VCr}}$. All the presently obtained interdiffusion coefficients are further validated by the following constraints[25]:

$$\tilde{D}^{\mathrm{Co}}_{\mathrm{CrCr}} + \tilde{D}^{\mathrm{Co}}_{\mathrm{VV}} > 0 \tag{12}$$

$$\tilde{D}^{\mathrm{Co}}_{\mathrm{CrCr}} \cdot \tilde{D}^{\mathrm{Co}}_{\mathrm{VV}} - \tilde{D}^{\mathrm{Co}}_{\mathrm{CrV}} \cdot \tilde{D}^{\mathrm{Co}}_{\mathrm{VCr}} \ge 0 \tag{13}$$

$$(\tilde{D}^{\mathrm{Co}}_{\mathrm{CrCr}} - \tilde{D}^{\mathrm{Co}}_{\mathrm{VV}})^2 + 4\tilde{D}^{\mathrm{Co}}_{\mathrm{CrV}} \cdot \tilde{D}^{\mathrm{Co}}_{\mathrm{VCr}} \ge 0 \tag{14}$$

Substituting the presently obtained interdiffusion coefficients into Eqs.(12~14), it is found that they satisfy these constraints. Therefore, the presently obtained interdiffusivities are considered to be reasonable.

Table 2 Experimental interdiffusion coefficients and DICTRA-extracted diffusivities in fcc Co-Cr-V alloys annealed at 1473 K for 259200 s

Intersection diffusion path	Composition/at%		Interdiffusion coefficient/×10^{-15} m^2·s^{-1}				DICTRA-extracted diffusivity/×10^{-15} m^2·s^{-1}			
	Cr	V	$\tilde{D}^{Co}_{\mathrm{CrCr}}$	$\tilde{D}^{\mathrm{Co}}_{\mathrm{CrV}}$	$\tilde{D}^{\mathrm{Co}}_{\mathrm{VV}}$	$\tilde{D}^{\mathrm{Co}}_{\mathrm{VCr}}$	$\tilde{D}^{\mathrm{Co}}_{\mathrm{CrCr}}$	$\tilde{D}^{\mathrm{Co}}_{\mathrm{CrV}}$	$\tilde{D}^{\mathrm{Co}}_{\mathrm{VV}}$	$\tilde{D}^{\mathrm{Co}}_{\mathrm{VCr}}$
A1-B1	4.58	2.96	7.602	1.368	9.790	1.341	9.321	–0.891	10.856	0.540
A1-B2	7.84	4.21	7.760	1.545	9.561	1.508	8.268	–0.534	11.131	–0.139
A1-B3	8.81	4.49	7.234	3.081	9.914	1.492	8.212	–0.405	11.255	–0.141
A2-B1	3.27	7.21	4.756	–0.430	12.434	0.531	4.724	–0.343	9.759	–0.319
A2-B2	4.34	8.79	5.398	–1.391	12.305	2.050	3.901	–0.360	9.690	–0.018
A2-B3	3.43	7.40	5.743	–1.060	11.582	2.165	4.616	–0.347	9.756	–0.275
B1-B3	2.92	7.75	6.982	0.377	13.877	3.314	4.311	–0.297	9.570	–0.280
B2-B3	6.76	5.53	5.183	–0.995	10.765	1.946	6.666	–0.518	10.781	–0.127

3.2 Assessment of atomic mobility

The thermodynamic description for Co-Cr-V system is obtained from the previous work of Zhao et al[26]. The calculated isothermal section of the Co-Cr-V system at 1473 K is presented in Fig.1. The end-members for pure Co are directly taken from Campbell et al[27]. And the atomic mobility parameters of Co-Cr and Co-V systems were assessed by Zhang et al[12] and Liu et al[28], respectively. Because the fcc phase of Cr-V system is metastable, there are no experimental data about it. For simplification, it is assumed that the impurity diffusion coefficient of Cr in the hypothetical fcc-V is equal to the self-diffusion coefficient of fcc-V, and the impurity diffusion coefficient of V 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 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 Co-Cr-V alloys were assessed by the PARROT module of the DICTRA software, and listed in Table 3 as well.

As can be seen in Table 2, the calculated interdiffusivities agree well with the experimental data. Fig.2 presents the

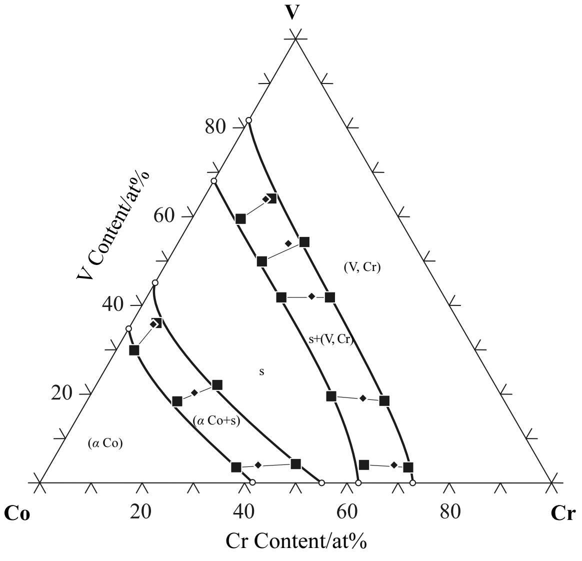

Fig.1 Calculated isothermal section at 1473 K in the Co-Cr-V system using the thermodynamic parameters of Zhao et al[26]

Table 3 Assessed mobility parameters for fcc Co-Cr-V alloys

Mobility	Parameter	Reference
Co	$Q_{\mathrm{Co}}^{\mathrm{Co}} = -286\,175 - 76T$	[27]
	$Q_{Co}^{\mathrm{Cr}} = -23\,5000 - 82T$	[12]
	$Q_{\mathrm{Co}}^{\mathrm{V}} = -197\,683.64 - 79.31T$	[28]
	$Q_{\mathrm{Co}}^{\mathrm{Co,Cr}} = -39\,154.49$	[12]
	$Q_{\mathrm{Co}}^{\mathrm{Co,V}} = 26\,129.87 - 283.98T$	[28]
	$Q_{\mathrm{Co}}^{\mathrm{Cr,V}} = 454\,292.09$	This work
Cr	$Q_{\mathrm{Cr}}^{\mathrm{Cr}} = -235\,000 - 82T$	[12]
	$Q_{\mathrm{Cr}}^{\mathrm{Co}} = -254\,464 - 91.3T$	[12]
	$Q_{\mathrm{Cr}}^{\mathrm{V}} = -197\,683.64 - 79.31T$	This work
	$Q_{\mathrm{Cr}}^{\mathrm{Cr,Co}} = -50\,243.34$	[12]
	$Q_{\mathrm{Cr}}^{\mathrm{Co,V}} = -323\,347.16$	This work
V	$Q_{\mathrm{V}}^{\mathrm{V}} = -197\,683.64 - 79.31T$	[28]
	$Q_{\mathrm{V}}^{\mathrm{Co}} = -282\,275.52 - 74.91T$	[28]
	$Q_{\mathrm{V}}^{\mathrm{Cr}} = -235\,000 - 82T$	This work
	$Q_{\mathrm{V}}^{\mathrm{V,Co}} = -132\,293.66 - 34.95T$	[28]
	$Q_{\mathrm{V}}^{\mathrm{Co,Cr}} = -48\,722.54$	This work

comparison between the main presently calculated diffusion coefficients and the experimental values. The calculated logarithmic values of main interdiffusion coefficients are equal to the experimental ones along the diagonal line, while the dashed lines refer to the diffusion coefficients with a factor of 2 or 0.5 from the model predicted main diffusion coefficients in this work. Such factor is a generally accepted experimental error for measuring the diffusivity, from which it can be indicated that the calculated 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 for predicting the concentration profile and diffusion path of ternary diffusion couples is performed. Fig. 3 presents the comparisons between the calculated concentration

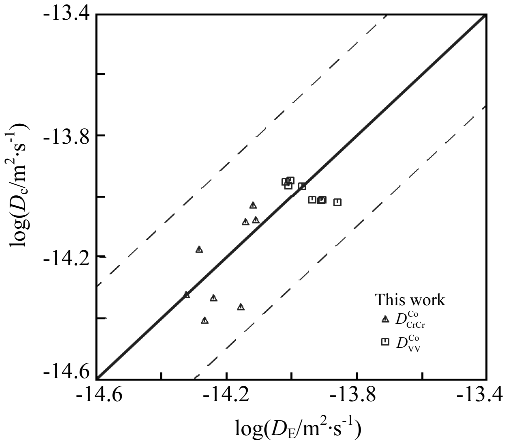

Fig.2 Comparison between the main calculated interdiffusion coefficients of the fcc Co-Cr-V system at 1473 K and the experimental values (dashed lines refer to the diffusion coefficients with a factor of 2 or 0.5 from the model-predicted ones)

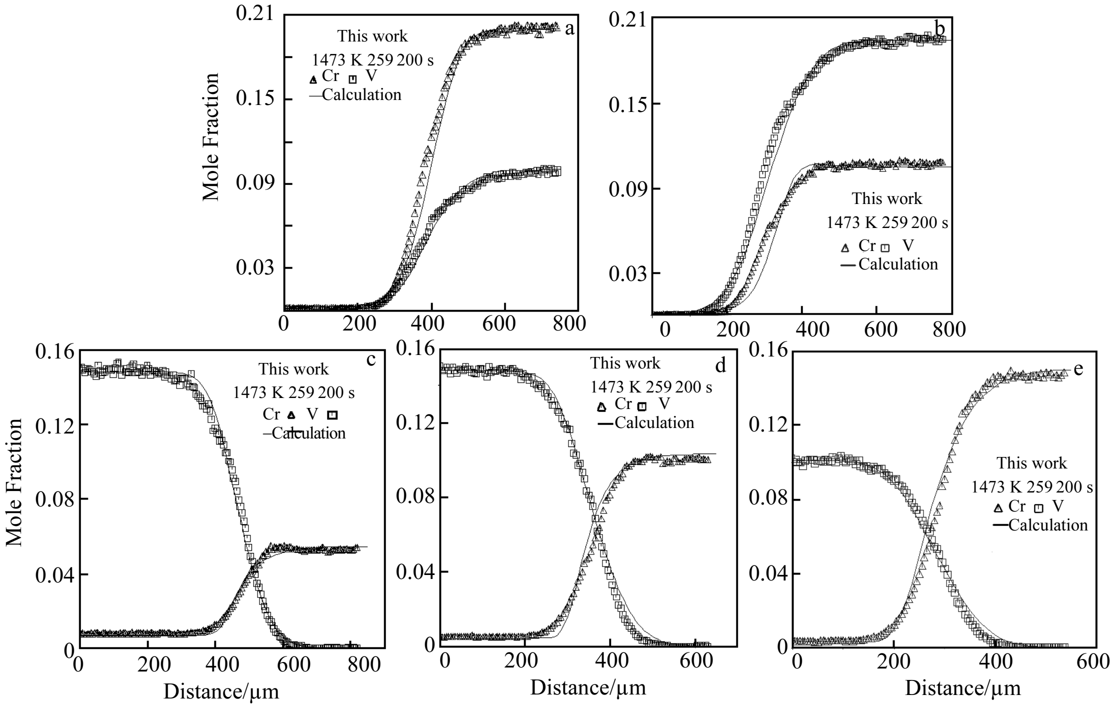

Fig. 3 Comparison between the calculated and the measured concentration profiles of Co/Co-20Cr-10V (a), Co/Co-10.06Cr-19.4V (b), Co-5.2Cr/Co-15V (c), Co-10Cr/Co-14.9V (d), and Co-14.7Cr/Co-10V (e) diffusion couple annealed at 1473 K for 259 200 s

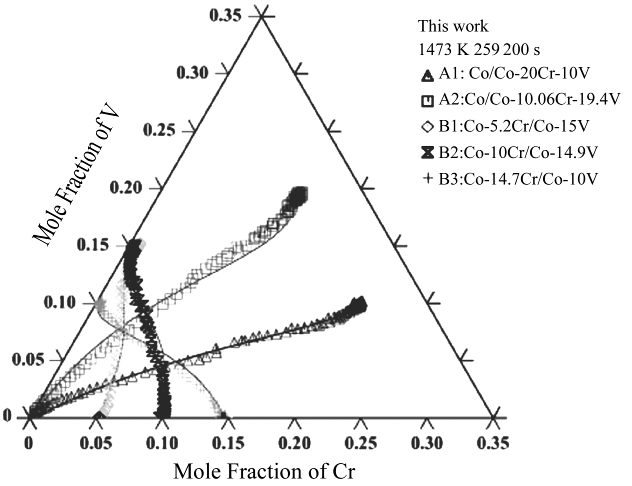

Fig.4 Calculated diffusion paths for various ternary Co-Cr-V diffusion couples annealed at 1473 K for 259200 s, compared with the experimental data measured in this work

-distance profiles of Cr and V in the diffusion couples (A1, A2, B1, B2, B3) annealed at 1473 K for 259200 s and the experimentally measured data. It is obvious that the calculated results are all in acceptable agreement with the experimental values, which confirms the reliability of the mobility parameters obtained in this work. As we can see from Fig.3b, V diffuses faster than Cr, due to the larger diffusion coefficient of V in fcc Co-Cr-V solution.

Fig.4 shows the calculated diffusion paths for various ternary diffusion couples (A1, A2, B1, B2, B3) annealed at 1473 K for 259200 s, compared with the corresponding experimental data. An S-shaped diffusion path can be observed, which is caused by the difference in diffusion coefficients and the mass balance of the diffusion species in solid-solid diffusion couplng [29]. As shown in the figure, there is a good agreement between the calculated results and the experimental values, which also proves the validity of the mobility parameters obtained in the present work.

4 Conclusions

1) Based on the ternary diffusion couples of fcc Co-Cr-V alloys annealed at 1473 K for 259200 s, the interdiffusion coefficients are determined in this work by EPMA together with Whittle and Green method.

2) The atomic mobilities in fcc Co-Cr-V alloys are assessed using the DICTRA software package with the aid of the experimental diffusivity data as well as the related thermodynamic description.

3) A good agreement is obtained by a comprehensive comparison between calculated interdiffusivities and measured ones. The obtained atomic mobility is further validated by successfully evaluating the concentration profiles and diffusion paths in the prepared diffusion couples. The atomic mobility parameters obtained in this work can be beneficial for establishing a general Co-based kinetic database for the design of high-temperature alloys.

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Co-Cr-V 三元系富 Co 侧 fcc 相的互扩散及原子迁移率参数研究

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摘 要：本研究制备了一系列 Co-Cr-V 合金，在 1200 ℃下扩散处理 259200 s。利用电子探针显微分析（EPMA）技术测定了各扩散偶的浓度-距离曲线，并根据测得的浓度-距离曲线用 Whittle and Green 方法计算了 Co-Cr-V 三元系在 1200 ℃下的互扩散系数。基于本研究的实验数据和文献报道的热力学信息和相关子二元系的动力学参数，利用 DICTRA 软件优化得到 Co-Cr-V 体系 fcc 相的原子迁移率参数。运用优化得到的原子迁移率参数计算互扩散系数，并与实验数据比对，取得较好的一致性，从而验证了所得迁移率参数的可靠性。同时运用该迁移率参数计算了各扩散偶的浓度-距离曲线和扩散路径，计算结果与实验数据均符合良好，进一步验证了参数的合理性和准确性。

关键词：Co-Cr-V合金；扩散偶；互扩散系数；DICTRA；原子迁移率参数

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