



## Assessment of atomic mobilities for fcc Co–Ti–V alloys

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### ABSTRACT

Based on the experimental interdiffusion coefficients from our previous work and the critically reviewed experimental diffusivities available in the literature, the atomic mobilities of Co, Ti and V in fcc Co–Ti–V alloys were assessed by means of DICTRA (Diffusion Controlled TRANSformation) software. Askill's empirical relations were utilized to assess the self-diffusion coefficients of fcc Ti and fcc V. Comprehensive comparisons between the DICTRA-calculated diffusivities and the experimental data indicate that the presently obtained atomic mobilities can reproduce most of the diffusivities in binary and ternary systems. In addition, a further verification on the obtained atomic mobilities was carried out through comparing the DICTRA-simulated concentration profiles/diffusion paths of the diffusion couples with the corresponding experimental ones. This work contributes to the establishment of a kinetic database for multi-component cemented carbide.

### 1. Introduction

Cemented carbides are widely used in industry as cutting tools and wear parts, in which fcc Co is often chosen as the binder phase [1]. It has been reported that certain addition of Ti and V can minimize the grain size of WC in Co-bonded cemented carbides, behaving as the grain growth inhibitors [2]. As is well known, diffusion plays a key role in the understanding of phenomena like precipitation, grain growth, homogenization, recrystallization, creep, etc. Therefore, the investigation of the composition-dependent diffusion characteristics is of vital importance in understanding how temperature, time and alloy composition affect the microstructure and properties of targeted materials [3]. Consequently, the investigation of diffusion in Co–Ti–V system, which is an important ternary system for cemented carbides, is of both technological and scientific interests. Traditional technique to compile diffusivities is to present them as composition- and temperature-dependent quantities, which are not convenient for data storage. With the rapid development of CALPHAD (CALculation of PHase Diagram) approach, diffusion data can be stored in the form of atomic mobilities and thermodynamic descriptions separately as functions of temperature

and composition [4,5]. However, there is no investigation on the atomic mobilities of the Co–Ti–V ternary system in the literature yet.

With the recent publication of our measured diffusivities in the Co–Ti–V ternary system [6] as well as experimental measured diffusivities in Co–Ti and Co–V binary systems [7,8], the atomic mobilities of this ternary system can be assessed as functions of temperature and composition.

The purposes of the present work are: (1) to assess all the atomic mobilities in sub-binary alloys using the experimental data available in the literature and Askill's empirical relations; (2) to evaluate the ternary atomic mobilities in fcc Co–Ti–V alloys by means of DICTRA software based on the experimental data, and (3) to verify the reliability of the presently obtained mobility parameters by comparing the DICTRA-calculated diffusivities, DICTRA-simulated concentration profiles and diffusion paths with the corresponding experimental data from various ternary diffusion couples.

### 2. Modeling of atomic mobility

According to the suggestion by Jönsson [9], the atomic mobility  $M_i$

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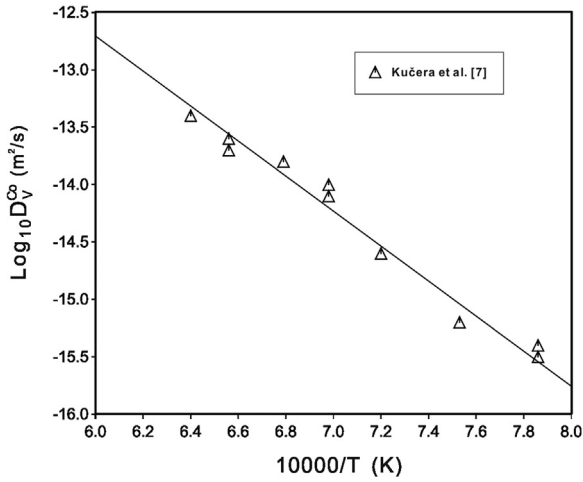


Fig. 1. Comparison between the DICTRA-calculated temperature dependence of impurity diffusion coefficients of V in fcc Co and the experimental values [7].

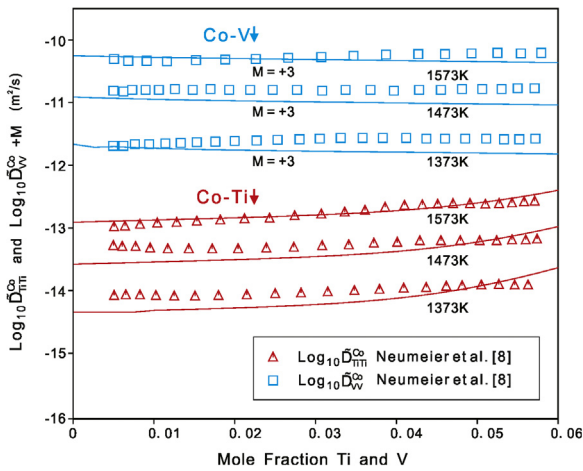


Fig. 2. Comparison between the DICTRA-calculated composition dependent interdiffusivities of fcc Co-Ti and Co-V alloys at 1373, 1473, and 1573 K and the experimental values [8], respectively.

of the component  $i$  could be expressed by an equation of the form:

$$M_i = \frac{M_i^0}{RT} \exp\left(\frac{-Q_i}{RT}\right)^{mg\Omega} \quad (1)$$

where  $R$  is the gas constant and  $T$  is the absolute temperature.  $^{mg\Omega}$  is a factor taking the ferromagnetic contribution into account, and the ferromagnetic contribution to diffusion is negligible for fcc phase. The frequency factor  $M_i^0$  and the activation energy  $Q_i$  are dependent on composition, temperature and pressure in general, and can be merged into one parameter  $\Phi_i$ , which can be expressed by:

$$\Phi_i = -Q_i + RT \ln(M_i^0) \quad (2)$$

According to the CALPHAD method, the composition dependence can be represented by a linear combination of the values at each endpoint of the composition space. Hence, the composition dependence  $-Q_i$  or  $RT \ln M_i^0$  can be described by the Redlich-Kister polynomial [10]:

Table 1

Summary of the atomic mobilities of fcc phase in the Co-Ti-V ternary system assessed in the present work.

Atomic mobilities	Parameters (J/mol)	References
Mobility of Co	$\Phi_{Co}^{Co} = -296542.9 - 74.48 * T$	[13]
	$\Phi_{Co}^{Ti} = -143640 - 80.85 * T$	This work
	$\Phi_{Co}^V = -197683.64 - 79.35 * T$	This work
	$\Phi_{Co}^{Co,Ti} = 950522.02$	This work
	$\Phi_{Co}^{Co,V} = -511752.79$	This work
	Mobility of Ti	$\Phi_{Ti}^{Ti} = -143640 - 80.85 * T$
$\Phi_{Ti}^V = -197683.64 - 79.35 * T$		This work
$\Phi_{Ti}^{Co} = -297017.57 - 58.32 * T$		This work
$\Phi_{Ti}^{Co,Ti} = -152887.73$		This work
$\Phi_{Ti}^{Co,V} = -277083.57$		This work
Mobility of V		$\Phi_V^V = -197683.64 - 79.35 * T$
	$\Phi_V^{Ti} = -143640 - 80.85 * T$	This work
	$\Phi_V^{Co} = -291937.79 - 68.08 * T$	This work
	$\Phi_V^{Co,V} = -244149.15$	This work
	$\Phi_V^{Co,Ti} = -330031.40$	This work

$$\Phi_i = \sum_j x_j \Phi_i^j + \sum_j \sum_{k>j} x_j x_k [\sum_{r=0}^m {}^r\Phi_i^{j,k} (x_j - x_k)^r] + \sum_j \sum_{k>j} \sum_{l>k} x_j x_k x_l [\sum_s v_{jkl}^s {}^s\Phi_i^{j,k,l}]; \quad (s = j, k, l) \quad (3)$$

where  $x_j$ ,  $x_k$  and  $x_l$  are the mole fraction of species  $j$ ,  $k$  and  $l$ , respectively.  $\Phi_i$  represents a temperature-dependent property, i.e.,  $-Q_i$  or/and  $RT \ln M_i^0$ .  $\Phi_i^j$  is the value of  $\Phi_i$  for  $i$  in pure  $j$  and thus represents the value of one endpoint in the composition space.  ${}^r\Phi_i^{j,k}$  and  ${}^s\Phi_i^{j,k,l}$  are binary and ternary interaction parameters need to be assessed.  ${}^r\Phi_i^{j,k}$  can also represent ternary interaction parameter when  $i$ ,  $j$  and  $k$  are not equal to each other. Each individual  $\varphi$  parameter, i.e.,  $\Phi_i^j$ ,  ${}^r\Phi_i^{j,k}$  or  ${}^s\Phi_i^{j,k,l}$ , can be expressed by a polynomial of temperature and pressure if necessary. The parameter  $v_{jkl}^s$  is given by:

$$v_{jkl}^s = x_s + (1 - x_j - x_k - x_l)/3 \quad (4)$$

where  $\varphi_{ave}$ ,  $\varphi_{ave} = (x_{CoSi}^1 - x_{CoSi}^0)^{-1} \cdot \int_{x_{CoSi}^0}^{x_{CoSi}^1} \varphi \cdot dx$ ,  $x_i$  and  $x_{CoSi}^1$  are mole fractions of elements  $j$ ,  $k$ ,  $l$  and  $s$ , respectively.

Assuming that there is a mono-vacancy mechanism for diffusion and correlation factors can be neglected, the tracer diffusivity  $D_i^*$  is related to the atomic mobility  $M_i$  by the Einstein relation [9]:

$$D_i^* = RTM_i \quad (5)$$

The interdiffusion coefficient  $\tilde{D}_{ij}^n$  ( $i, j = 1, 2, \dots, n-1$ ) is modeled with the atomic mobilities by [11]:

$$\tilde{D}_{ij}^n = \sum_i (\delta_{ik} - x_k) x_i M_i \left( \frac{\partial \mu_i}{\partial x_j} - \frac{\partial \mu_i}{\partial x_n} \right) \quad (6)$$

where  $x_i$ ,  $\mu_i$  and  $M_i$  is the mole fraction, chemical potential and atomic mobility of the component  $i$ , respectively.  $\delta_{ik}$  is the Kronecker delta ( $\delta_{ik} = 1$  if  $i = k$ , otherwise  $\delta_{ik} = 0$ ).

### 3. Result and discussion

#### 3.1. Establishment of atomic mobility

The atomic mobility parameters for fcc Co-Ti-V alloys were optimized in the PARROT module of the DICTRA software based on the experimental diffusivities and thermodynamic database. The thermodynamic description of the Co-Ti-V ternary system used in the present

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