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Assessment of Atomic Mobilities for bcc Phase of Ti-Al-V System

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Experimental diffusion data in the literature, in conjunction with existing CALPHAD-based thermodynamic parameters, were used to assess the atomic mobilities for the bcc phase of the Ti-Al-V system by using the DICTRA software. Good agreement was obtained from a comprehensive comparison between the calculated and experimental diffusion coefficients. The atomic mobilities database developed was further validated by appropriate predictions of some diffusion behavior resulting from interdiffusion, especially the concentration profile of diffusion couples.

Keywords atomic mobility, critical assessment, DICTRA modeling, diffusion, Ti-Al-V

1. Introduction

Ti-based alloys have been widely used as aerospace materials, with the Ti-Al-V alloy as one of model materials, due to the excellent combination of their unique mechanical and physical properties, such as high strength-to-weight ratio, high strength under static and fatigue loads, good corrosion resistance, and weldability.[1] It is well known that the microstructures and mechanical properties of the titanium alloys are largely governed by the heat treatment schedule.[2] The knowledge of thermo-kinetics is of crucial importance to design of the heat treatment schedule for the alloys and understanding the microstructural development. The study of thermo-kinetic property is also driven by increasing demands for computer simulation of microstructural evolution, with the phase field approach as one of representatives, developing toward a quantitative model.[3] The DICTRA software (diffusion controlled transformation)[4,5] uses the atomic mobility as a base, rather than various diffusion coefficients, thus technically develops an effective phenomenological way to study diffusion problems with what the CALPHAD approach (calculation of phase diagram) does for phase diagrams.[6] So far, there are currently two commercial thermodynamic databases available for titanium alloys[7,8] and the atomic mobility descriptions for some of the constituent binary systems of the Ti-based alloys[9–11]; however, the mobility database is still missing for the ternary Ti-Al-V system. The purposes of the present work are to assess the atomic mobility for the bcc phase of the Ti-Al and Al-V binaries and then extend the assessment to the Ti-Al-V ternary system by using the DICTRA software, and finally provide insight into diffusion characteristic with simulation of some diffusion couples by applying the assessed atomic mobility parameters.

2. Modeling Description

As suggested by Andersson and Ågren[12] and later modified by Jönsson,[13] the atomic mobility M_i of species i could be described from the absolute reaction rate theory[14] by,

$$M_i = M_i^0 \exp\left(\frac{-Q_i^S}{RT}\right)\frac{1}{RT}{}^{mg}\Gamma, \qquad \text{(Eq 1)}$$

where M_i^0 is the frequency factor, Q_i^S is the activation energy, ${}^{mg}\Gamma$ is the ferromagnetic factor, R is the gas constant, and T is temperature in Kelvin. The first two parts of the mobility parameter can be grouped into a single parameter, i.e., $Q_i = -Q_i^S + RT\ln M_i^0$ if without ferromagnetic effect. Similar to the phenomenological CALPHAD approach, the parameter Q_i is approximated to be compositionally dependent and this can be expressed by a Redlich-Kister polynomial,[15] i.e.,

$$Q_i = \sum_p x_p Q_i^p + \sum_p \sum_{q>p} x_p x_q \left[\sum_{r=0,1,2,\ldots} {}^rQ_i^{p,q}(x_p - x_q)^r\right] + \sum_p \sum_{q>p} \sum_{v>q} x_p x_q x_v \left[v_{pqv}^s \, {}^sQ_i^{p,q,v}\right], \quad (s = p, q, v), \qquad \text{(Eq 2)}$$

where x_p is the mole fraction of species p, Q_i^p is the value Q_i of species i in pure species p, ${}^rQ_i^{p,q}$ and ${}^sQ_i^{p,q,v}$ are the binary and ternary interaction parameters.

Various diffusivities can be directly related to the atomic mobility, e.g., the tracer diffusion coefficient D_i^* is

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rigorously related to the atomic mobility, M_i, by a simple relation,

$$D_i^* = RTM_i, \qquad \text{(Eq 3)}$$

the intrinsic diffusion coefficient, e.g., for a binary alloy with a constant molar volume, by

$$D_i = x_i M_i \left(\frac{\partial \mu_i}{\partial x_i} - \frac{\partial \mu_i}{\partial x_j} \right), \quad j \neq i, \qquad \text{(Eq 4)}$$

where μ_i is the chemical potential of species i, and the interdiffusion coefficients, $\tilde{D}^n_{pq}$, relative to dependent species n, is derived by a form[13]

$$\tilde{D}^n_{pq} = \sum_{i=1}^{n-1} (\delta_{ip} - x_p) x_i M_i \left(\frac{\partial \mu_i}{\partial x_q} - \frac{\partial \mu_i}{\partial x_n} \right), \qquad \text{(Eq 5)}$$

where the Kronecker marker $\delta_{ip} = 1$ when $i = p$ and 0 otherwise. Upon the proposed relations, the mobility parameters in Eq 2, i.e., $Q_i^p, {}^rQ_i^{p,q}$, and ${}^sQ_i^{p,q,v}$, can be numerically assessed by fitting to the experimental diffusion coefficients.

The composition, varying with the diffusion time t in the diffusion zone of diffusion couple, can be described by the equation of continuity,

$$\frac{1}{V_m} \frac{\partial x_i}{\partial t} + \nabla \cdot \tilde{J}_i = 0, \qquad \text{(Eq 6)}$$

where V_m is the molar volume which is generally treated as constant, and $\tilde{J}_i$ is the interdiffusion flux of component i. With different initial conditions and boundary conditions, Eq 6 can be solved numerically to express the form of the concentration profile. If the diffusion process is controlled by a vacancy mechanism, the intrinsic diffusion flux J_i, measured in the lattice-fixed frame of reference, can be introduced to describe the nonuniform one-dimension velocity field $v(z, t)$, i.e.,

$$v(z,t) = -V_m(J_A + J_B) = (D_B - D_A)\frac{\partial x_B}{\partial z}. \qquad \text{(Eq 7)}$$

3. Evaluation of Experimental Data

Some experimental diffusion data are available for the Ti-Al-V bcc alloys, including tracer, impurity, and interdiffusion coefficient.[16-22] In the subsections that follow, the data are evaluated system by system.

3.1 Ti-Al

Goold[16] reported the first comprehensive study of the interdiffusion in the Ti-Al system. Two diffusion couples, Ti/Ti-4 mass% Al and Ti/Ti-8 mass% Al, were made to measure the interdiffusion coefficients over the temperature range, 1107-1523 K, and Kirkendall markers were included in the diffusion couples. Ouchi et al.[17] conducted similar interdiffusional studies in the temperature range between 973 and 1523 K. The interdiffusional coefficients were determined by the Boltzmann-Mantano method without accounting for variation of molar volumes in the concentration. The Al-Ti binary phase diagram shows that the αTi (hcp) → βTi (bcc) allotropic transition occurs near 1155 K and that Al additions raise the transition temperature to ~1125 K for 4 mass% Al and to ~1325 K for 8 mass% Al. Thus at temperatures below the pure Ti transition temperature the diffusion couples were hcp Ti abutting hcp Ti-Al alloys, at intermediate temperatures above the Ti allotropic transition the couples were between bcc Ti and hcp Ti-Al alloys, and at higher temperatures between bcc Ti and bcc Ti-Al alloys. The interesting feature of this investigation was that the Kirkendall markers moved toward the Ti side when the crystallographic structure of both sides was the same but moved toward the Al alloy side when the crystallographic nature differed.

Ti tracer diffusion was studied by Gerold and Herzig[18] for the $Ti_{90}Al_{10}$ and $Ti_{70}Al_{30}$ bcc alloys numerical values in at.%. The results revealed that, similar to the self-diffusivity in bcc-Ti, the Arrhenius plots of the Ti tracer diffusivity were anomalously curved for the two alloys and exhibit negligible concentration dependence within the experimental uncertainty. Interdiffusion coefficients were also determined from these single-phase diffusion couples by using the Boltzmann-Matano method. It was pointed out that Ti diffuses faster than Al when the Al content is less than 25 at.% Al whereas Al becomes a faster diffuser as the Al content increases when $T > 1720$ K. This finding is inconsistent with the previous experimental observations.[16,17]

Araki et al.[19] measured the interdiffusion coefficients from the Ti/Ti-2.1at.%A1 diffusion couple between 1223 and 1573 K by using the Boltzmann-Matano method and by the Hall method for the low composition alloys. Other work using similar techniques was reported by Kainuma and Inden[20] for the temperatures between 1494 and 1591 K. This set of data was extracted from multiphase diffusion couples it likely that interphase boundary diffusion contributed to results; those results were not used in the present work. There is no experimental Al impurity diffusivity in bcc-Ti available because of low-specific activity of ^{26}Al and the difficulty of coating ^{26}A1 on a surface of a pure Ti sample.

All interdiffusion coefficients for the Ti-Al bcc alloys accepted in this work are illustrated in Fig. 1 for comparison. The data from Ouchi et al.,[17] Gerold and Herzig,[18] and Araki et al.[19] agree reasonably over the whole temperature range and were then given the highest weights during the optimizing process, while the other[16] with less agreement and poor purity of raw materials was given a low weight.

3.2 Al-V

Maslov et al.[21] investigated the impurity diffusion of Al in bcc-V over the temperature range 1273-1773 K by the x-ray method.

3.3 Ti-Al-V Ternary System

The ternary interdiffusion coefficients have been recently measured for the Ti-rich ternary bcc alloys over the

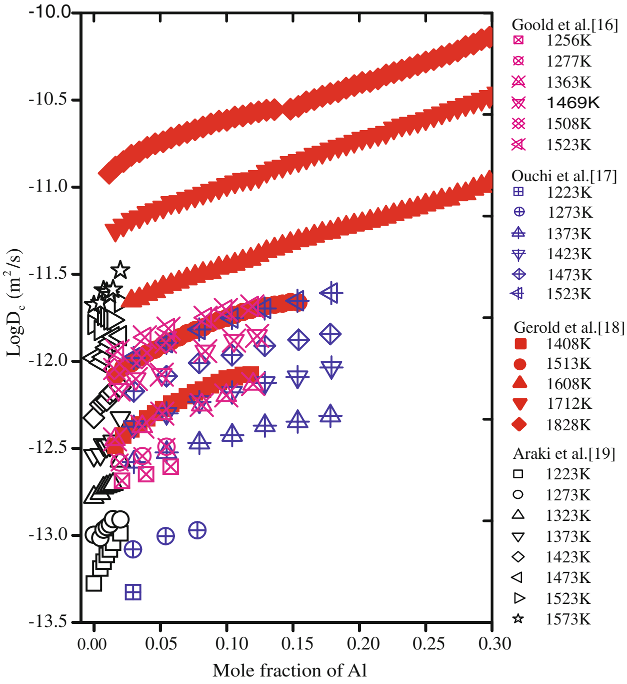

Fig. 1 Experimental information on the interdiffusion coefficients in the Ti-Al system

temperatures from 1323 to 1473 K[22] by the Matano-Kirkaldy (MK) and the modified Hall methods for the coefficients at the composition limits. All the main interdiffusion coefficients (D^{Ti}_{AlAl} and D^{Ti}_{VV}) and most of the cross coefficients (D^{Ti}_{AlV} and D^{Ti}_{VAl}) are positive in the ternary alloys that have been studied and exhibit a weak concentration dependence. All these data were used to derive the ternary interaction mobility parameters; however, the cross coefficients were given only a very low weight, this will be addressed in details in Section 5.

Table 1 Assessed atomic mobilities for the BCC alloys of the Ti-Al-V ternary system (all in SI units)

Mobility	Parameter, J/mole	Reference
Mobility of Al		
Q^{Al}_{Al}	$-215000 - 80.2 * T$	34
Q^{Ti}_{Al}	$R * T * \mathrm{Ln}(5.19e{-}10 * \exp(-96000/R/T) + 5.51E{-}6 * \exp(-204000/R/T))$	Present work
Q^{V}_{Al}	$-268200 - 97.2 * T$	Present work
${}^{0}Q^{Al,Ti}_{Al}$	$-499946.15 + 333.87 * T$	Present work
${}^{1}Q^{Al,Ti}_{Al}$	$-407271.50 + 286.27 * T$	Present work
${}^{0}Q^{Al,V}_{Al}$	-751405.09	Present work
${}^{0}Q^{Ti,AL,V}_{Al}$	-308901.62	Present work
Mobility of Ti		
Q^{Al}_{Ti}	$-196948.34 - 87.54 * T$	Present work
Q^{Ti}_{Ti}	$-151989.95 - 127.37 * T$	9
Q^{V}_{Ti}	$-329983.49 - 65.25 * T$	9
${}^{0}Q^{Ti,V}_{Ti}$	$174277.27 - 62.90 * T$	9
${}^{1}Q^{Ti,V}_{Ti}$	-27605.20	9
${}^{0}Q^{Ti,AL,V}_{Ti}$	1721802.68	Present work
Mobility of V		
Q^{Al}_{V}	$-325008.12 - 73.99 * T$	Present work
Q^{Ti}_{V}	$-179392.69 - 106.68 * T$	9
Q^{V}_{V}	$-325008.12 - 73.99 * T$	9
${}^{0}Q^{Al,V}_{V}$	-1300707.37	Present work
${}^{0}Q^{Ti,V}_{V}$	$159507.07 - 48.62 * T$	9
${}^{1}Q^{Ti,V}_{V}$	-10551.39	9

4. Optimization Process

The thermodynamic descriptions, used for deriving the thermodynamic factor for diffusion coefficients, were taken from the existing CALPHAD-type works. The Ti-Al binary system has been assessed several times.[23–31] The latest one by Witusiewicz et al.,[31] updated with the most recent experimental data, was accepted in this work. Those for two other binaries, i.e., Ti-V and Al-V, were taken from Hari Kumar et al.[32] and Gong et al.,[33] respectively. The description of the Ti-Al-V ternary system was extrapolated from the three sub-binaries since there is currently no assessed thermodynamic data for the ternary.

The mobility parameters of the Ti-V binary system were taken from a recent work.[9] The mobility of the Al self-diffusivity was taken from the work of Helander and Ågren[34] to keep compatibility between the present work and existing mobility database. To account for the Al impurity diffusion in bcc-Ti with a strongly curved Arrhenius plot, one can either use a piecewise polynomial or fit it by $D = D_1 \exp(-Q_1/RT) + D_2 \exp(-Q_2/RT)$. The latter gives a clearer physical meaning and can be readily incorporated in any CALPHAD-base thermo-kinetic database and was therefore accepted in this work. As no experimental data were available for fixing the requisite parameters, they were extracted from the Ti-Al binary interdiffusion coefficients.

All the other parameters were optimized by fitting to the selected experimental tracer diffusivity and interdiffusion coefficients by using the DICTRA software. The process was performed as follows: optimization of the parameter Q^{Al}_{Ti} of Ti diffusion in bcc-Al was done by fitting to the Ti tracer diffusivity in the Ti-Al binary alloys, and the interaction parameters ${}^{0}Q^{Al,Ti}_{Al}$ and ${}^{1}Q^{Al,Ti}_{Al}$ of Al diffusion were fitted to the Ti-Al interdiffusion coefficients; then the parameter Q^{V}_{Al} was obtained by using the Al impurity diffusivity in bcc-V. The other parameters of the Al-V binary, for a lack of experimental data, were optimized together with those of the Ti-Al-V ternary system by fitting to the ternary interdiffusion coefficients. All mobility parameters obtained in this work, together with those for Ti-V,[9] are listed in Table 1.

5. Results and Discussion

5.1 Ti-Al and Al-V Binaries

Validation of the assessed mobility parameters can be primarily done by using them for deriving various diffusion coefficients. The calculated Al impurity diffusivity in the bcc-Ti is compared in Fig. 2(a) compared with the data extrapolated from experimental interdiffusion coefficients.[17,19] Figure 2(b) presents the Arrhenius plot of the Ti tracer diffusivity in the binary Ti-Al alloys and is compared with observed data of Gerold and Herzig[18] It is clear from Fig. 2 that the agreement is satisfactory.

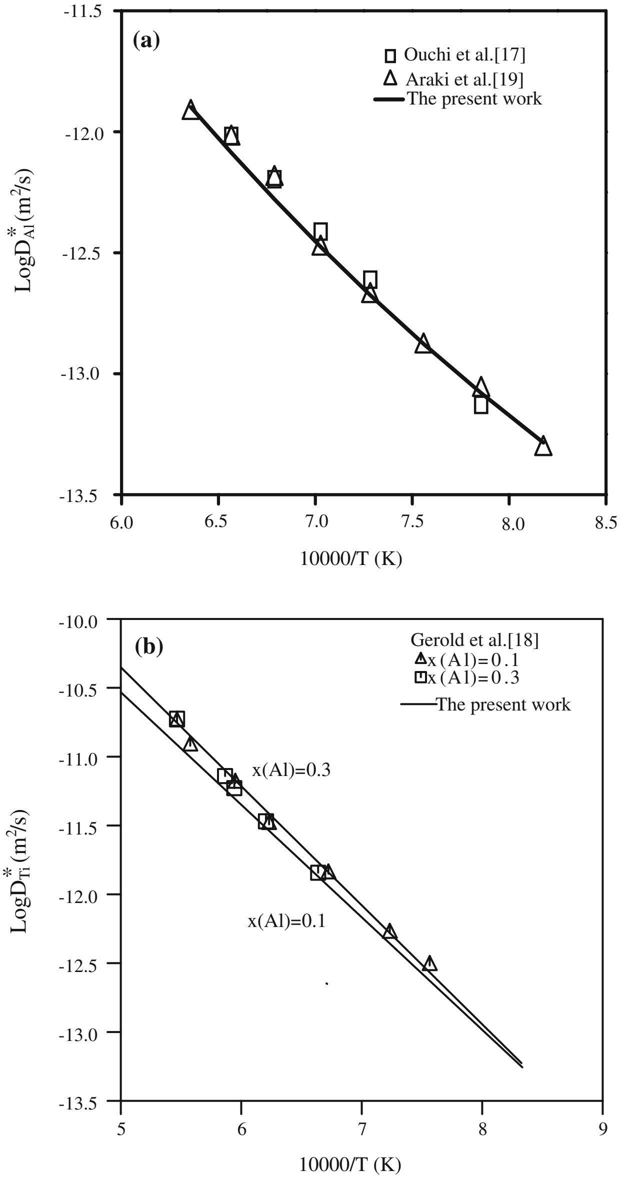

Fig. 2 (a) Arrhenius plot of Al impurity diffusion in bcc-Ti compared with data extrapolated from experimental interdiffusion coefficients; (b) Arrhenius plot of Ti tracer diffusion in bcc-Ti alloys compared with the experimental data

Comparisons of the interdiffusion coefficients are given in Fig. 3 between the calculated data and experimental points.[17-19] As can be seen, general agreement is obtained though it is less good at two low temperatures. Further validation can be made by comparing the predicted in-depth diffusion behavior resulting from interdiffusion with some measured data. In conjunction with the thermodynamic database, solving Eq 6 numerically enables much of diffusion processes, particularly in the diffusion-couple

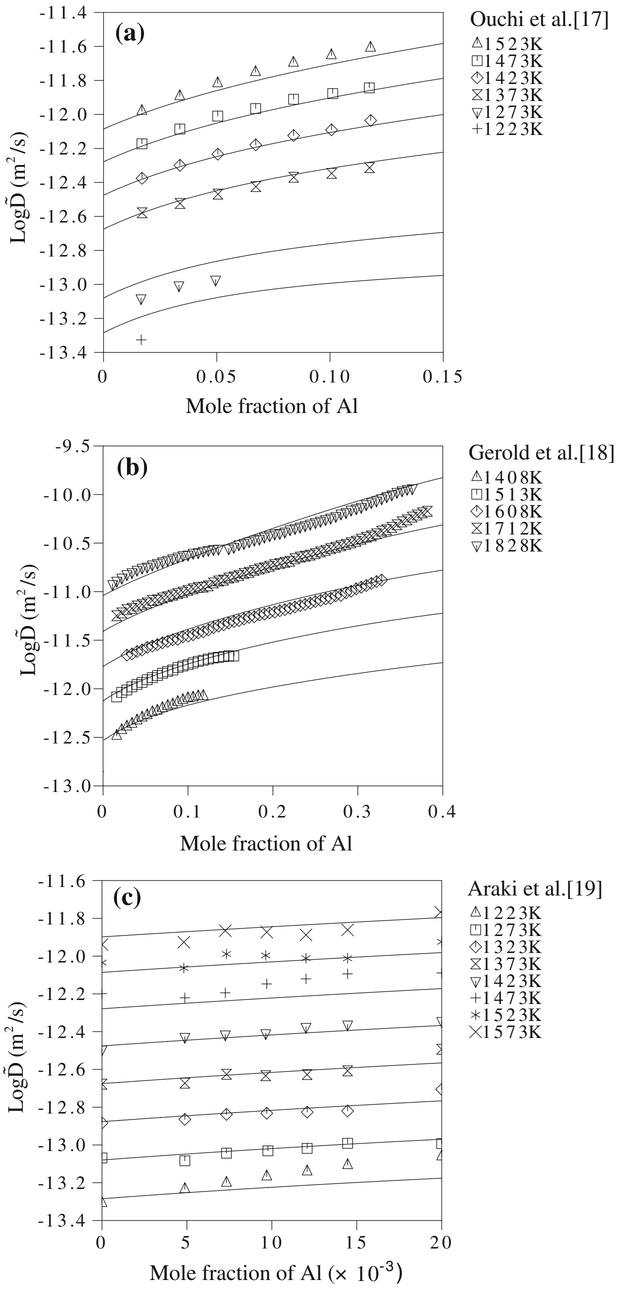

Fig. 3 Calculated interdiffusion coefficients of the bcc Ti-Al-V ternary system with respect to different temperatures and concentrations compared with the experimental measurements of (a) Ouchi et al.,[17] (b) Gerold et al.,[18] and (c) Araki et al.[19]

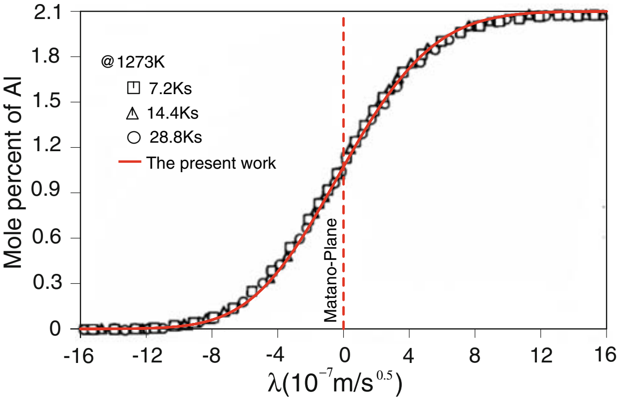

Fig. 4 Simulated concentration profiles of Ti/Ti-2.1at%Al diffusion couple after annealing at 1273 K for 10500 s compared with the experimental measurement (*symbols*)

experiment, to be predicted. Figure 4 illustrates such an example for a semi-infinite Ti/Ti-2.1%Al diffusion couple annealed at 1273 K. Note that the simulated concentration profiles represent the measured points[16] very well.

As indicated by Eq 7, the velocity of the inert maker displacement occurring in a diffusion couple experiment could be determined from the knowledge of the intrinsic diffusivities and the composition gradient at the marker position. Figure 5(a) shows variations in the tracer and intrinsic diffusivities with composition at 1523 K and the interdiffusion coefficient as well. Note that the ratio of the two intrinsic diffusivities, $D_{\mathrm{Al}}/D_{\mathrm{Ti}}$, are about 0.533-0.626 over the composition range from 0 to 40 at.% Al and is weakly composition dependent, therefore indicating that Ti is always the fast diffuser if a diffusion couple is made within this composition range. Figure 5(b) shows velocity of the Matano plane inset with the Kirkendall shift of the Ti-4at.%Al/Ti diffusion couple. The present calculation is in

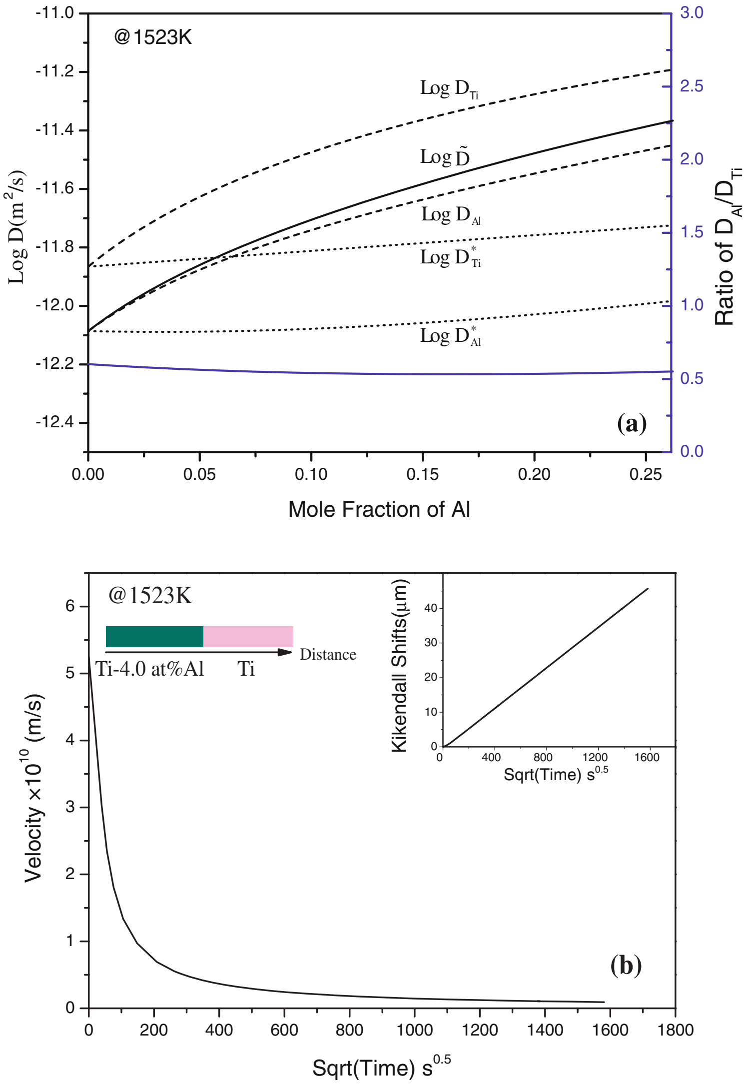

Fig. 5 (a) Calculated relations of tracer, intrinsic, and interdiffusion diffusivities for the Ti-Al system at 1523 K; (b) the predicted velocity of the Matano plane (Kirkendall shift in the inset) for the Ti-4at.%Al/Ti diffusion couple

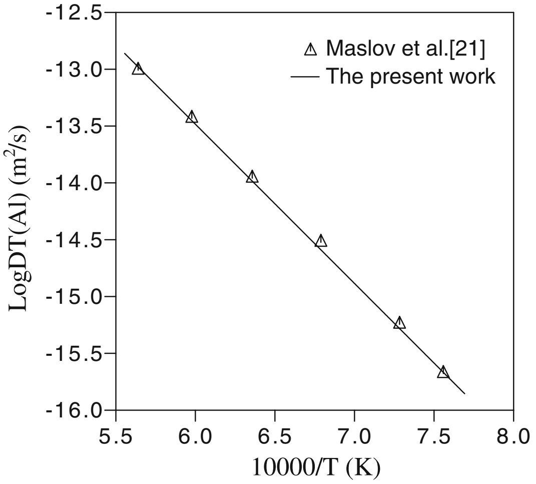

Fig. 6 Arrhenius plot of Al diffusion coefficients in bcc-V compared with the experimental data (*symbols*)[21]

accord with the finding of Gerold and Herzig,[18] however, does not agree with the other observation, i.e., the inert maker at 4.0 at% Al shifted to the Al-rich side by Ouchi.[17] As indicated from the experimental observations,[16,17] it seems that an ideal D_{Al}/D_{Ti} ratio should occur in such a way that it is larger than 1 at the Al-rich side while dropping to <1 as the Ti content rises. Our attempt failed to reproduce such a tendency as long as we choose to trust the tracer

Table 2 Calculated four interdiffusion coefficients based on experimental data[22]

	Takahashi et al.[22]	Matano-Kirkaldy method[35]	Whittle-Green method[36]
D^{Ti}_{AlAl}, m²/s	7.4×10^{-13}	8.2×10^{-13}	8.1×10^{-13}
D^{Ti}_{AlV}, m²/s	1.2×10^{-13}	-1.6×10^{-13}	-1.0×10^{-13}
D^{Ti}_{VAl}, m²/s	1.7×10^{-13}	-0.06×10^{-13}	-0.12×10^{-13}
D^{Ti}_{VV}, m²/s	4.1×10^{-13}	6×10^{-13}	5.9×10^{-13}

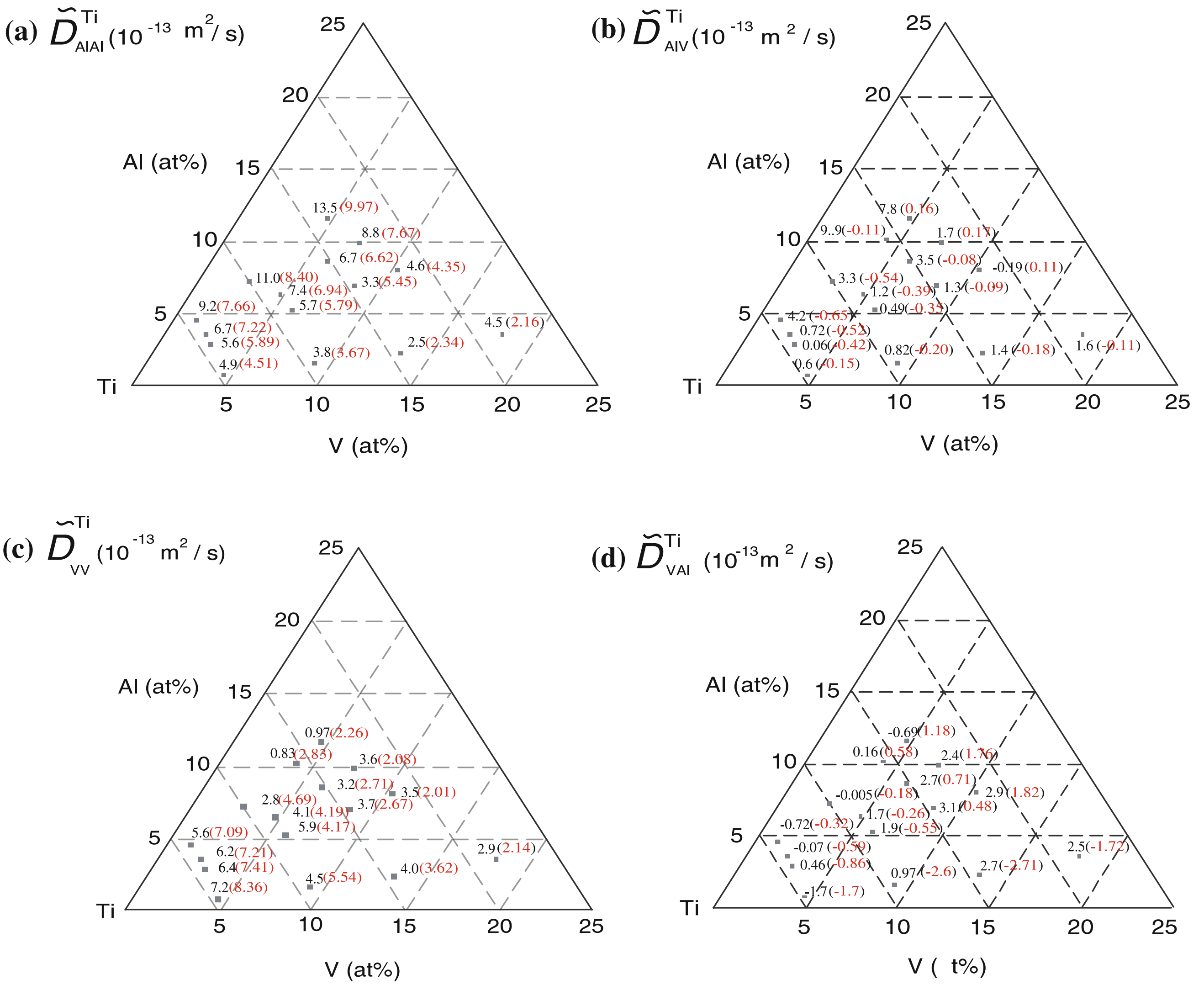

Fig. 7 Calculated interdiffusion coefficients (in *brackets*) of the ternary Ti-Al-V bcc alloys at 1473 K compared with the experimental measurements[22] (a) D^{Ti}_{AlAl}, (b) D^{Ti}_{AlV} (c) D^{Ti}_{VV}, and (d) D^{Ti}_{VAl}

diffusion data; however, it is well known that the tracer diffusivity generally has the least uncertainty in determination of diffusion coefficients. The discrepancy of the Kirkendall shift between the prediction and different experimental resources indicates that further experimental effort is needed. It should also be noted that the current phenomenological treatment is a simplified treatment without any kinetic considerations.

The calculated Al impurity diffusivity in bcc-V is compared with the experimental data[21] in Fig. 6. There is a good agreement.

5.2 Ti-Al-V Ternary

The main ternary interdiffusion coefficients, $D^{\mathrm{Ti}}_{\mathrm{AlAl}}$ and $D^{\mathrm{Ti}}_{\mathrm{VV}}$, and the cross coefficients, $D^{\mathrm{Ti}}_{\mathrm{AlV}}$ and $D^{\mathrm{Ti}}_{\mathrm{VAl}}$ were

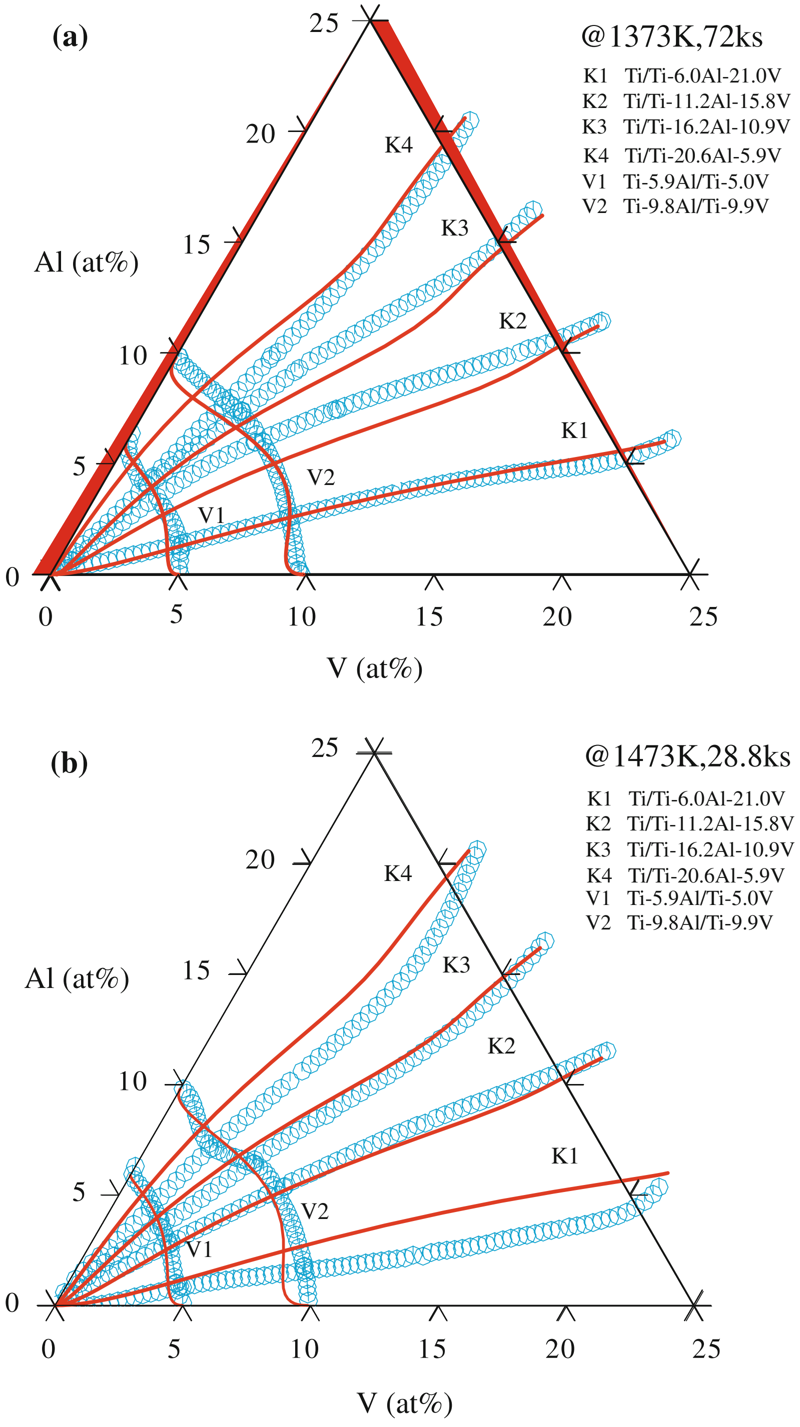

Fig. 8 Simulated diffusion paths for ternary couples compared with the experimental measurements (*symbols*)[22] (a) 1373 K and (b) 1473 K

calculated, and are shown in Fig. 7 for a comparison with the experimental data[22] at 1473 K. The agreement is good for the main coefficients, specifically, the experimental coefficients $D^{\mathrm{Ti}}_{\mathrm{AlAl}}$ and $D^{\mathrm{Ti}}_{\mathrm{VV}}$ are ranged over $2.5\text{-}13.5\times10^{-13}$ and $0.82\text{-}7.2\times10^{-13}$ $\mathrm{m^2/s}$ at 1473 K, respectively, whereas the calculated values are $2.16\text{-}9.97\times10^{-13}$ and $2.01\text{-}8.36\times10^{-13}$ $\mathrm{m^2/s}$, respectively. However, the agreement for the two cross coefficients $D^{\mathrm{Ti}}_{\mathrm{AlV}}$ and $D^{\mathrm{Ti}}_{\mathrm{VAl}}$ is not good, particularly, some of the calculated values are negative while the experimental work showed the positive values. Our careful examination shows that the cross coefficient, even its sign, is sensitive to the raw data set that are chosen for calculation, see Table 2 for a comparison of the four diffusion coefficients at the intersection point of the K3/V2 couples using the MK method[35] and the Whittle-Green (WG) method[36] and those due to Takahashi et al.[22] It is apparent that there is a good agreement for the two main terms among the three calculations. However, Takahashi et al.[22] showed the positive values for the two cross terms whereas our calculations, either by the MK or the WG method, gave the two cross terms the negative values, therefore, indicating that the cross terms have relatively larger uncertainty of determination. This is further verified by a fact that our attempt to give a closer fit to the cross coefficients has never been achieved without using unrealistic mobility parameters while still keeping the fit to the binary systems acceptable. Simulated diffusion paths for the diffusion couples made by Takahashi et al.[22] were compared with the experimental curves. It was noticed that agreement is generally good at one temperature while it is unfavorable at another for most of the ternary couples (see Fig. 8), for example, the couple Ti/Ti-6.0Al-21.0V (at.%).[22] Close inspection reveals that a comprehensive assessment of the atomic mobility of the Ti-Al-V ternary, together with the sub-binaries, does not allow a significant temperature dependence of the ternary diffusion data as indicated by the diffusion paths measured by Takahashi et al.[22] unless an unrealistically large temperature term is generally used for the optimized ternary mobility parameters. The predicted concentration profiles of the couples Ti/Ti-16.2Al-10.9V and Ti-9.8Al/Ti-9.9V are compared with the experimental points in Fig. 9. There is a good agreement, but as same as for the diffusion paths, the agreement is much less good for some of the other couples for much the same reason.

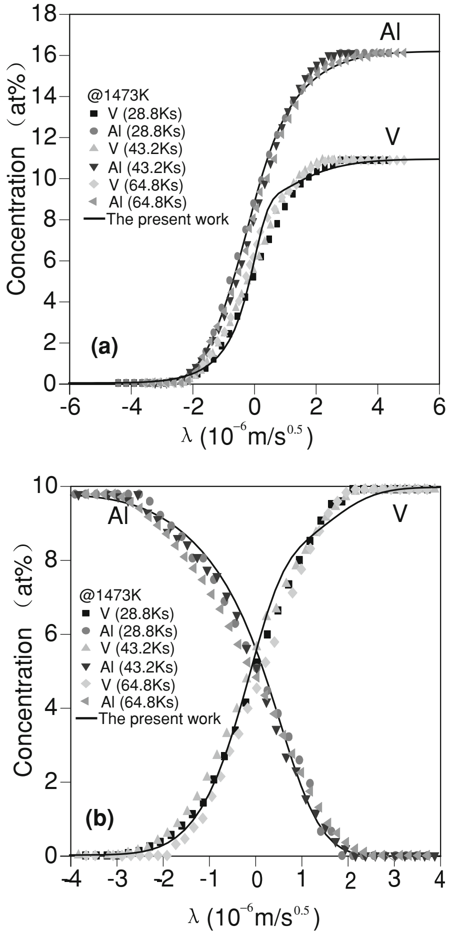

Fig. 9 Simulated concentration profiles for ternary diffusion couples at 1473 K compared with the experimental measurements[22]: (a) Ti/Ti-16.2Al-10.9V and (b) Ti-9.8Al/Ti-9.9V

6. Conclusion

The atomic mobilities for the bcc phase of the Ti-Al and Al-V binaries and the Ti-Al-V ternary were assessed by fitting to the evaluated experimental data. Reasonable agreement was obtained from comprehensive comparisons made between the calculated and experimental diffusion coefficients. The assessed mobilities were further validated by the simulations of some diffusion couple experiments.

Acknowledgments

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