

Assessment of the Atomic Mobilities in fcc Cu-Fe and Cu-Ti Alloys

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The experimentally measured diffusion coefficients of fcc Cu-Fe and Cu-Ti alloys in the published literature were reviewed critically in the present work. On the basis of the available thermodynamic information, the atomic mobilities of Cu, Fe, and Ti in fcc Cu-Fe and Cu-Ti alloys as a function of temperature and composition were assessed in terms of the CALPHAD method using the DICTRA[®] software. The optimized mobility parameters are presented. The calculated diffusion coefficients show an excellent agreement with the experimental data. The composition-distance profiles of the Cu-Ti binary diffusion couples reported in the literature were also predicted using the assessed mobility parameters. Overall good agreement is achieved between the experimental results and simulations.

Keywords atomic mobility, CALPHAD, Cu-based alloys, DICTRA, diffusion

1. Introduction

Brazing diamond grits onto a metal substrate in the form of a single-layer configuration is an effective technique to manufacture high performance monolayer diamond abrasive tools.^[1–11] Cu-Sn-Ti filler metals have been used widely to braze diamond grits onto a steel substrate due to their relatively high strength and erosion resistance when compared to Ag-Cu-based alloys, and their lower melting point when compared to Ni-based alloys.^[7–11] The diffusion behavior between the filler metal and the diamond or the steel substrate affects the microstructure evolution and the formation of intermetallic compounds at the interfaces, which has significant influence on the performance of braze joints. In order to better understand the interdiffusion between filler metals and diamond/steel substrate, thermodynamic and kinetic information of the whole system is necessary to control the interfacial microstructure evolution and thus to design and optimize brazing processes.

The DICTRA[®] (diffusion controlled transformation) software has been developed and operates under the CALPHAD framework.^[12–16] On the basis of the local equilibrium hypothesis, the DICTRA[®] software has been used successfully to simulate various diffusion controlled phase transformation processes such as cementite dissolution during austenitization, solidification and carburization, coarsening of carbides as well as the growth of intermetallic

compounds.^[17–22] In many cases, the diffusion data measured experimentally from different sources are not consistent with each other, which affect significantly the quality of the DICTRA simulation. Therefore, the available and compatible mobility databases for multi-component systems need to be developed. Recently, the atomic mobilities in the fcc Cu-based binary alloys such as Cu-Au and Cu-Pt,^[23] Cu-Co,^[24] Cu-Ni,^[25] Cu-Sn,^[26] and Al-Cu^[27] have been assessed. As a contribution to establish a general mobility database including Cu-based filler metals and steel substrates, the present work aims to assess the atomic mobilities in fcc Cu-Fe and Cu-Ti alloys by means of the CALPHAD-type procedure using the DICTRA[®] software.^[12–16]

2. Experimental Information

2.1 The Cu-Fe System

Many experimental investigations of the impurity diffusion coefficients of Fe in fcc Cu have been performed.^[28–35] Mackliet^[28] measured the impurity diffusion coefficients of Fe in fcc Cu single crystals (purity 99.998%) in the temperature range from 973 to 1348 K using the radioactive tracer ⁵⁹Fe and the lathe sectioning method. With the same method, Mullen^[29] determined the impurity diffusion coefficients of Fe in pure fcc Cu single crystals (purity 99.998%) between 990 and 1329 K. Barreau et al.^[30] reported the impurity diffusion coefficients of Fe in pure fcc Cu single crystals and polycrystals (purity 99.995%) between 923 and 1343 K using ⁵⁹Fe and the residual activity method. Bernardini and Cabane^[31] investigated the impurity diffusion of Fe in fcc Cu single crystals (purity 99.995%) from 1005 to 1297 K through ⁵⁹Fe and electrolytic sectioning technique. Sen et al.^[32] measured the impurity diffusion coefficients of Fe in fcc Cu polycrystals by the resistometric technique in the temperature range from 1063 to 1273 K. Salje and Feller-Kniepmeier^[33] studied the impurity diffusion of Fe from 923 to 1323 K by vapor-deposition of Fe on

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pure fcc Cu single crystals (purity 99.999%) with the electron probe micro-analysis (EPMA) method. Almazouzi et al.^[34] investigated the impurity diffusion coefficient of Fe in fcc Cu from 651 to 870 K by means of Fe sputter-deposited on pure fcc Cu single crystals (purity 99.999%) with the ion-beam sputtering technique and with secondary-ion mass spectroscopy (SIMS). Tomono and Ikushima^[35] employed the tracer ⁵⁵Fe with the lathe sectioning method to determine the impurity diffusion coefficients of Fe in fcc Cu single crystals (purity 99.99%) in the high temperature range (1130-1320 K). The impurity diffusion coefficients of Fe in pure Cu reported by Mackliet,^[28] Mullen,^[29] Barreau et al.,^[30] Bernardini and Cabane,^[31] Sen et al.,^[32] Salje and Feller-Kniepmeier,^[33] and Almazouzi et al.^[34] are self-consistent in both the high and the low temperature range, but are significantly higher than that the measured values by Tomono and Ikushima.^[35] Considering the compatibility of the experimental results, the data as given in references^[28-34] were employed in the present optimization, while the data of Tomono and Ikushima^[35] was rejected.

On the other hand, Speich et al.^[36] measured the impurity diffusion coefficients of Cu in fcc Fe polycrystals (purity 99%) between 1183 and 1293 K by EPMA. Rothman et al.^[37] investigated the impurity diffusion coefficients of Cu in fcc Fe single crystals (purity 99%) from 1558 to 1641 K by means of ⁶⁴Cu and grinder sectioning method. Salje and Feller-Kniepmeier^[38] studied the impurity diffusion coefficients of Cu from 923 to 1323 K by vapor-deposition of Cu on pure fcc Fe polycrystals (purity 99.9%) with EPMA. Using ⁶⁴Cu as a tracing element and the residual activity method, Majima and Mitani^[39] determined the impurity diffusion coefficients of Cu in fcc Fe polycrystals (purity 99%) between 1378 and 1483 K. Using the lathe sectioning with atomic absorption analysis, Taguchi et al.^[40] measured the impurity diffusion coefficients of Cu in fcc Fe polycrystals (purity 99.9%) from 1203 to 1283 K. The experimental data^[36-40] mentioned above are in good agreement with each other and were used in the present optimization.

Using serial-sectioning experiments, Bocquet^[41] measured the tracer diffusion coefficients of Cu in various fcc Cu-Fe alloys (up to 2.40 at.% Fe) in the temperature range from 1265 to 1351 K. Tsuji and Yamanaka^[42] investigated interdiffusion coefficients in fcc Cu-Fe alloys in the temperature range between 1133 and 1283 K using the diffusion couple method. The experimental information of the tracer diffusion coefficients of Cu and interdiffusion coefficients in fcc Cu-Fe alloys^[41,42] was also taken into account in the present work.

2.2 The Cu-Ti System

According to a thorough literature review, the diffusion coefficients in fcc Cu-Ti alloys have been scarcely measured because of the narrow solubility of the Cu-rich fcc alloys and the unstable structure of fcc Ti in Ti-rich alloys at 298.15 K and 1 bar. Only Iijima et al.^[43] determined interdiffusion coefficients in the Cu-rich fcc alloys in the temperature range between 973 and 1283 K using the Cu/Cu-1.98 at.% Ti diffusion couple and Matano's method.

3. Modeling of Atomic Mobility

In the volume-fixed frame of reference, the diffusional flux of the specie, J_k , in a multicomponent system is given by the Fick-Onsager law as:

$$J_k = - \sum_{j=1}^{n-1} D_{kj}^n \nabla C_j \quad (\text{Eq 1})$$

where D_{kj}^n is the chemical diffusion coefficient. The summation is performed over $(n-1)$ independent concentration as the dependent n component may be taken as the solvent. In a substitutional solution phase, D_{kj}^n can be given by^[14,15] as:

$$D_{kj}^n = \sum_i (\delta_{ik} - x_k) x_i M_i \left(\frac{\partial \mu_i}{\partial x_j} - \frac{\partial \mu_i}{\partial x_n} \right) \quad (\text{Eq 2})$$

where δ_{ik} is the Kroneker delta ($\delta_{ik} = 1$ if $i = k$, otherwise $\delta_{ik} = 0$); x_i is the mole fraction, μ_i is the chemical potential of element i , and M_i is the composition dependent atomic mobility.

From the absolute reaction rate theory and neglecting the ferromagnetic effect on mobilities of fcc alloys, the mobility parameters M_k for the element k , can be divided into a frequency factor M_k^0 and an activation enthalpy Q_k as suggested by Jönsson^[44-47]:

$$M_k = \exp\left(\frac{-Q_k + RT \ln M_k^0}{RT}\right) \frac{1}{RT} = \exp\left(\frac{\Delta G_k}{RT}\right) \frac{1}{RT} \quad (\text{Eq 3})$$

where R is the gas constant and T is the temperature. Similar to the phenomenological CALPHAD method, Andersson and Ågren^[15] suggested that the parameter ΔG_k can be assumed to be a function of composition, which can be expressed by the Redlich-Kister polynomial^[48]:

$$\Delta G_k = \sum_i x_i \Delta G_k^i + \sum_i \sum_{j>i} x_i x_j \left[\sum_r \Delta^r G_k^{ij} (x_i - x_j)^r \right] \quad (\text{Eq 4})$$

where ΔG_k^i and $\Delta^r G_k^{ij}$ are the mobility parameters of the end-members and the interaction for diffusion between the elements i and j , respectively.

The tracer diffusion coefficient of the element i , D_i^* , can be related to the atomic mobility M_i by Einstein's relation:

$$D_i^* = RT M_i \quad (\text{Eq 5})$$

In the A-B binary system, D_i^* can be applied to calculate the chemical diffusion coefficient \tilde{D} by Darken's equation^[49]:

$$\tilde{D} = (x_B D_A^* + x_A D_B^*) \phi \quad (\text{Eq 6})$$

where ϕ is the thermodynamic factor, which can be expressed as:

$$\begin{aligned} \phi &= 1 + \frac{d \ln \gamma_A}{d \ln x_A} = \frac{x_A}{RT} \frac{\partial \mu_A}{\partial x_A} = \frac{x_A(1-x_A)}{RT} \frac{d^2 G_m}{dx_A^2} \\ &= 1 + \frac{d \ln \gamma_B}{d \ln x_B} = \frac{x_B}{RT} \frac{\partial \mu_B}{\partial x_B} = \frac{x_B(1-x_B)}{RT} \frac{d^2 G_m}{dx_B^2} \end{aligned} \quad (\text{Eq 7})$$

Section I: Basic and Applied Research

where μ_A , μ_B , γ_A , γ_B , x_A , and x_B are the chemical potential, activity coefficient and mole fraction of component A and B, respectively; G_m is the molar Gibbs energy; R is the gas constant, and T is the temperature in Kelvin.

The temporal profile of the diffusing specie k is given by the Fick's law in the mass conservation form as follows:

$$\frac{\partial C_k}{\partial t} + \nabla \cdot J_k = 0 \quad (\text{Eq 8})$$

where C_k is the concentration in moles per volume.

4. Results and Discussion

In order to perform the assessment of the atomic mobilities in fcc Cu-Fe and Cu-Ti alloys, reasonable thermodynamic parameters are necessary to calculate the thermodynamic factor. Thermodynamic parameters of fcc Cu-Fe and Cu-Ti alloys optimized by Chen and Jin^[50] and Kumar et al.,^[51] respectively, were used in the present work, which can reproduce the phase diagram and most of thermodynamic data.

According to the available experimental data of self-diffusion coefficients in both fcc Cu and fcc Fe, the mobility parameters of Cu and Fe have been assessed by Ghosh^[52] and Jönsson,^[47] respectively, which can reproduce most of the experimental data and are consistent with the extrapolation of high-order related systems. The mobility parameters of Cu and Fe in the above references^[47,52] were thus employed in the present work. On the other hand, the self-diffusion coefficient of Ti in the hypothetical fcc Ti cannot be determined by experimental methods because of its unstable structure at 298.15 K and 1 bar. The self-diffusion coefficient of Ti was assumed by Matan et al.^[53] and was later included in the mobility database for multi-component Ni-based super-alloys developed by Campbell et al.^[54] through an empirical analysis. The mobility parameter of Ti by Matan et al.^[53] was thus used in the present work. Meanwhile, the impurity diffusion of Cu in hypothetical fcc Ti can also not be measured experimentally but is required during the optimization according to Eq 4. Using a similar approximation in references,^[26,53-55] it is assumed to be

equal to the self-diffusion coefficient of Ti in hypothetical fcc Ti in the present work.

The optimizations for obtaining the atomic mobilities have been performed with the PARROT module of the DICTRA[®] software.^[12-16] This module works by minimizing the square sum of the differences between experimental data and calculated values. In the present optimization, the experimental data of impurity diffusion coefficients, tracer diffusion coefficients and interdiffusion coefficients were employed to assess the mobility parameters of fcc Cu-Fe and Cu-Ti alloys. The mobility parameters used and obtained finally in the present work are summarized in Table 1.

4.1 The Cu-Fe System

Figure 1 is the calculated phase diagram of the Cu-Fe binary system and Fig. 2 shows the calculated thermodynamic factor (ϕ) of the fcc Cu-Fe alloys at different

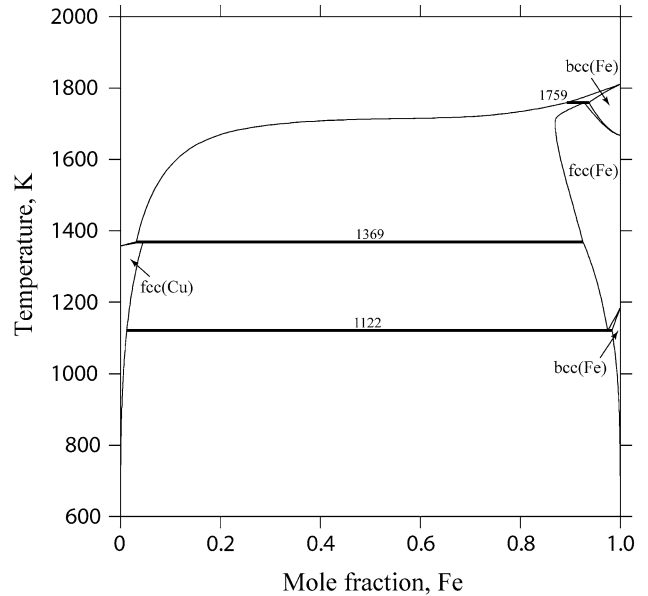


Fig. 1 Calculated phase diagram of the Cu-Fe binary system by Chen and Jin^[50]

Table 1 Mobility parameters of the face-centered cubic Cu-Fe and Cu-Ti alloys

Mobility	Parameters	Reference
Mobility of Cu	$\Delta G_{\text{Cu}}^{\text{Cu}} = -205,872 + RT \ln (4.889 \times 10^{-5})$	[52]
	$\Delta G_{\text{Cu}}^{\text{Fe}} = -273,718 + RT \ln (2.478 \times 10^{-5})$	This work
	$\Delta G_{\text{Cu}}^{\text{Ti}} = -256,900 + RT \ln (8.600 \times 10^{-5})$	[53]
	$\Delta^0 G_{\text{Cu}}^{\text{Cu,Fe}} = -25,965$	This work
Mobility of Fe	$\Delta G_{\text{Fe}}^{\text{Fe}} = -286,000 + RT \ln (7.000 \times 10^{-5})$	[47]
	$\Delta G_{\text{Fe}}^{\text{Cu}} = -207,421 + RT \ln (5.267 \times 10^{-5})$	This work
	$\Delta^0 G_{\text{Fe}}^{\text{Cu,Fe}} = -1,218,512$	This work
Mobility of Ti	$\Delta G_{\text{Ti}}^{\text{Ti}} = -256,900 + RT \ln (8.600 \times 10^{-5})$	[53]
	$\Delta G_{\text{Ti}}^{\text{Cu}} = -195,958 + RT \ln (6.931 \times 10^{-5})$	This work

Note: The units are J/(mol atoms), while the parameters R and T are the gas constant and temperature, respectively

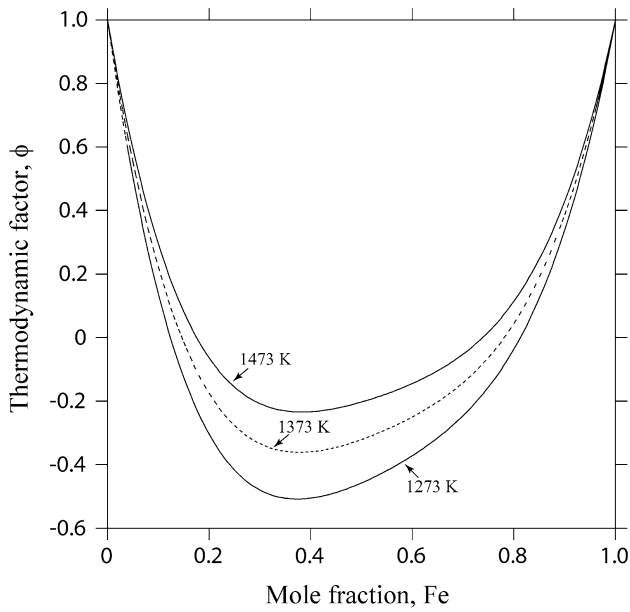


Fig. 2 Calculated thermodynamic factor (ϕ) of the fcc phase in the Cu-Fe binary system using the data by Chen and Jin^[50]

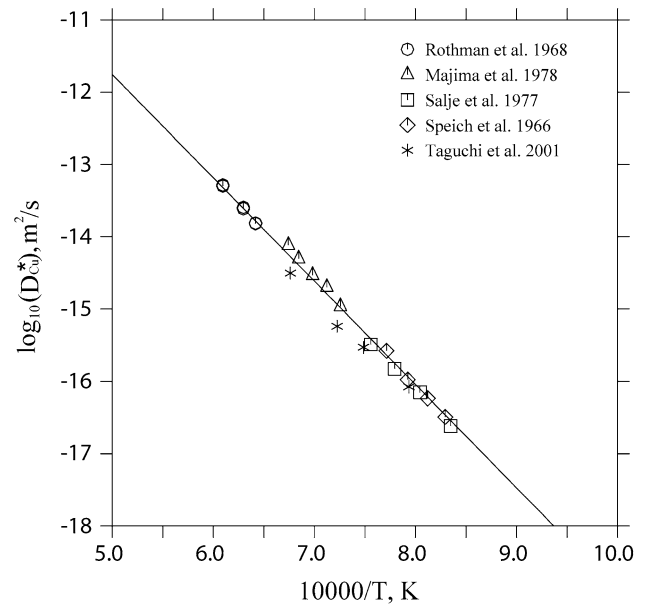


Fig. 4 Calculated temperature dependence of impurity diffusion coefficient of Cu in pure fcc Fe with the experimental data^[36-40]

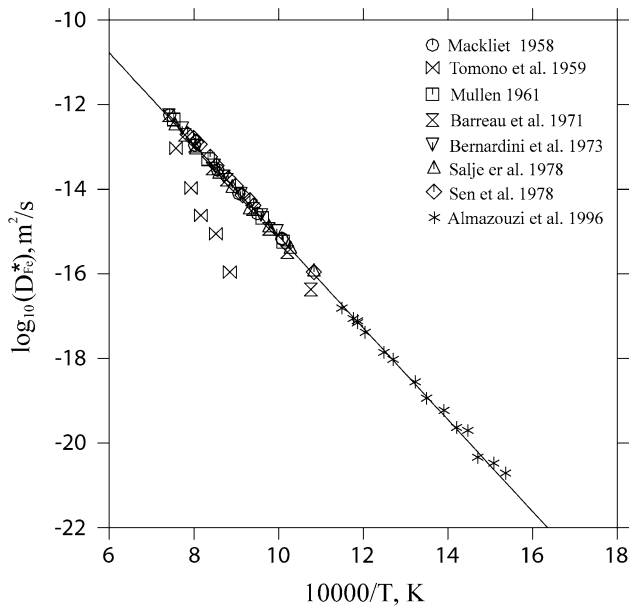


Fig. 3 Calculated temperature dependence of impurity diffusion coefficient of Fe in pure fcc Cu with the experimental data^[28-35]

temperatures using the thermodynamic parameters assessed by Chen and Jin.^[50]

Figure 3 presents the calculated temperature dependence of Fe impurity diffusion coefficients in fcc Cu with the experimental data.^[28-35] The calculated results are in good agreement with the experimental data measured by Mackliet,^[28] Mullen,^[29] Barreau et al.,^[30] Bernardini and Cabane,^[31] Sen et al.,^[32] Salje and Feller-Kniepmeier,^[33] and Almazouzi et al.,^[34] but show obvious deviation

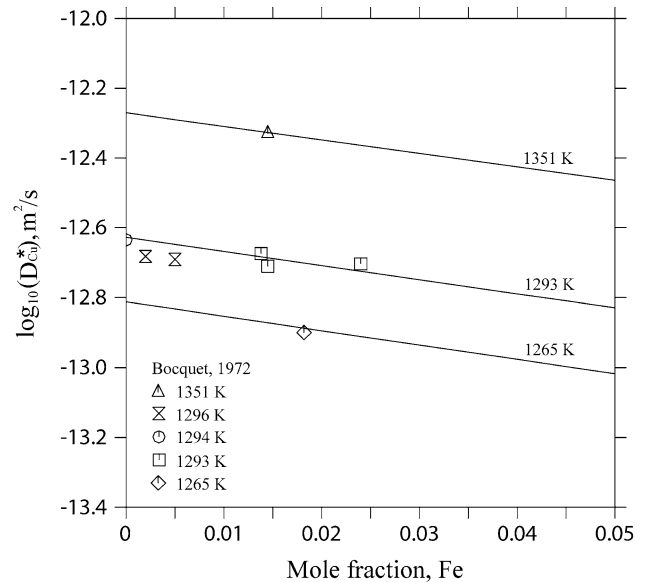


Fig. 5 Calculated tracer diffusion coefficient of Cu in fcc Cu-Fe alloys at different temperatures with the experimental data^[41]

from the experimental data by Tomono and Ikushima.^[35] Comparison between the calculated impurity diffusion coefficients of Cu in fcc Fe with the temperature dependence and the experimental data^[36-40] is given in Fig. 4. As can be seen, the calculated results agree well with the measured experimental data by Speich et al.,^[36] Rothman et al.,^[37] Salje and Feller-Kniepmeier,^[38] Majima and Mitani,^[39] and Taguchi et al.^[40]

Figure 5 shows the calculated tracer diffusion coefficients of Cu in fcc Cu-Fe alloys at different temperatures

Section I: Basic and Applied Research

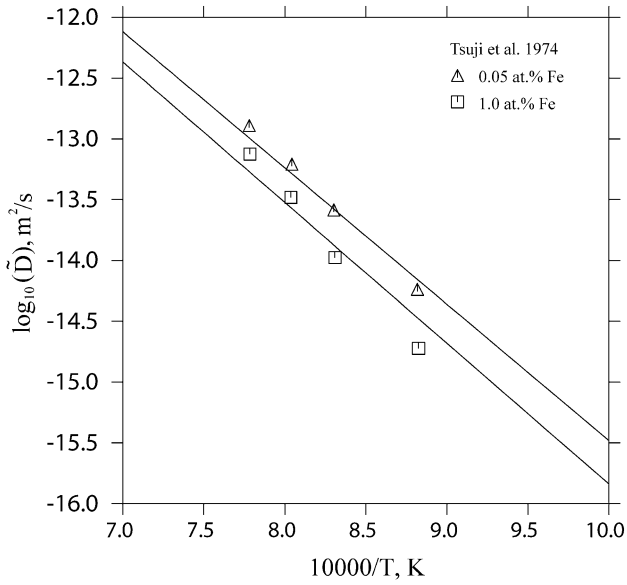


Fig. 6 Calculated temperature dependence of interdiffusion coefficient in fcc Cu-Fe alloys with the experimental data^[42]

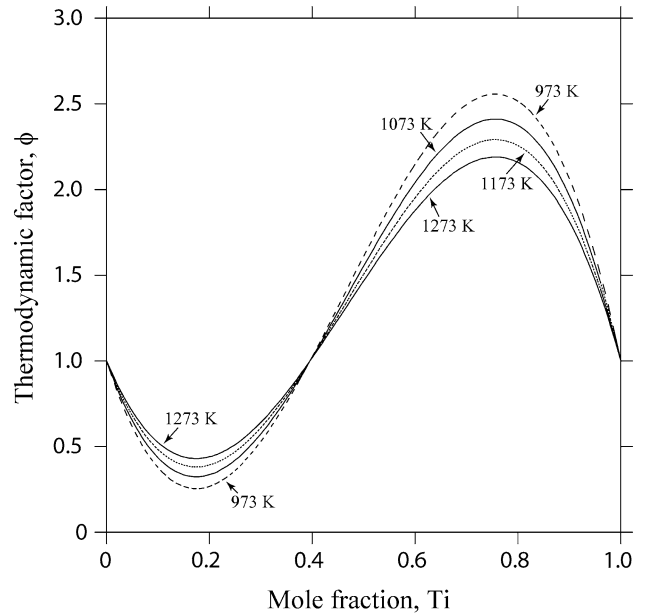


Fig. 8 Calculated thermodynamic factor (ϕ) of the fcc phase in the Cu-Ti binary system using the data by Kumar et al.^[51]

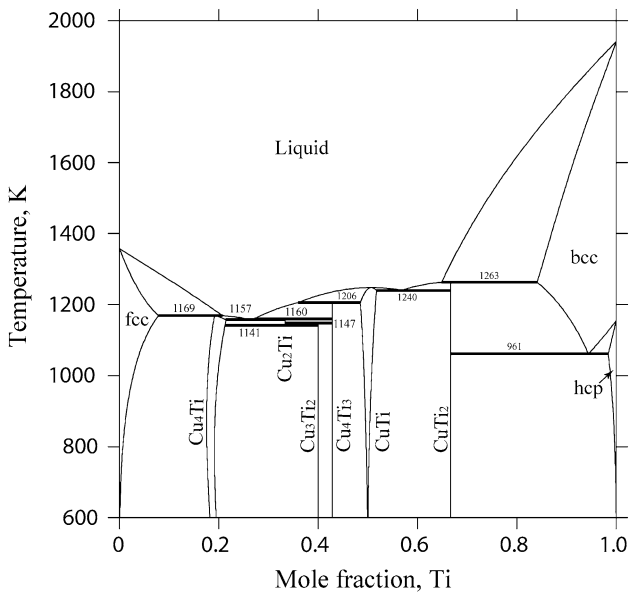


Fig. 7 Calculated phase diagram of the Cu-Ti binary system by Kumar et al.^[51]

(1265, 1293, and 1351 K) together with the experimental data.^[41] It is evident that the calculated values are quite consistent with the measured ones by Bocquet,^[41] although there is the small solubility of Fe in fcc Cu.

The calculated temperature dependence of interdiffusion coefficients in fcc Cu-Fe alloys is compared with the experimental data measured by Tsuji and Yamanaka^[42] as shown in Fig. 6. It can be seen that the calculated interdiffusion coefficients as a function of temperature at Cu-0.05 at.% Fe alloys are in good agreement with the

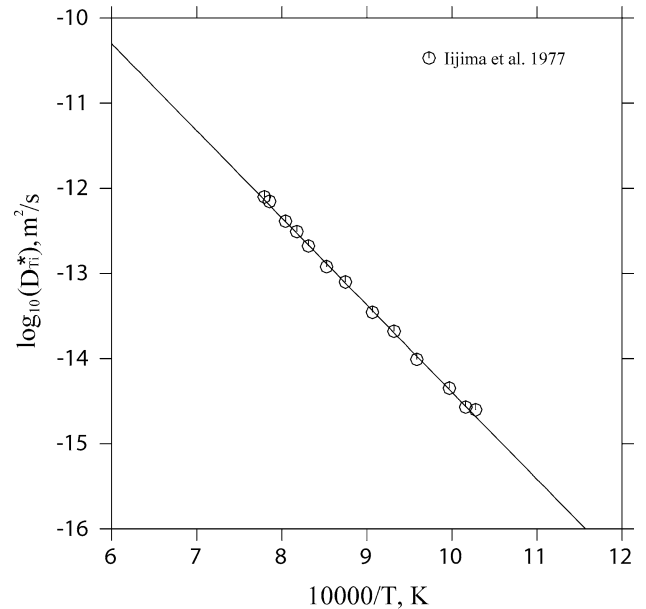


Fig. 9 Calculated temperature dependence of impurity diffusion coefficient of Ti in pure fcc Cu with the experimental data^[43]

experimental data. Although a small difference exists between the calculated values and the measured data by Tsuji and Yamanaka,^[42] the calculated interdiffusion coefficients for Cu-0.10 at.% Fe alloys are acceptable in the present work if considering that the experimental error of diffusion coefficients can be in the range of one or two orders of magnitude.

4.2 The Cu-Ti System

Figure 7 is the calculated phase diagram of the Cu-Ti binary system and Fig. 8 shows the calculated thermodynamic factor (ϕ) of the fcc Cu-Ti alloys at different temperatures using the thermodynamic parameters optimized by Kumar et al.^[51] As mentioned in the experimental section, there is only one paper reporting on the experimental measurement of diffusion coefficients in the Cu-Ti binary system. Therefore, the interaction parameters were not used in the present work.

Figure 9 compares the calculated temperature dependence of the impurity diffusion coefficients of Ti in fcc Cu

with the experimental data.^[43] Figure 10 presents the calculated interdiffusion coefficients with the temperature in various fcc Cu-Ti alloys. Figure 11 shows the comparison between the calculated interdiffusion coefficients and the experimental data at different temperatures. The calculated results for both impurity diffusion coefficient of Ti and interdiffusion coefficients are in excellent agreement with the experimental data measured by Iijima et al.^[43]

Further validation of the atomic mobility parameters obtained in the present work was performed by checking whether the parameters can describe satisfactorily the

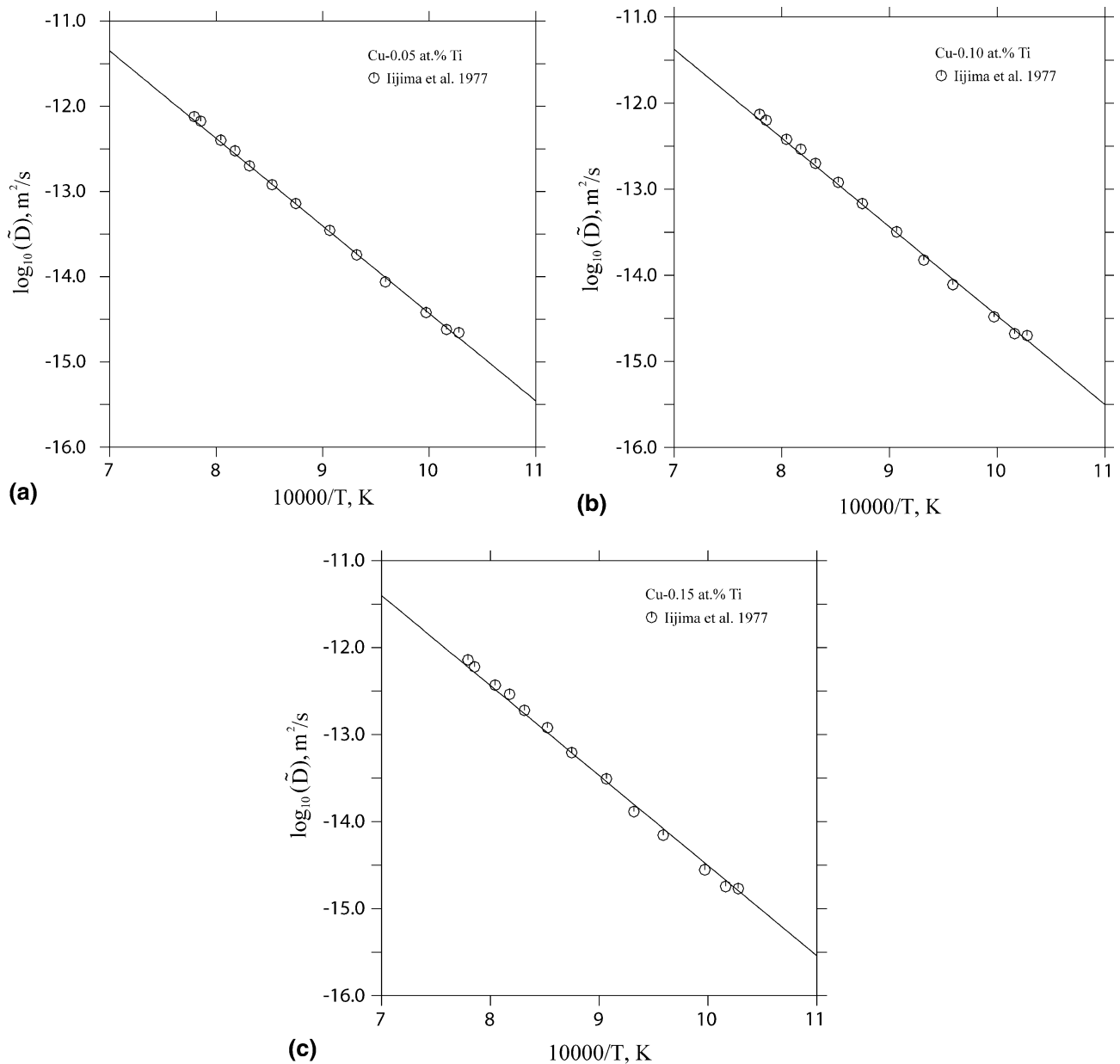


Fig. 10 Calculated temperature dependence of interdiffusion coefficient in fcc Cu-Ti alloys with the experimental data.^[43] (a) Cu-0.05 at.% Ti, (b) Cu-0.10 at.% Ti, (c) Cu-0.15 at.% Ti

Section I: Basic and Applied Research

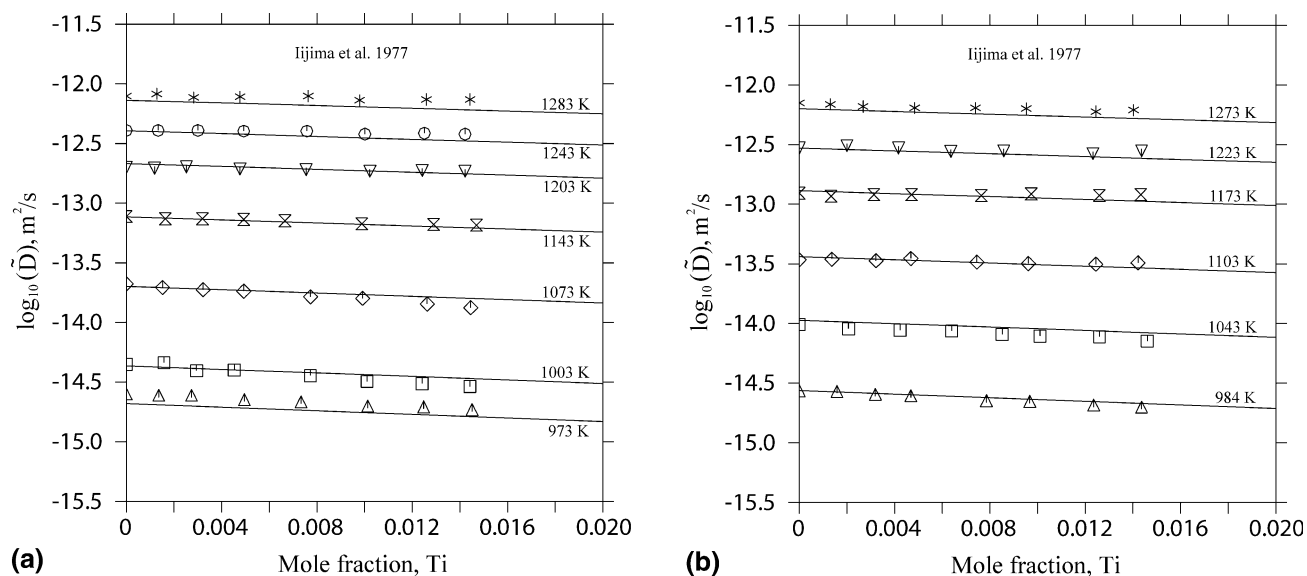


Fig. 11 Comparison of the calculated interdiffusion coefficients in fcc Cu-Ti alloys at different temperatures with the experimental data^[43]

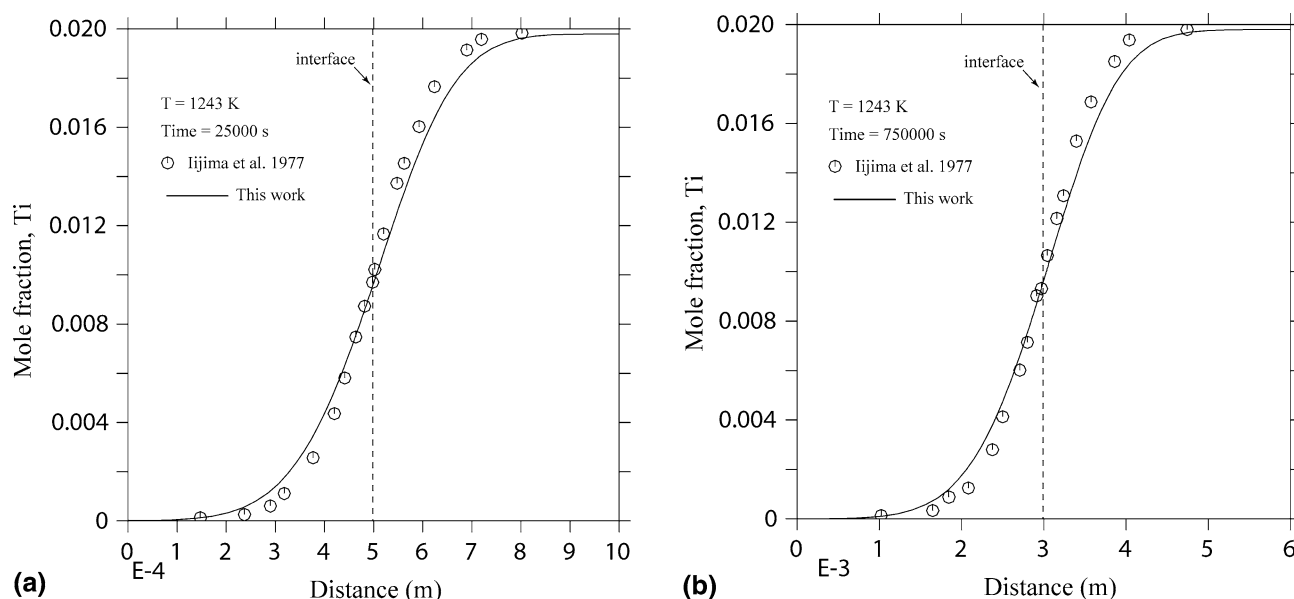


Fig. 12 Comparison between calculated concentration-distance profiles of the Cu/Cu-1.98 at.% Ti diffusion couple at 1243 K with the experimental data.^[43] (a) 25,000 s, (b) 750,000 s

composition-distance profiles in Cu-Ti binary diffusion couples. Using the optimized mobility parameters through the DICTRA[®] software package,^[12-16] the composition-distance profiles of the Cu/Cu-1.98 at.% Ti diffusion couples were simulated at 1243 K for different time as shown in Fig. 12. As can be seen, the present simulations agree well with the experimental data measured by Iijima et al.^[43] This confirms the validity of the mobility parameters obtained in the present assessment.

5. Conclusion

Combined with the available thermodynamic information and various experimental diffusion coefficients, the atomic mobilities of Cu, Fe and Ti in fcc Cu-Fe and Cu-Ti alloys as a function of temperature and composition have been assessed using the DICTRA[®] software. The optimized mobility parameters can be employed to reproduce

satisfactorily most of the experimental information on the measured diffusion coefficients in both Cu-Fe and Cu-Ti alloys. Furthermore, the composition-distance profiles in the Cu-Ti binary diffusion couple reported in the published literature can also be predicted well.

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Section I: Basic and Applied Research

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