

## **INTERDIFFUSION COEFFICIENTS AND ATOMIC MOBILITIES IN FCC Cu-Fe-Mn ALLOYS**

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### **Abstract**

*In the present work, the interdiffusion coefficients in fcc Cu-Fe-Mn alloys were experimentally determined via a combination of solid/solid diffusion couples, electron probe microanalysis (EPMA) technique and Matano-Kirkaldy method. Based on the reliable thermodynamic description of fcc phase in the Cu-Fe-Mn system available in the literature as well as the ternary diffusion coefficients measured in the present work, the atomic mobilities in fcc Cu-Fe-Mn alloys were assessed by utilizing the DICTRA (Diffusion Controlled TRAnsformation) software package. The calculated interdiffusion coefficients based on the assessed atomic mobilities agree well with most of the experimental data. The comprehensive comparison between various model-predicted diffusion properties and the measured data, including the concentration penetration profiles, interdiffusion flux profile, and diffusion paths, further verify the reliability of the presently obtained atomic mobilities.*

*Key words: Diffusion; Atomic mobility; Fcc Cu-Fe-Mn alloys; DICTRA; Diffusion path*

### **1. Introduction**

As an alloying element, Fe is important for improving the damping properties and workability for Cu-Mn based alloys [1,2], while Cu is an important alloying element and influential factor in steel [3]. The Cu-Fe-Mn ternary system is one of the important systems in both Fe-Cu based magnetic alloys [4] and Cu-based shape memory alloys [5]. Besides, the three elements (Cu, Fe and Mn) are also important for the aluminum alloy since the aluminides of transition metals have high-melting points, good mechanical properties, low cost and better corrosion resistance and weldability [6]. In order to achieve a better optimization of alloy composition and control process condition in Cu-Fe-Mn alloys, accurate thermodynamic and kinetic data in the Cu-Fe-Mn system are indispensable. Nowadays, two thermodynamic descriptions for the Cu-Fe-Mn system have been established [4,7] by means of the CALPHAD (CALculation of PHase Diagram) technique. From such thermodynamic descriptions, various thermodynamic properties over wide composition and temperature ranges can be easily calculated. However, this is not the case for kinetics. Up to now, only the kinetic databases, also known as the atomic mobility database [8,9], in binary fcc Cu-

Fe, Fe-Mn, and Cu-Mn alloys have been evaluated by Liu et al. [10,11] and Zhang et al. [12]. As for the ternary system, there has been no any report up to now. The major obstacle for establishment of atomic mobility databases in ternary Cu-Fe-Mn system is the lack of various reliable experimental diffusion coefficients. Thus, it is urgent to remedy this situation.

Consequently, fcc Cu-Fe-Mn ternary alloys are chosen as the target in the present work. The major objectives of this work are: (i) to measure the interdiffusion coefficients in fcc Cu-Fe-Mn alloys at 1273 K using the Matano-Kirkaldy method; (ii) to evaluate the atomic mobilities of fcc Cu-Fe-Mn alloys by means of DICTRA (Diffusion Controlled TRAnsformation) based on the presently obtained experimental diffusion coefficients; and (iii) to further verify the reliability of the obtained atomic mobilities *via* the comprehensive comparison between the simulated and measured diffusion properties, i.e., concentration profiles, interdiffusion flux profile, and diffusion paths of various diffusion couples. The obtained atomic mobilities of fcc Cu-Fe-Mn alloys will be incorporated in the atomic mobility database for multi-component Al alloys pursued in our research group [9,13-15] *via* a combined approach of experiment, DICTRA assessment and first-principle calculations since 2009.

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## 2. Experimental procedure

The detail experimental procedure in the present work is similar to our previous work [9,13], and thus concisely described here. Cu (purity: 99.99 wt.%), Fe (purity: 99.97 wt.%), and Mn (purity: 99.9 wt.%) were used as starting materials. By arc melting of the pure elements under a high-purity argon atmosphere using a non-consumable tungsten electrode, button samples of Fe-Mn and Cu-Fe-Mn alloys were prepared. The nominal compositions of the prepared alloys are listed in Table 1. They were re-melted four times in order to improve the homogeneity of the buttons. Then, the buttons were cut into blocks of approximate dimension  $4 \times 4 \times 6 \text{ mm}^3$  and sealed in quartz tubes with vacuum atmosphere, and then homogenized at 1273 K for 30 days in an L4514-type diffusion furnace (Qingdao Instrument & Equipment Co. Ltd., China), followed by quenching in water. The polished and cleaned blocks were bound together by molybdenum wires to form the 6 diffusion couples according to the assembly listed in Table 1. These couples were then sealed in quartz tubes under vacuum atmosphere, and annealed at 1273 K for 15 days in the L4514-type diffusion furnace. Subsequently, the couples were quenched into cold water. After standard metallographic preparation, the concentration profiles were measured by means of electron probe microanalysis (EPMA) technique (JXA-8230, JEPL, Japan) on the polished section. The concentrations were obtained by comparing with standards of pure elements Cu, Fe and Mn, after absorption and fluorescence correction (ZAF corrections). The uncertainty of the experimental concentration profiles for each component in the 6 samples is within 2 at. %.

## 3. Evaluation of ternary diffusivities and diffusion modeling

### 3.1 Evaluation of interdiffusion coefficients in fcc Cu-Fe-Mn alloys

The interdiffusion flux of component  $i$ ,  $\tilde{J}_i$ , in a fictitious 1-2-3 ternary system can be expressed as [16]:

$$\tilde{J}_i = -\tilde{D}_{i1}^3 \frac{\partial C_1}{\partial x} - \tilde{D}_{i2}^3 \frac{\partial C_2}{\partial x} \quad (i = 1, 2), \quad (\text{Eq 1})$$

where  $i$  is the solute, and 3 is the solvent, which is usually treated as the dependent element.  $C_1$  and  $C_2$  are the concentrations of solutes 1 and 2, respectively.  $x$  is the distance relative to the Matano interface.  $\tilde{D}_{i1}^3$  and  $\tilde{D}_{i2}^3$  are the main interdiffusion coefficients, while the other two are the cross interdiffusion coefficients. Here, the symbols, 1, 2 and 3, represent Cu, Mn and Fe, respectively.

The Boltzmann-Matano method was successfully extended into ternary and even higher-order systems by Kirkaldy [17]. With the method from Kirkaldy [17], it is then possible to obtain the interdiffusion coefficients at the intersection point of diffusion paths of two designed couples. According to the Matano-Kirkaldy method [18,19], one can obtain equations like

$$\int_{C_i^\infty}^{C_i} x dC_i = -2t \left[ \tilde{D}_{i1}^3 \frac{\partial C_1}{\partial x} + \tilde{D}_{i2}^3 \frac{\partial C_2}{\partial x} \right]_{C_i} \quad (i = 1, 2), \quad (\text{Eq 2})$$

in a ternary system by expressing interdiffusion flux of component  $i$  as

$$\tilde{J}_i = \frac{1}{2t} \int_{C_i^\infty}^{C_i} x dC_i \quad (i = 1, 2). \quad (\text{Eq 3})$$

In Eqs. 2 and 3, the definition of the Matano plane, which is the reference of the distance, can be expressed in such a way [20]

$$x_M = \frac{1}{C_i^\infty - C_i^{+\infty}} \int_{C_i^\infty}^{C_i^{+\infty}} x dC_i \quad (i = 1, 2), \quad (\text{Eq 4})$$

### 3.2 Diffusion modeling

From the absolute reaction rate theory arguments, the atomic mobility of element  $k$ ,  $M_k$ , can be divided into a frequency factor  $M_k^0$  and an activation enthalpy  $Q_k$  [21,22]. As further suggested by Jönsson [22], one should expand the logarithm of the frequency factor,  $\ln M_k$ , rather than the value itself. The mobility,  $M_k$ , is thus expressed as

$$M_k = \exp\left(\frac{RT \ln M_k^0}{RT}\right) \exp\left(\frac{-Q_k}{RT}\right) \frac{1}{RT} \text{ m}^2 \text{ s}^{-1}, \quad (\text{Eq 5})$$

**Table 1.** Annealing schedule for the prepared diffusion couples in the Cu-Fe-Mn alloys

Couple number	Nominal composition of the diffusion couples / at. %	Diffusion temperature / K	Time / s
1#	Fe-4.3Cu-18.4Mn / Fe-20.2Mn	1273	1296000
2#	Fe-4.6Cu-29.4Mn / Fe-0.4Cu-35.6Mn	1273	1296000
3#	Fe-4.7Cu-32.7Mn / Fe-46.3Mn	1273	1296000
4#	Fe-2.4Cu-32.8Mn/Fe	1273	1296000
5#	Fe / Fe-2.4Cu-26.5Mn	1273	1296000
6#	Fe-4.3Cu-3.4Mn / Fe-1.8Cu-37.4Mn	1273	1296000

where  $R$  is the gas constant,  $T$  is the temperature in Kelvin, and  $^{mg}Q$  is the factor taking into account the contribution of ferromagnetic ordering. The ferromagnetic contribution can be neglected for the disordered fcc phase [23]. Thus the corresponding atomic mobility parameters for a certain element  $B$  in the DICTRA notation,  $RT \ln M_B^0$  and  $Q_B$ , can be merged into one parameter, i.e.,  $\Phi_B = -Q_B + RT \ln M_B^0$ , which in general depends on composition, temperature, and pressure. Therefore,  $\Phi_B$  for disordered fcc phase in the Cu-Fe-Mn system can be represented by the Redlich-Kister polynomial [24]:

$$\Phi_B = \sum_i x_i \Phi_B^i + \sum_i \sum_{j>i} x_i x_j \left[ \sum_{r=0}^n (x_i - x_j)^r \cdot \Phi_B^{i,j,r} \right] + \sum_i \sum_{j>k} x_i x_j x_k \left( \sum_s v_{ijk}^s \Phi_B^{i,j,k,s} \right) \quad (s = i, j, k), \quad (\text{Eq 6})$$

where  $x_i$  is the mole fraction of component  $i$ .  $\Phi_B^i$  is the value of  $\Phi_B$  for  $B$  in pure  $i$ , while  $^r \Phi_B^{i,j}$  and  $^s \Phi_B^{i,j,k}$  are the respective binary and ternary interaction parameters to be evaluated on the basis of the experimental data. In Eq. 6, the parameter  $v_{ijk}^s$  can be expressed as:

$$v_{ijk}^s = x_s + (1 - x_i - x_j - x_k) / 3. \quad (\text{Eq 7})$$

The interdiffusion coefficient,  $\tilde{D}_{ij}^n$ , which is related to the flux of element  $k$  with the gradient of component  $j$  and reference component  $n$ , can be given by [21,22]:

$$\tilde{D}_{ij}^n = \sum_i (\delta_{ik} - x_k) \cdot x_i \cdot M_i \cdot \left( \frac{\partial \mu_i}{\partial x_j} - \frac{\partial \mu_i}{\partial x_n} \right), \quad (\text{Eq 8})$$

where  $\delta_{ik}$  is the Kronecker delta ( $\delta_{ik} = 1$  if  $i = k$ , otherwise  $\delta_{ik} = 0$ ).  $x_i$  and  $\mu_i$  are the mole fraction and the chemical potential of element  $i$ , respectively. Assuming the mono-vacancy atomic exchange mechanism, the tracer diffusion coefficients,  $D_i^*$ , relates to the atomic mobility *via* the Einstein relation

$$D_i^* = RTM_i. \quad (\text{Eq 9})$$

#### 4. Results and discussion

##### 4.1 Determination of interdiffusion coefficients at 1273 K

Figure 1 presents the calculated isothermal section of the Cu-Fe-Mn system at 1273 K in Fe-rich region according to the thermodynamic description by Zhang et al. [7]. All the diffusion couples are superimposed on the isothermal section. The concentration profiles of all the diffusion couples were determined by EPMA. The variation in alloy composition is determined to be within  $\pm 0.5$  at.% for each component. Considering that all the concentration profiles measured in the present work are symmetric, the Boltzmann function was used to fit the experimental data. The Matano-Kirkaldy method was used to evaluate the interdiffusion coefficients. Table 2 shows the obtained interdiffusion coefficients,

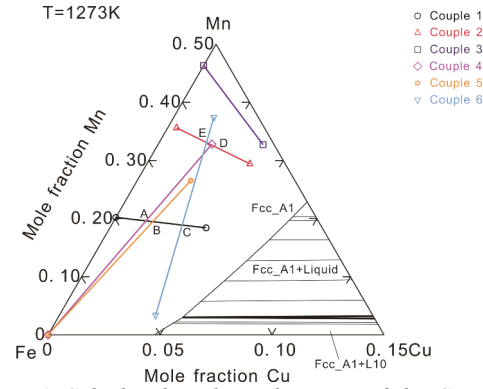


Figure 1. Calculated isothermal section of the Cu-Fe-Mn system in Fe-rich region at 1273 K due to the thermodynamic parameters from [7]. The nominal compositions of all the diffusion couples are also superimposed

including  $\tilde{D}_{CuCu}^{Fe}$ ,  $\tilde{D}_{CuMn}^{Fe}$ ,  $\tilde{D}_{MnCu}^{Fe}$  and  $\tilde{D}_{MnMn}^{Fe}$  at the 5 intersection points of the Cu-Fe-Mn diffusion couples. As can be seen in the table, the main interdiffusion coefficients,  $\tilde{D}_{CuCu}^{Fe}$  and  $\tilde{D}_{MnMn}^{Fe}$ , are positive and generally larger than the absolute values of the cross ones,  $\tilde{D}_{CuMn}^{Fe}$  and  $\tilde{D}_{MnCu}^{Fe}$ .

Before their usage for assessment of atomic mobility, these experimental interdiffusion coefficients should be validated by the following constraints, which express the stability of solid solution [25]:

$$\tilde{D}_{CuCu}^{Fe} + \tilde{D}_{MnMn}^{Fe} > 0, \quad (\text{Eq 13})$$

$$\tilde{D}_{CuCu}^{Fe} \cdot \tilde{D}_{MnMn}^{Fe} - \tilde{D}_{CuMn}^{Fe} \cdot \tilde{D}_{MnCu}^{Fe} \geq 0, \quad (\text{Eq 14})$$

$$\left( \tilde{D}_{CuCu}^{Fe} - \tilde{D}_{MnMn}^{Fe} \right)^2 + 4 \cdot \tilde{D}_{CuMn}^{Fe} \cdot \tilde{D}_{MnCu}^{Fe} \geq 0. \quad (\text{Eq 15})$$

The calculations indicate that all the measured interdiffusion coefficients listed in Table 2 satisfy these constraints.

Table 2. The presently obtained ternary interdiffusion coefficients in fcc Cu-Fe-Mn alloys at 1273 K

Diffusion couple	Composition / at. %		Interdiffusion coefficients $\times 10^{-16} / \text{m}^2 \text{s}^{-1}$			
	Cu	Mn	$\tilde{D}_{CuCu}^{Fe}$	$\tilde{D}_{CuMn}^{Fe}$	$\tilde{D}_{MnCu}^{Fe}$	$\tilde{D}_{MnMn}^{Fe}$
1#~4# (A)	1.6	19.3	2.06	-0.0847	0.0325	1.94
1#~5# (B)	1.8	19.3	2.08	0.0203	-0.0913	1.66
1#~6# (C)	3.7	19.0	2.18	-0.372	4.40	7.99
2#~4# (D)	2.3	32.3	7.25	-0.722	-13.0	5.39
2#~6# (E)	2.7	32.0	7.93	-0.0258	-10.6	7.75

##### 4.2 Assessment of atomic mobility

The assessment of ternary atomic mobilities in fcc Cu-Fe-Mn alloys was conducted in the PARROT module of the DICTRA software package [26,27]

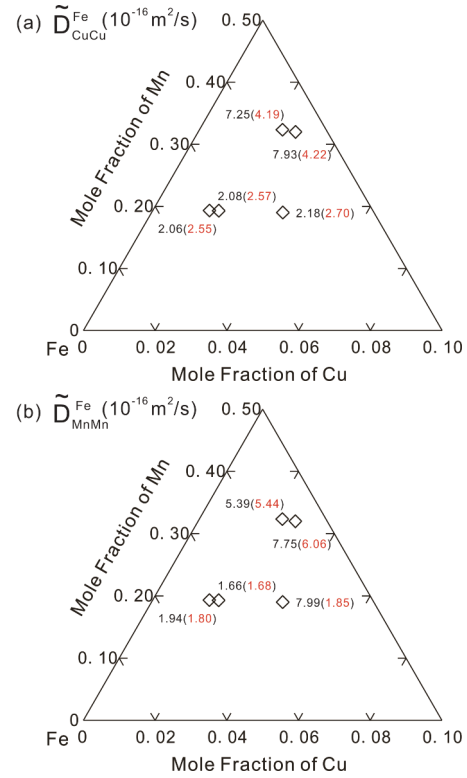
based on the experimental interdiffusion coefficients at 1273 K obtained in the present work. The atomic mobilities in binary fcc Cu-Fe and Fe-Mn alloys are taken from the assessments by Liu et al. [10,11], while those in binary fcc Fe-Mn alloys are from Zhang et al. [12]. The finally obtained atomic mobility parameters for fcc Cu-Fe-Mn alloys, as well as those in boundary binaries from the literature, are listed in Table 3.

**Table 3.** Summary of the atomic mobilities for the fcc phase in the Cu-Fe-Mn system obtained in the present work

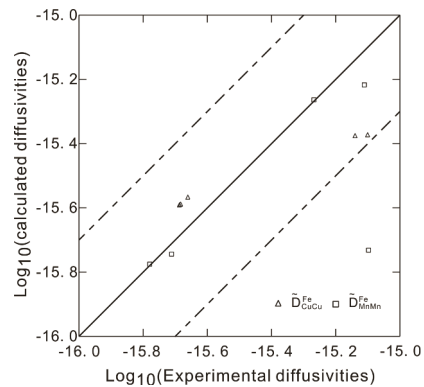
Mobilities	Parameter (J/mol)	Reference
Mobility of Cu	$\Phi_{Cu}^{Cu} = -205872.0 - 82.52 \times T$	[28]
	$\Phi_{Cu}^{Fe} = -277188.5 - 85.65 \times T$	[10]
	$\Phi_{Cu}^{Mn} = -212755.9 - 98.07 \times T$	[12]
	${}^0\Phi_{Cu}^{Cu,Mn} = -2905.0 - 11.91 \times T$	[12]
	${}^0\Phi_{Cu}^{Fe,Mn} = -23348.6$	This work
Mobility of Fe	$\Phi_{Fe}^{Cu} = -206123.2 - 82.61 \times T$	[10]
	$\Phi_{Fe}^{Fe} = -286000.0 - 79.55 \times T$	[29]
	$\Phi_{Fe}^{Mn} = -212755.9 - 98.07 \times T$	[11]
	${}^0\Phi_{Fe}^{Cu,Mn} = 1760055.5$	This work
	${}^0\Phi_{Fe}^{Fe,Mn} = -10711.1 - 26.32 \times T$	[11]
	${}^1\Phi_{Fe}^{Fe,Mn} = 16312.2$	[11]
Mobility of Mn	$\Phi_{Mn}^{Cu} = -193085.3 - 81.86 \times T$	[12]
	$\Phi_{Mn}^{Fe} = -246512.7 - 104.56 \times T$	[11]
	$\Phi_{Mn}^{Mn} = -212755.9 - 98.07 \times T$	[30]
	${}^0\Phi_{Mn}^{Cu,Fe} = -1370227.5$	This work
	${}^0\Phi_{Mn}^{Cu,Mn} = -16533.2 + 130.19 \times T$	[12]
	${}^0\Phi_{Mn}^{Fe,Mn} = -24655.6 + 25.32 \times T$	[11]
	${}^1\Phi_{Mn}^{Fe,Mn} = -32017.56$	[11]

The calculated main interdiffusion coefficients (red digits in brackets) of the ternary fcc Cu-Fe-Mn alloys at 1273 K based on the presently obtained atomic mobilities are compared with the presently experimental measurements of  $\tilde{D}_{CuCu}^{Fe}$  and  $\tilde{D}_{MnMn}^{Fe}$ , as presented in Fig. 2. The schematic diagram of the comparison between the calculated main interdiffusion coefficients and the experimental data

is presented in Fig. 3. The dashed lines, which refer to the diffusivities with a factor of 2 or 0.5 from the model-predicted ones, are also superimposed in the figure. As can be seen in both figures, the calculated results are in good agreement with the experimental data except one for Mn. One possible reason might be the relatively scattered Mn concentration points in



**Figure 2.** Calculated main interdiffusion coefficients (digits in brackets) of (a) Cu and (b) Mn of the ternary Cu-Fe-Mn fcc alloys at 1273 K due to the presently obtained atomic mobilities compared with the experimental measurements



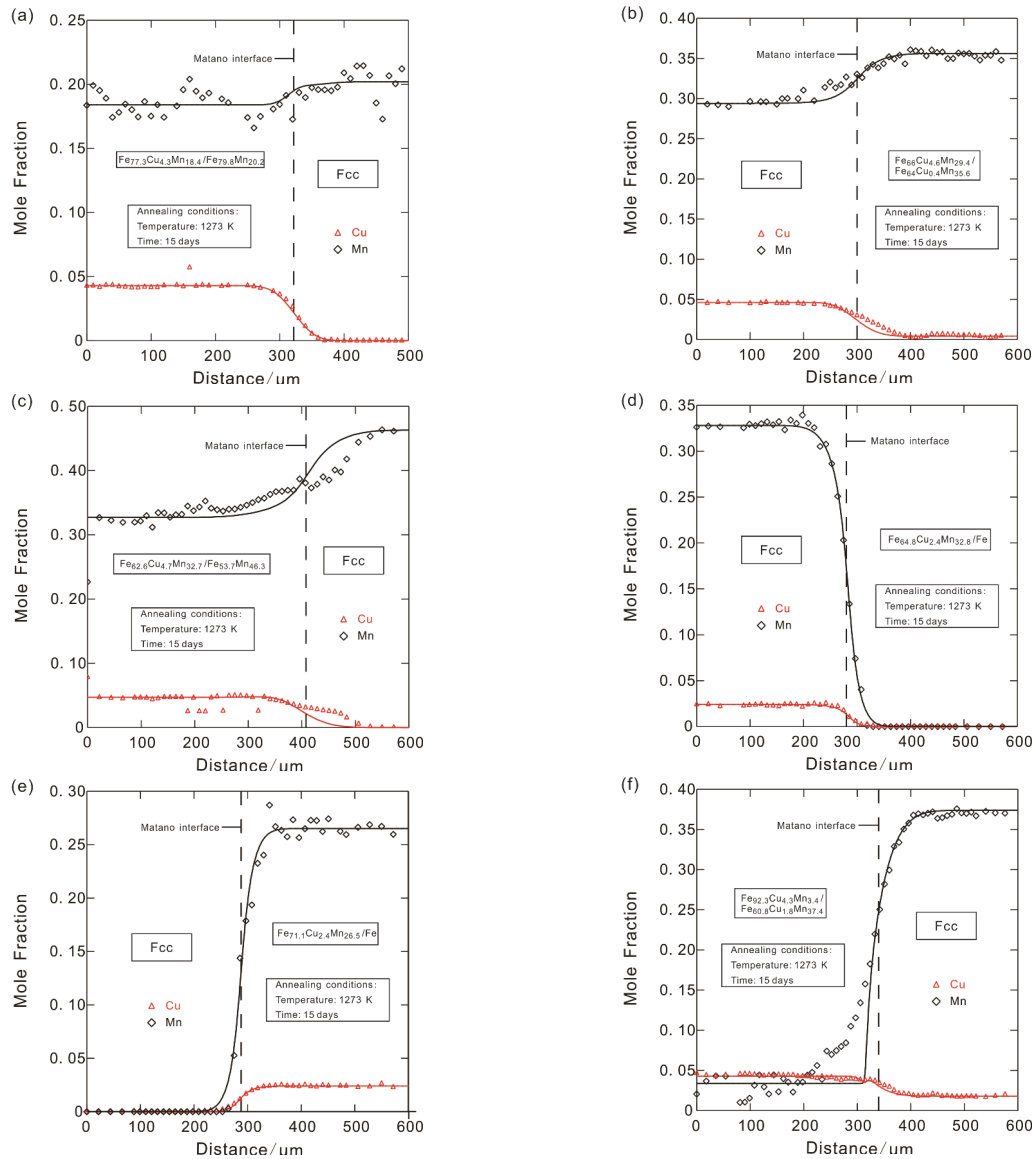
**Figure 3.** Comparison between the calculated main interdiffusion coefficients of the fcc Cu-Fe-Mn system at 1273 K and the experimental values. Dashed lines refer to the diffusion coefficients with a factor of 2 or 0.5 from the model-predicted ones

couple 6#, which leads to a large uncertainty of the determined interdiffusion coefficients.

Based on the presently evaluated atomic mobilities together with the thermodynamic description, the concentration profiles and diffusion paths in various diffusion couples as well as the interdiffusion flux profiles can be calculated. This kind of simulation is also an effective way to verify the reliability of the obtained atomic mobilities.

Figure 4(a-f) shows the model-predicted concentration profiles for the 6 diffusion couples annealed at 1273 K for 15 days, compared with the presently measured data. As can be seen in the figures,

the agreement between the model-predicted concentration profiles and the experimental data is generally good considering the scattered experimental points. The model-predicted and the experimental interdiffusion fluxes of Cu, Fe and Mn in couple 5# are presented in Fig. 5(a-d). The position of the average Matano plane is also given in the figures. As can be seen in Fig. 5, the calculated interdiffusion fluxes are in consistent with the experimental data. Though the same plots can be made for other couples, they are not shown here for saving the space. As shown in Figs. 4 and 5, the good agreement between the model-predicted diffusion properties and the



**Figure 4.** The model-predicted concentration profiles for the 6 diffusion couples annealed at 1273 K for 15 days, compared with the presently measured data: (a) Fe-4.3 at.% Cu-18.4 at.% Mn / Fe-20.2 at.% Mn, (b) Fe-4.6 at.% Cu-29.4 at.% Mn / Fe-0.4 at.% Cu-35.6 at.% Mn, (c) Fe-4.7 at.% Cu-32.7 at.% Mn / Fe-46.3 at.% Mn, (d) Fe-2.4 at.% Cu-32.8 at.% Mn / Fe, (e) Fe-2.4 at.% Cu-26.5 at.% Mn / Fe, and (f) Fe-4.3 at.% Cu-3.4 at.% Mn / Fe-1.8 at.% Cu-37.4 at.% Mn

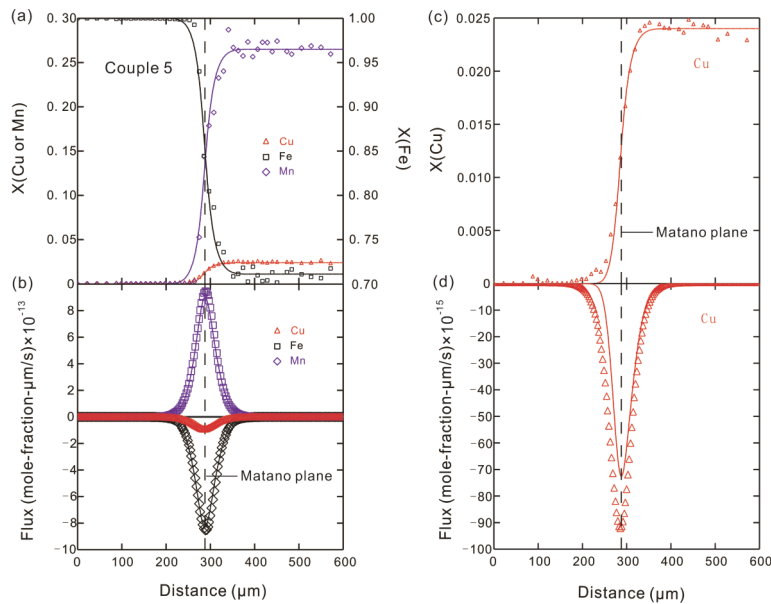


experimental data indicate the reliability of the presently obtained atomic mobilities.

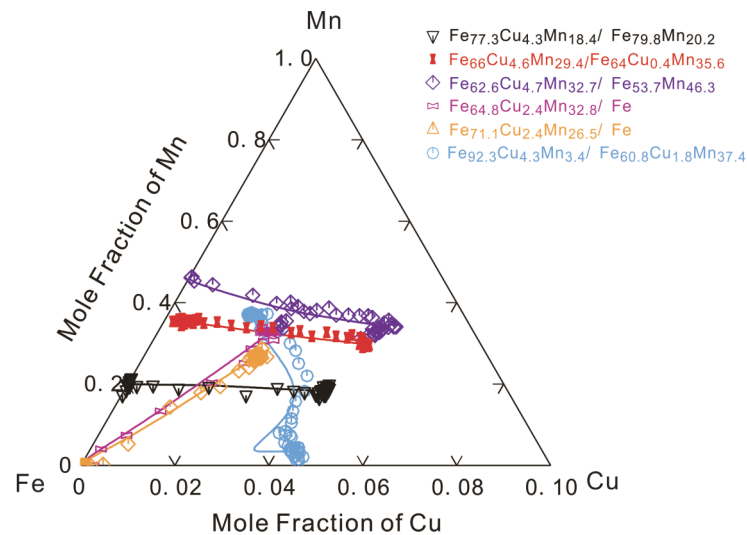
Diffusion paths are loci for concentration profiles in diffusion couples, and their corresponding concentration relations can be concisely presented on the phase diagram. The model-predicted diffusion paths for these 6 ternary couples annealed at 1273 K for 15 days are presented in Fig. 6, compared with the corresponding experimental data. As shown in Fig. 6, all the calculated diffusion paths are consistent with the experimental data. Moreover, the reason for the marked bend in the diffusion path of couple 6# is due to the difference between the diffusion rates of Cu and Mn.

## 5. Conclusions

By employing the diffusion couple technique together with the Matano-Kirkaldy method, the interdiffusion coefficients of fcc Cu-Fe-Mn alloys at 1273 K were determined in the present work. Based on the measured interdiffusion coefficients as well as the available thermodynamic description, atomic mobilities in fcc Cu-Fe-Mn alloys were assessed by using the DICTRA software package. The calculated interdiffusion coefficients agree well with the experimental ones. Moreover, the comprehensive comparisons between the model-predicted and the measured concentration penetration



**Figure 5.** Model-predicted interdiffusion flux profiles of Cu, Fe and Mn of couple 5# (Fe-2.4 at.% Cu-26.5 at.% Mn / Fe) annealed at 1273 K for 15 days, compared with the corresponding experimental data



**Figure 6.** Calculated diffusion paths for the 6 ternary diffusion couples annealed at 1273 K for 15 days, compared with the corresponding experimental data. Symbols denote the experimental data

profiles/interdiffusion flux profile/diffusion paths of diffusion couples, the reliability of the presently obtained atomic mobilities was further verified. The good agreement between the calculations and the experiments indicates that the presently obtained atomic mobilities are reliable.

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