Assessment of Atomic Mobility for the Bcc Phase of the Ti-Al-Mo System

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Abstract. The atomic mobility for the bcc phase of the Ti-Al-Mo ternary system was developed by critical assessment of the experimental diffusion data by using the DICTRA software. The results showed the calculated diffusion coefficients presented the good agreements by the comprehensive comparisons with the experimental diffusion coefficients. The developed Ti-Al-Mo ternary atomic mobility was subsequently validated by appropriate prediction of the interdiffusion behavior with comparison of the diffusion-couple experiments in the literature.

1. Introduction

β titanium alloy exhibits excellent formability thanks to its sustainability of 100% β when quenched from β phase area [1], yet offers significantly higher strengths by separating out the α phase when aged at α+β phase area [2, 3], which are widely used in aerospace and automotive industries [1-3]. The microstructure of the β-Ti alloys are largely depended on the recrystallization, phase transformation and grain growth process, while much of these processes are governed by the diffusion interaction [4-6] during thermomechanical processing and the follow heat treatment. Therefore, knowledge of diffusion kinetics is critical to understand the influence of alloying additions, schedule and optimize the heat treatment parameters and control of microstructural development for new type Ti-based alloys.

Nowadays, by combined with computational thermodynamics, the computational diffusion kinetics [7, 8] can predict the kinetic process of high quality for many commercially important alloy systems by using the DICTRA software, in which the atomic mobility database of the alloy system should be used [8]. More importantly, the mobility database can be applied for simulation the full diffusion picture of titanium alloys of interest without extra experimental measurements by combining the CALPHAD-base (Calculation of Phase Diagram) thermodynamic database [11-14].

The ternary Ti-Al-Mo system is an important base system of many titanium alloys such as Ti-5553 [15] and β-21S [16]. Due to the missing of the mobility database, the aim of this work is to assess the atomic mobility for the bcc phase of the Ti-Al-Mo ternary system by using the DICTRA software, and finally obtain the diffusion characteristic of the Ti-Al-Mo system with simulation of some diffusion couples by applying the acquired atomic mobility parameters.

2. Model Description

The atomic mobility $M_i$ is suggested by Andersson and Ågren first [16] and later modified by Jönsson[17], which is expressed as

$$M_i = M_i^0 \exp \left( \frac{-Q_i^s}{RT} \right) \frac{1}{RT} m \theta \Gamma,$$

(1)
where \( Q^F \) is the activation energy, \( M_i^0 \) is the frequency factor, \( T \) is the temperature and \( R \) is the gas constant, and \( m^q T \) is the effect of ferromagnetic ordering. If there is no ferromagnetic effect, we combined the first two parts of the mobility parameter into a single parameter, i.e., \( Q_i = -Q_i^F + RT \ln M_i^0 \). This parameter \( Q_i \) is approximated to be of composition dependence, which can be similar treated in the phenomenological CALPHAD approach by using the Redlich-Kister polynomial [18], i.e.,

\[
Q_i = \sum_{p} x_p Q_i^p + \sum_{p} \sum_{q>p} x_p x_q \left[ \sum_{r=0,1,2,...} r Q_i^{p,q} (x_p - x_q)^r \right] + \sum_{p} \sum_{q>p} \sum_{v>q} x_p x_q x_v \left[ v_{pqv} \sum_{s} Q_i^{p,q,v,s} \right], \quad (S = p, q, v),
\]

where the \( Q_i^p \) is the value \( Q_i \) of species \( i \) in pure species \( p \) and the \( x_p \) is the mole fraction of species \( p \), while the \( r Q_i^{p,q} \) and \( r Q_i^{p,q,v} \) are the binary and ternary interaction parameters.

All the diffusivities can be expressed to the atomic mobility \( M_i \), e.g., the tracer diffusivity \( D_i^* \) is directly related to the atomic mobility by the follow equation,

\[
D_i^* = RT M_i, \quad (3)
\]

and the interdiffusion coefficient \( D_{pq}^n \) can be expressed as,

\[
D_{pq}^n = \sum_{i=1}^{n-1} (\delta_{ip} - x_p) x_i M_i \left( \frac{\partial \mu_i}{\partial x_q} - \frac{\partial \mu_i}{\partial x_p} \right), \quad (4)
\]

where the \( \delta_{ip} \) is equal to 1 when \( i=p \) and otherwise equal to 0, and in which \( \mu_i \) is the chemical potential of species \( i \). By fitting to experimental obtained diffusion coefficients, those binary and ternary mobility parameters, \( Q_i^p \), \( Q_i^{p,q} \) and \( Q_i^{p,q,v} \), can be numerically assessed upon the proposed relations.

In the diffusion couple, the composition is varying with the diffusion time \( t \) in the diffusion zone, which can be expressed as [19],

\[
\frac{1}{V_m} \frac{\partial x_i}{\partial t} + \nabla \cdot \mathbf{J}_i = 0, \quad (5)
\]

where \( \mathbf{J}_i \) is the interdiffusion flux and the molar volume \( V_m \) is generally treated as a constant. By adding the different boundary conditions and initial conditions, this equation can be solved numerically to present the form of the concentration profile.

3. Evaluation of experimental diffusion data

By applying the Matano-Kirkaldy and the modified Hall methods, the interdiffusion and impurity diffusion coefficients of the bcc phase of the Ti-Al-Mo ternary alloys at the Ti-rich corner have been recently determined at the temperature of 1523 K [20]. Before using those to optimize the ternary interaction parameters in this work, all those interdiffusion coefficients were examined and obey the thermodynamic constraints [21].

4. Optimization procedure

During the optimization procedure, the thermodynamic factor of diffusion should be obtained first by using CALPHAD-base thermodynamic database. In this paper, the thermodynamic parameters of the Ti-Al-Mo ternary were provided from CompuTherm [22] for calculation.

The mobility parameters of the bcc phase of Ti-Al binary was taken from the works of Chen et al. [23] was accepted by this work whereas the descriptions of the Ti-Mo binary assessed by Huang et al. [24] was used in this work. Then, by using DICTRA software [25], all the other mobility parameters were optimized by fitting to the selected experimental diffusion coefficients [20]. Table 1 shows the accessed mobility parameters of the Ti-Al-Mo ternary system.
Table 1. Assessed atomic mobilities for the BCC phase of the Ti-Al-Mo ternary system.

| Mobility Parameter (J/mole) | Reference |
|-----------------------------|-----------|
| Mobility of Al              |           |
| $Q_{Al}^{Al}$                | -215000-80.2*T | [23]   |
| $Q_{Al}^{Ti}$                | -154855.1839-129.012*T | Present work |
| $Q_{Al}^{Mo}$                | -215000-80.2*T | Present work |
| $Q_{Al}^{ALMo}$              | 0         | Present work |
| $Q_{Al}^{TLAl}$              | -488445.3+78.3*T | Present work |
| $Q_{Al}^{TLMo}$              | -262410.72-182.65*T | Present work |
| $Q_{Al}^{TLMo}$              | -389841   | Present work |
| Mobility of Mo              |           |
| $Q_{Mo}^{Al}$                | -448004.86-74.69*T | Present work |
| $Q_{Mo}^{Ti}$                | -196255.4-105.21*T | Present work |
| $Q_{Mo}^{Mo}$                | -448004.86-74.69*T | Present work |
| $Q_{Mo}^{ALMo}$              | 0         | Present work |
| $Q_{Mo}^{TLMo}$              | 172696.72-101.96*T | [24]   |
| $Q_{Mo}^{TLMo}$              | -162707.90 | [24]   |
| $Q_{Mo}^{TLAl}$              | 46667     | Present work |
| Mobility of Ti              |           |
| $Q_{Ti}^{Al}$                | -199404.05-90.78*T | [23]   |
| $Q_{Ti}^{Ti}$                | -151989.95-127.37*T | [23]   |
| $Q_{Ti}^{Mo}$                | -207422.23-178.30*T | [24]   |
| $Q_{Ti}^{TLMo}$              | 247023.39-161.01*T | [24]   |
| $Q_{Ti}^{TLMo}$              | 189952.94 | [24]   |
| $Q_{Ti}^{TLAl}$              | -223061.6+184.84*T | Present work |
| $Q_{Ti}^{TLAl}$              | 304789.2-194.43*T | Present work |

5. Results and discussions

5.1 The Ti-Al-Mo ternary

In order to validation of the assessed mobility parameters, the diffusion coefficients are calculated and then compared with the experimental data. Figure 1 shows the calculated main ternary interdiffusion coefficients, $D_{AlAl}^{Ti}$ and $D_{MoMo}^{Ti}$, and the cross coefficients, $D_{AlMo}^{Ti}$ and $D_{MoAl}^{Ti}$, which are compared with the experimental data [20] at 1523 K. It can be seen that the agreements are very reasonable, which reviews particularly good for the main coefficients. However, it shows some minor discrepancy for the cross interdiffusion coefficients, which is mainly due to the usual scatter and relatively larger uncertainty of the experimental cross interdiffusion coefficients. In this work, the calculated cross interdiffusion coefficients $D_{AlMo}^{Ti}$ and $D_{MoAl}^{Ti}$ reviews the regularly change rather than abnormally changing with the variation of the composition, which means our calculations allow the variation of interdiffusion coefficients in the concentration to be appropriately predicted, i.e., the main interdiffusion coefficients of Al increase with increasing the Al content or decreasing the Mo content; however, decreasing the Al or Mo content both leads to a rise of the main interdiffusion coefficients of Mo. The calculated results also show the cross interdiffusion coefficients of Al and Mo increase with increasing both the Al and Mo content.
5.2 Simulation of diffusion couple experiments

The accuracy of the assessed mobility parameters can be further validated by comparing the predicted in-depth diffusion behavior arising from interdiffusion with the available diffusion experiment. By combining the obtained mobility parameters of the Ti-Al-Mo ternary the thermodynamic parameters, the diffusion couple experiment can be predicted by solving Eq. (5) numerically. Figure 2 shows the examples of the Ti-Al-Mo ternary diffusion couple for the concentration profile of Ti/Ti-22.83Al-5.94Mo in Fig. 2 (a) and Ti-5Mo/Ti-15.09Al in Fig. 2 (b) both at 1523 K with the experimental data [20] for comparison. The results show the agreement is apparently very satisfactory. Figure 3 compares the simulated diffusion paths with the experimental, the curves on the ternary isotherm mapping the locus of the compositions in planes parallel to the couple interface throughout the diffusion zone, with the experimental points measured from the diffusion couples at 1523 K [20]. The results also show the good agreement for a majority of the diffusion couples.

Figure 1. Calculated interdiffusion coefficients (in italic font) of the Ti-Al-Mo bcc ternary alloys at 1523 K in a comparison with the experimental measurement [20] (a) $D_{AlAl}^{Ti}$, (b) $D_{AlMo}^{Ti}$, (c) $D_{MoAl}^{Ti}$, (d) $D_{MoMo}^{Ti}$.

6. Conclusion

The DICTRA software was used for developing the diffusion mobility for the bcc phase of the Ti-Al-Mo ternary by assessing the experimental diffusion data. The comprehensive comparisons were made between the calculated diffusion coefficients and the available experimental data, which show the general satisfactory agreements. By combining with the CALPHAD-base thermodynamic parameters, the developed atomic mobility database has been successfully validated through further predicting of a number of ternary diffusion experiments.
Figure 2. Simulated concentration profiles for (a) Ti/Ti-22.83Al-5.94Mo and (b) Ti-5Mo/Ti-15.09Al diffusion couples at 1523K in a comparison with the experimental measurement [20].

Figure 3. Simulated diffusion paths for ternary couples at the temperatures of 1523K compared with the experimental measurement (symbols) [20].

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