Vol. 14 № 5 Trans. Nonferrous Met. Soc. China Oct. 2004

Article ID: 1003-6326(2004)05-0875-05

Calculation of activity coefficients for components in ternary Ti alloys and intermetallics as matrix of composites①

ZHU Yan(朱 艳)[1,2,3], YANG Yan-qing(杨延清)[2], SUN Jun(孙 军)[1]
(1. State Key Laboratory for Mechanical Behavior of Materials,
College of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China;
2. Department of Materials Science and Engineering,
Northwestern Polytechnical University, Xi'an 710072, China;
3. College of Environment and Chemical Engineering,
Xi'an University of Engineering Science and Technology, Xi'an 710048, China)

Abstract: Based on Kohler's ternary solution model and Miedema's model for calculating the formation heat of binary solution, the integral equation was established for calculating the activity coefficients in ternary alloys and intermetallics. The activity coefficients for components in alloy Ti-5Al-2.5Sn, Ti-6Al-4V and intermetallics TiAl, Ti_3Al and Ti_2AlNb were calculated with the equations. The calculated data coincide well with the experimental ones found in literatures. According to the calculated activity coefficients and activities, it can be predicted that the interfacial reaction in SiC/Ti_3Al composite is more severe than that in composites SiC/Ti_2AlNb and SiC/TiAl.

Key words: activity coefficient; thermodynamics; Ti-alloy; intermetallics; interfacial reaction

CLC number: TB 331 **Document code:** A

1 INTRODUCTION

Activity and activity coefficient can be directly used to calculate the evaporation loss of alloying elements during melting[1, 2] and to calculate thermodynamic properties in studying interfacial reaction mechanism of metal-matrix composites[3]. Because there are some difficulties to measure the activity coefficient experimentally[4, 5], it is necessary to get it by calculation. Some research works have been done to predict or calculate activities and activity coefficients in systems of a number of components[6]. However, up to now, for the solution systems consisting of elements more than 3, it is still difficult to get those activity coefficients precisely. Although two main ternary solution models and formulas have been set up, the calculated data from one set formulas do not coincide well with the experimental ones found in Ref.[7] and there are some mistakes in another set formulas[8]. Besides, although thermocalc software can be used in calculating activity coefficients in ternary alloys, the price of the data base is expensive and the number of elements in the data base are limited.

In this paper, based on Kohler's ternary solution model and Miedema's model of calculating formation heat, ΔH_{ij}, of binary system, the integral equation was established for calculating the activity coefficients in ternary alloys and intermetallics with thermodynamic methods. The activity coefficients for components in ternary alloy Ti-5Al-2.5Sn, Ti-6Al-4V and intermetallics TiAl, Ti_3Al and Ti_2AlNb were obtained with the equation, and compared with experimental data in literatures. The calculated results agree with experimental values although there are a little flaws in both of the starting models. Interfacial reaction tendency of SiC/TiAl, SiC/Ti_3Al and SiC/Ti_2AlNb composites was predicted according to the activity coefficients.

2 CALCULATION MODEL

For i-j-k ternary system, under the condition of certain temperature and pressure, the activity coefficient of solute i would be expressed as[9]:

$$\ln \gamma_i = \ln \gamma_i^0 + \sum_{j=2}^{3} \varepsilon_i^j x_j + \sum_{j=2}^{3} \rho_i^j x_j^2 + \sum_{i=2}^{3}\sum_{j=2}^{3} \rho_i^{ij} x_i x_j + o(x^3) \quad (1)$$

The definition of each coefficient is as follows:

$$\ln \gamma_i^0 = \frac{1}{RT}(\bar{G}_i^{\mathrm{E}})_{x_j=0,\ x_k\to 1} \quad (2)$$

$$\varepsilon_i^i = \left[\frac{\partial \ln \gamma_i}{\partial x_i}\right]_{x_j=0,\ x_k\to 1} = \frac{1}{RT}\left[\frac{\partial \bar{G}_i^{\mathrm{E}}}{\partial x_i}\right]_{x_j=0,\ x_k\to 1} \quad (3)$$

---

① **Foundation item:** Project(locality-02191) supported by the Key Foundation of Ministry of Education of China; project(2002B20) supported by the Natural Science Foundation of Shaanxi Province; project(02JK117) supported by the Foundation of Shaanxi Education Committee

Received date: 2004-02-05; **Accepted date:** 2004-05-08

Correspondence: ZHU Yan, Professor, PhD; Tel: +86-29-88061297; E-mail: yan_zhu0863@sina.com

$$\varepsilon_i^j = \left[\frac{\partial \ln \gamma_i}{\partial x_j}\right]_{x_k \to 1} = \frac{1}{RT}\left[\frac{\partial \bar{G}_i^{\mathrm{E}}}{\partial x_j}\right]_{x_k \to 1} \tag{4}$$

$$\rho_i^i = \frac{1}{2}\left[\frac{\partial^2 \ln \gamma_i}{\partial x_i^2}\right]_{x_j = 0,\ x_k \to 1} = \frac{1}{2RT}\left[\frac{\partial^2 \bar{G}_i^{\mathrm{E}}}{\partial x_i^2}\right]_{x_j = 0,\ x_k \to 1} \tag{5}$$

$$\rho_i^j = \frac{1}{2}\left[\frac{\partial^2 \ln \gamma_i}{\partial x_j^2}\right]_{x_k \to 1} = \frac{1}{2RT}\left[\frac{\partial^2 \bar{G}_i^{\mathrm{E}}}{\partial x_j^2}\right]_{x_k \to 1} \tag{6}$$

$$\rho_i^{ij} = \frac{1}{RT}\left[\frac{\partial^2 \bar{G}_i^{\mathrm{E}}}{\partial x_i \partial x_j}\right]_{x_k \to 1} \tag{7}$$

In the ternary system, there exist the equations as:

$$\begin{cases} \bar{G}_i^{\mathrm{E}} = G^{\mathrm{E}} - x_j \dfrac{\partial G^{\mathrm{E}}}{\partial x_j} + (1 - x_i)\dfrac{\partial G^{\mathrm{E}}}{\partial x_i} \\ \bar{G}_j^{\mathrm{E}} = G^{E} - x_i \dfrac{\partial G^{\mathrm{E}}}{\partial x_i} + (1 - x_j)\dfrac{\partial G^{\mathrm{E}}}{\partial x_j} \\ \bar{G}_k^{\mathrm{E}} = G^{\mathrm{E}} - x_i \dfrac{\partial G^{\mathrm{E}}}{\partial x_i} - x_j \dfrac{\partial G^{\mathrm{E}}}{\partial x_j} \end{cases} \tag{8}$$

where x_i, x_j and x_k are the mole fractions of components i, j and k; $\bar{G}_i^{\mathrm{E}}$, $\bar{G}_j^{\mathrm{E}}$, $\bar{G}_k^{\mathrm{E}}$ are the partial mole excess free energy of components i, j, k; ε_i^i, ε_i^j are the first-order international coefficients between i and i, j; ρ_i^i, ρ_i^j, ρ_j^{ij} are the second-order international coefficients between i and i, j; G^E is the excess free energy of ternary system; γ_i is the activity coefficient of component i; γ_i^0 is the zero-order activity coefficient of component i. From Eqns. (1)−(8), it is obvious that, if the relationship between G^E and x_i, x_j and x_k can be built up, the activity coefficient of component i can be calculated. The following Kohler's equation just serves the purpose:

$$\begin{aligned} G^{\mathrm{E}} = {} & (x_i + x_j)^2 G_{ij}^{\mathrm{E}}\left[\frac{x_i}{1 - x_i - x_j}, \frac{x_j}{1 - x_i - x_j}\right] + \\ & (1 - x_j)^2 G_{ik}^{\mathrm{E}}\left[\frac{x_i}{1 - x_j}, \frac{1 - x_i - x_j}{1 - x_j}\right] + \\ & (1 - x_i)^2 G_{jk}^{\mathrm{E}}\left[\frac{x_j}{1 - x_i}, \frac{1 - x_i - x_j}{1 - x_i}\right] \end{aligned} \tag{9}$$

$$\left.\begin{aligned} G_{ij}^{\mathrm{E}} &= H_{ij}^{\mathrm{E}} - TS_{ij}^{\mathrm{E}} = \Delta H_{ij} - TS_{ij}^{\mathrm{E}} \\ G_{ik}^{\mathrm{E}} &= H_{ik}^{\mathrm{E}} - TS_{ik}^{\mathrm{E}} = \Delta H_{ik} - TS_{ik}^{\mathrm{E}} \\ G_{jk}^{\mathrm{E}} &= H_{jk}^{\mathrm{E}} - TS_{jk}^{\mathrm{E}} = \Delta H_{jk} - TS_{jk}^{\mathrm{E}} \end{aligned}\right\} \tag{10}$$

where G_{ij}^{E}, G_{ik}^{E}, G_{jk}^{E} are the excess free energies of these binary systems (i, j), (j, k) and (i, k). ΔH_{ij}, ΔH_{ik}, ΔH_{jk} are the formation heats during the alloying process between component i and j, i and k, j and k, respectively; S_{ij}^{E}, S_{ik}^{E}, S_{jk}^{E} are the excess entropies of component i and j, i and k, j and k, respectively.

$$S_{ij}^{\mathrm{E}} = 0.1 \times \Delta H_{ij}\left[\frac{T_{mi} + T_{mj}}{T_{mi}T_{mj}}\right] \tag{11}$$

$$G_{ij}^{\mathrm{E}} = \alpha_{ij} \times \Delta H_{ij} \tag{12}$$

where $\alpha_{ij} = 1 - 0.1T\left[\dfrac{T_{mi} + T_{mj}}{T_{mi}T_{mj}}\right]$, T_{mi} and T_{mj} are the melting points of the components i and j, respectively. According to the Miedema's Model[10], ΔH_{ij} could be written as:

$$\Delta H_{ij} = \frac{f_{ij} x_i[1 + \mu_i x_j(\phi_i - \phi_j)]}{M_{ij}} \cdot \frac{x_j[1 + \mu_j x_i(\phi_j - \phi_i)]}{M_{ij}} \tag{13}$$

where

$$f_{ij} = 2pV_i^{2/3}V_j^{2/3} \times \left\{\frac{9.4[(n_{ws}^{1/3})_j - (n_{ws}^{1/3})_i]^2}{(n_{ws}^{1/3})^{-1} + (n_{ws}^{1/3})_j^{-1}} - \frac{(\phi_j - \phi_i)^2 + a(r/p)}{(n_{ws}^{1/3})^{-1} + (n_{ws}^{1/3})_j^{-1}}\right\}$$

$$\begin{aligned} M_{ij} = {} & x_i V_i^{2/3}[1 + \mu_i x_j(\phi_i - \phi_j)] + \\ & x_j V_j^{2/3}[1 + \mu_j x_i(\phi_j - \phi_i)] \end{aligned}$$

where V_i, V_j, V_k are the mole volume of i, j and k; $(n_{ws})_j$ the electron-densities of i and j; ϕ_i, ϕ_j, ϕ_k the electron-negativity of i, j and k; p, r, μ the experimental constants. Substituting Eqns. (12), (13) into Eqns. (2−8), and making $F_{ij} = \alpha_{ij} \times f_{ij}$, we can get the following expressions.

$$\ln \gamma_i^0 = \frac{1}{RT}A \tag{14}$$

$$\ln \gamma_j^0 = \frac{1}{RT}D \tag{15}$$

$$\varepsilon_i^i = \frac{1}{RT}(2B - 2C) \tag{16}$$

$$\varepsilon_j^j = \frac{1}{RT}(2B' - 2C') \tag{17}$$

$$\varepsilon_i^j = \varepsilon_j^i = \frac{1}{RT}(-A - D) \tag{18}$$

$$\rho_i^i = \frac{1}{2RT}(-E + J) \tag{19}$$

$$\rho_j^j = \frac{1}{2RT}(-F + J') \tag{20}$$

$$\rho_i^j = \frac{1}{2RT}(-F) \tag{21}$$

$$\rho_j^i = \frac{1}{2RT}(-F') \tag{22}$$

$$\rho_i^{ij} = \rho_j^{ij} = \frac{1}{RT}(A + D) \tag{23}$$

$$A = F_{ik}[1 + \mu_i(\phi_i - \phi_k)]/V_k^{2/3} \tag{24}$$

$$\begin{aligned} B = {} & F_{ik}[-1 - (2\mu_i + \mu_k)(\phi_i - \phi_k) - \\ & \mu_i\mu_k(\phi_i - \phi_k)^2]/V_k^{2/3} \end{aligned} \tag{25}$$

$$\begin{aligned} B' = {} & F_{jk}[-1 - (2\mu_j + \mu_k)(\phi_j - \phi_k) - \\ & \mu_j\mu_k(\phi_j - \phi_k)^2]/V_k^{2/3} \end{aligned} \tag{26}$$

$$\begin{aligned} C = {} & F_{ik}[1 + \mu_i(\phi_i - \phi_k)] \cdot \\ & \{V_i^{2/3}[1 + \mu_i(\phi_i - \phi_k)] + \\ & V_k^{2/3}[-1 + \mu_k(\phi_k - \phi_i)]\}/(V_k^{2/3})^2 \end{aligned} \tag{27}$$

$$\begin{aligned} C' = {} & F_{jk}[1 + \mu_j(\phi_j - \phi_k)] \cdot \\ & \{V_j^{2/3}[1 + \mu_j(\phi_j - \phi_k)] + \\ & V_k^{2/3}[-1 + \mu_k(\phi_k - \phi_j)]\}/(V_k^{2/3})^2 \end{aligned} \tag{28}$$

$$D = F_{jk}[1 + \mu_j(\phi_j - \phi_k)]/V_k^{2/3} \tag{29}$$

$$\begin{aligned} E = {} & F_{ik}\{[(4\mu_i + 2\mu_k)(\phi_k - \phi_i)] - \\ & 2 - 2\mu_i\mu_k(\phi_k - \phi_i)^2]/V_k^{2/3} - \\ & 2[1 + \mu_i(\phi_i - \phi_k)][V_i^{2/3}(1 + \end{aligned}$$

$$
\begin{aligned}
&\mu_i(\phi_i - \phi_k)) + V_k^{2/3}(-1+ \\
&\mu_k(\phi_k - \phi_i))]/(V_k^{2/3})^2\} \qquad (30)
\end{aligned}
$$

$$
\begin{aligned}
F = {}& F_{jk}\{[(4\mu_j + 2\mu_k)(\phi_k - \phi_j)] - \\
&2 - 2\mu_j\mu_k(\phi_k - \phi_j)^2]/V_k^{2/3} - \\
&2[1 + \mu_j(\phi_j - \phi_k)][V_j^{2/3}(1+ \\
&\mu_j(\phi_j - \phi_k)) + V_k^{2/3}(-1+ \\
&\mu_k(\phi_k - \phi_j))]/(V_k^{2/3})^2\} \qquad (31)
\end{aligned}
$$

$$
\begin{aligned}
F' = {}& F_{ik}\{[(4\mu_i + 2\mu_k)(\phi_k - \phi_i)] - \\
&2 - 2\mu_i\mu_k(\phi_k - \phi_i)^2]/V_k^{2/3} - \\
&2[1 + \mu_i(\phi_i - \phi_k)][V_i^{2/3}(1+ \\
&\mu_i(\phi_i - \phi_k)) + V_k^{2/3}(-1+ \\
&\mu_k(\phi_k - \phi_i))]/(V_k^{2/3})^2\} \qquad (32)
\end{aligned}
$$

$$
\begin{aligned}
J = {}& F_{ik}\{6\mu_i(\phi_i - \phi_k)/V_k^{2/3} + \\
&6\mu_i\mu_k(\phi_i - \phi_k)^2/V_k^{2/3} + \\
&6\mu_i(\phi_i - \phi_k)Z/(V_k^{2/3})^2 + 6[1+ \\
&\mu_i(\phi_i - \phi_k)]\mu_k(\phi_i - \phi_k)/V_k^{2/3} + \\
&6[1 + \mu_i(\phi_i - \phi_k)]Z/(V_k^{2/3})^2 + 6[1+ \\
&\mu_i(\phi_i - \phi_k)]\mu_k(\phi_i - \phi_k)Z/(V_k^{2/3})^2 - \\
&3[1 + \mu_i(\phi_i - \phi_k)]Y/(V_k^{2/3})^2 + 6[1+ \\
&\mu_i(\phi_i - \phi_k)]Z^2/(V_k^{2/3})^3\} \qquad (33)
\end{aligned}
$$

$$
\begin{aligned}
J' = {}& F_{jk}\{6\mu_j(\phi_j - \phi_k)/V_k^{2/3} + \\
&6\mu_j\mu_k(\phi_j - \phi_k)^2/V_k^{2/3} + \\
&6\mu_j(\phi_j - \phi_k)Z'/(V_k^{2/3})^2 + 6[1+ \\
&\mu_j(\phi_j - \phi_k)]\mu_k(\phi_j - \phi_k)/V_k^{2/3} + \\
&6[1 + \mu_j(\phi_j - \phi_k)]Z'/(V_k^{2/3})^2 + 6[1+ \\
&\mu_j(\phi_j - \phi_k)]\mu_k(\phi_j - \phi_k)Z'/(V_k^{2/3})^2 - \\
&3[1 + \mu_j(\phi_j - \phi_k)]Y'/(V_k^{2/3})^2 + 6[1+ \\
&\mu_j(\phi_i - \phi_k)]Z'^2/(V_k^{2/3})^3\} \qquad (34)
\end{aligned}
$$

$$
\begin{aligned}
Z = {}& V_i^{2/3}[1 + \mu_i(\phi_i - \phi_k)] + \\
&V_k^{2/3}[-1 + \mu_k(\phi_k - \phi_i)] \qquad (35)
\end{aligned}
$$

$$
\begin{aligned}
Y = {}& V_i^{2/3}[-2\mu_i(\phi_i - \phi_k)] + \\
&V_k^{2/3}[-2\mu_k(\phi_k - \phi_i)] \qquad (36)
\end{aligned}
$$

$$
\begin{aligned}
Z' = {}& V_j^{2/3}[1 + \mu_j(\phi_j - \phi_k)] + \\
&V_k^{2/3}[-1 + \mu_k(\phi_k - \phi_j)] \qquad (37)
\end{aligned}
$$

$$
\begin{aligned}
Y' = {}& V_j^{2/3}[-2\mu_j(\phi_j - \phi_k)] + \\
&V_k^{2/3}[-2\mu_k(\phi_k - \phi_j)] \qquad (38)
\end{aligned}
$$

In order to obtain the activity of each component in intermetallics with higher solute concentration, the following Eqn.[11] can be used to calculate the activity coefficient of solvent:

$$
\begin{aligned}
\ln \gamma_k = {}& \left[\frac{\varepsilon_i^i x_i^2 + \varepsilon_i^j x_i x_j + \varepsilon_j^j x_j^2}{(x_i + x_j)^2}\right]\left[(x_i + x_j) + \right. \\
&\left.\ln x_k\right] + 2\left[\ln x_k + (x_i + x_j) + \right. \\
&\left.\frac{(x_i + x_j)^2}{2}\right] \cdot \left[\frac{x_i^3\rho_i^i + x_i x_j^2 \rho_i^j}{(x_i + x_j)^3} + \right. \\
&\left.\frac{x_i^2 x_j \rho_i^{ij} + x_j x_i^2 \rho_j^i + x_j^2 x_i \rho_j^{ij} + x_j^3 \rho_j^j}{(x_i + x_j)^3}\right] \qquad (39)
\end{aligned}
$$

The activity coefficients of solutes i and j are calculated according to the following formulae which were derived from Eqn. (1):

$$
\begin{aligned}
\ln \frac{\gamma_i}{\gamma_i^0} = {}& \ln \gamma_k + \varepsilon_i^i x_i + \varepsilon_i^j x_j + \\
&\rho_i^i x_i^2 + \rho_i^j x_j^2 + \rho_i^{ij} x_i x_j \qquad (40)
\end{aligned}
$$

$$
\begin{aligned}
\ln \frac{\gamma_j}{\gamma_j^0} = {}& \ln \gamma_k + \varepsilon_j^i x_i + \varepsilon_j^j x_j + \\
&\rho_j^i x_i^2 + \rho_j^j x_j^2 + \rho_j^{ij} x_i x_j \qquad (41)
\end{aligned}
$$

3 RESULTS AND DISCUSSION

Using Eqns. (39), (40) and (41), the activity coefficients, γ_i of Ti-5Al-2.5Sn, Ti-6Al-4V alloy and Ti_3Al, TiAl intermetallics are calculated and compared with experimental data. For calculation, the values of electron-densities ϕ, electron-negativity n_{ws}, mole volumes V and some parameters (r/p, μ, q/p and P) come from Ref. [12]. Due to the lower solute concentration in Ti-5Al-2.5Sn alloy, it is not necessary to consider the revisory term $\ln \gamma_k$ in Eqns. (40) and (41). The activity coefficients of components in Ti-5Al-2.5Sn melt at 2 100 K and Ti-6Al-4V melt at 2 100 K are computed with empirical constant $a = 0.73$[12], as listed in Table 1 together with the measured ones[13]. It can be found that the calculated and the measured are in close agreement with each other. For Ti_3Al and TiAl in solid state, if $a = 1$ as reported in Refs. [7, 12], a large deviation can be found between the calculated and the measured data. However, by the way of try and error, if $a = 0.32$, as shown in Table 1, the calculated activity coefficients of Ti in Ti_3Al and TiAl are in good accordance with the measured ones.[14] The difference of activity coefficient between melt and solid depends on empirical constant a, which in some system may be larger than that in others by calculating with different a.

Table 1 Comparison of calculated activity coefficients with measured ones

Alloy	Elements	Calculated	Measured
Ti-5Al-2.5Sn (2 100 K, $a = 0.73$)	Al Sn	0.014 0.052	0.016 0.066
Ti-6Al-4V (2 100 K, $a = 0.73$)	Al V	0.117 9 0.891 3	0.011 0.713
TiAl (1 000 K, $a = 0.32$)	Ti	0.176 9	0.157
Ti_3Al (1 000 K, $a = 0.32$)	Ti	0.635 3	0.716

The activity coefficients of intermetallics Ti_3Al, TiAl and Ti_2AlNb at different temperatures are then calculated as shown in Figs. 1, 2 and 3, respectively. The results show that the activity coefficients of Ti and Al in the three Ti-Al intermetallics are less than 1. The activity coefficients of Ti in both TiAl and Ti_2AlNb are much smaller than those in Ti_3Al, indicating that the atomic binding energy in both TiAl and Ti_2AlNb is larger. So it can be forecasted that

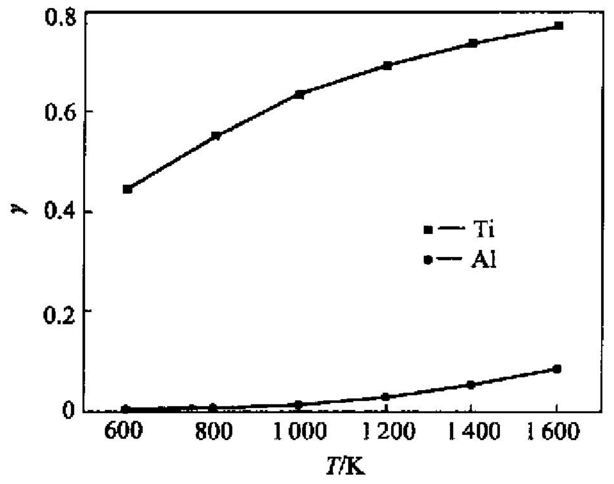

Fig. 1 Activity coefficient of elements in Ti_3Al at different temperatures

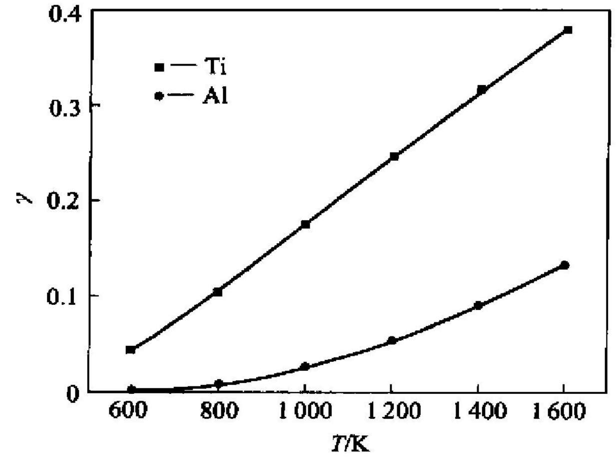

Fig. 2 Activity coefficient of elements in TiAl at different temperatures

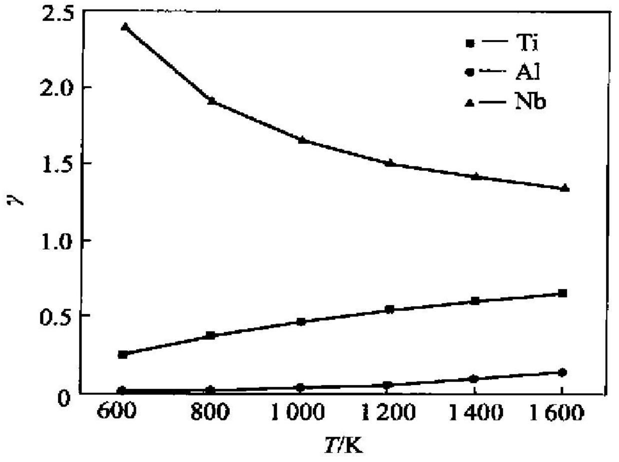

Fig. 3 Activity coefficient of elements in Ti_2AlN_b at different temperatures

Ti atoms in Ti_3Al are more active.

For a chemical reaction, according to thermodynamic criterion, $\Delta_r G = \Delta_r G^{\ominus} + RT\ln J_a$, in which $\Delta_r G^{\ominus}$ is determinated, $\Delta_r G$ depends on J_a which is in inverse proportion with activities, namely the larger the activities are, the more negative $\Delta_r G$ are, and the easier the reaction occurs. Based on some experiments on the interfacial reaction of SiC/Ti-Al matrix composites[14-16], there exist some binary products of Ti and C and of Ti and Si and ternary products of Ti, C and Al at the interface. Considering the influence of Ti and Al in matrix, according to γ_i values calculated in this paper and the formula $a_i = \gamma_i x_i$, the activities of Ti and Al in Ti_3Al, TiAl and Ti_2AlNb are $a(Ti) = 0.476\,5$, $a(Al) = 0.002\,844$; $a(Ti) = 0.088\,45$, $a(Al) = 0.013\,57$; $a(Ti) = 0.231\,8$, $a(Al) = 0.007\,07$, respectively, at 1 000 K. One can find that the activities of Ti in Ti_3Al, Ti_2AlNb and TiAl decrease in turn. Therefore, it can be predicted that the interfacial reaction in SiC/Ti_3Al composite is more severe than that in composites SiC/Ti_2AlNb and SiC/TiAl, in other words, the thickness of interfacial reaction products in composites SiC/Ti_2AlNb and SiC/TiAl should be thinner than that in SiC/Ti_3Al. Fig. 4 shows the thickness of the interfacial reaction zone in SCS-6 SiC/Ti_3Al and in SCS-6 SiC/Ti_2AlNb exposed at 800 ℃, which was measured with transmission electron microscope by one of the present authors[15, 16]. It is in good accordance with the predictions. The above results mean that the thermodynamic prediction may be helpful for choosing the matrix alloys of the composites.

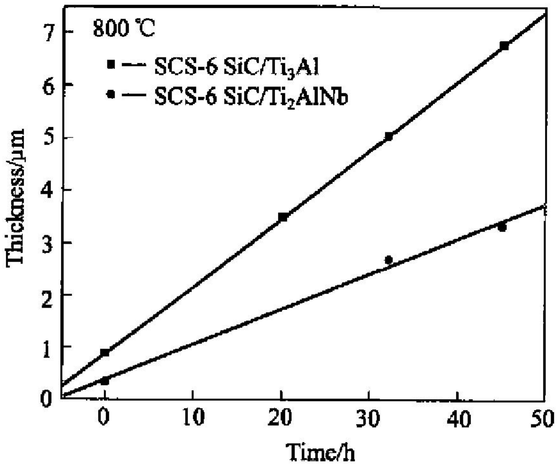

Fig. 4 Thickness of interfacial reaction zone in SCS-6 SiC/Ti_3Al and SCS-6 SiC/Ti_2AlNb

4 CONCLUSIONS

1) The formulae of calculating activity coefficient of ternary alloy and intermetallic have been developed, which are suitable to calculate activity coefficient of binary, ternary alloys and intermetallics. The empirical constants (a) of 0.73 for ternary melt and 0.32 for solid ternary system were determined.

2) The calculated activity coefficients of Ti and Al in Ti_3Al, TiAl and Ti_2AlNb are less than 1, indicating a negative deviation from Raoult law and at-

tractive force between atoms.

3) By comparing the calculated activities in Ti_3Al, TiAl and Ti_2AlNb, it can be predicted that the interfacial reactions in SiC/Ti_3Al composite at about 1 000 K are more severe than those in SiC/Ti_2AlNb and SiC/TiAl, namely the thickness of interfacial reaction layer in SiC/Ti_2AlNb and SiC/TiAl composites is thinner than those in SiC/Ti_3Al composite.

REFERENCES

[1] GUO Jing-jie, LIU Yuan, SU Yan-qing. Evaporation behavior of aluminium in Ti-24Al-11Nb melt during induction skull melting(ISM) process [J]. Acta Metallurgica Sinica, 1999, 35(4): 416 - 420. (in Chinese)

[2] LIU Gui-zhong, SU Yan-qing, GUO Jing-jie, et al. Evaporation loss of components in Ti-13Al-29Nb-2. 5Mo melt during ISM process[J]. Rare Metal Materials and Engineerting, 2003, 32(2): 108 - 112. (in Chinese)

[3] ZHU Yan, YANG Yan-qing, MA Zhi-jun, et al. Thermodynamic studies on interfacial reaction of SiC/Ti-matrix composites[J]. Rare Met Mater Eng, 2002, 31(4): 279 - 282. (in Chinese)

[4] SUN Cheng-wen, CHEN Shen, YANG Zhi-zhou. Thermodynamic properties of Na-Pb alloys by using a sodium beta-alumina [J]. The Chinese Journal of Nonferrous Metals, 2000, 10(6): 877 - 881. (in Chinese)

[5] LE Qi-chi, ZHANG Xin-jian, CUI Jian-zhong. Progression of research on thermodynamic model of metallic alloy melts[J]. Acta Metallurgica Sinica, 2003, 39(1): 35 - 42. (in Chinese)

[6] DING Xue-yong, WANG Wen-zhong. A new thermodynamic calculation formula for activity of component in binary system [J]. Acta Metallurgica Sinica, 1994, 30B (10): 444 - 447. (in Chinese)

[7] DING Xue-yong, FAN Peng, HAN Qi-yong. Models of activity and activity interaction parameter in ternary metallic melt [J]. Acta Metallurgica Sinica, 1994, 30B (2): 49 - 59. (in Chinese)

[8] SU Yan-qing, LIU Yuan, GUO Jing-jie. Calculation of activity coefficients for components in Ti-15-3 melt [J]. Journal of Harbin Institute of Technology, 1999, 6(1): 54 - 57.

[9] Lupis C H P, Elliott J F. Generalized interaction coefficients [J]. Acta Met, 1966, 14: 529 - 538.

[10] Midema A R, De Chatel P F, De Boer F R. Cohesion in alloys-fundamentals of a semi-empirical model[J]. Physica, 1980, 100B: 1 - 28.

[11] Chronister D J, Scott S W, Stickle D R. Induction skull melting of titanium and other reactive alloy[J]. JOM, 1986, 38(9): 51 - 54.

[12] GUO Jing-jie, SU Yan-qing. The Themodynamic and Kinetic Analysis of Ti alloys during the ISM Process [M]. Harbin: Harbin Institute of Technology Press, 1998, 12. (in Chinese)

[13] KONG Fan-ya, YANG Ke-nu. Concentration distribution of alloying element in surface layer of Ti alloy melts [J]. Acta Metallurgica Sinica, 1991, 27B (5): 361 - 363. (in Chinese)

[14] SI Wei-min. Investigation on the Interface of Titanium Aluminides Composites [D]. Shanghai: Shanghai Jiaotong University, 1992. (in Chinese)

[15] YANG Yan-qing, ZHU Yan, MA Zhi-jun, et al. Formation of interfacial reaction products in SCS-6 SiC/Ti_2AlNb composites [J]. Scripta Materialia, 2004, 51: 385 - 389.

[16] YANG Yan-qing , Dudek H J. Interfacial stability in SCS-6 SiC/super α_2 composites [J]. Scripta Materialia, 1997, 37: 503 - 510.

(Edited by LONG Huai-zhong)