THERMODYNAMIC MODELING OF THE Bi–M (M = Ti, Cr, V) SYSTEMS

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Abstract

The Bi–M (M = Ti, Cr, V) systems have been critically reviewed and modeled by means of the CALPHAD technique. All the intermetallics ($BiTi_3$, $BiTi_2$, Bi_9Ti_8, Bi_3Ti_2 and Bi_2Ti) were treated as stoichiometric compounds. The enthalpy of formation at 0 K for $BiTi_2$ was computed via first-principles calculations to assist the thermodynamic modeling. The gas phases for the Bi–Cr and Bi–V systems were treated as ideal gas. A set of self-consistent thermodynamic parameters has been finally obtained for each of these binary systems. Comparisons between the calculated and measured phase diagrams as well as first-principles calculations show that most of experimental data can be satisfactorily reproduced by the present thermodynamic descriptions.

Key words: Bi–Ti; Bi–Cr; Bi–V; Thermodynamic modeling; First-principles calculations

1. Introduction

Al alloys are widely used in building, automobile and aviation industry due to their good mechanical properties. A small addition of Bi, Ti, Cr, and V in Al alloys can significantly affect their mechanical properties. Bi is a good self-lubricating element which could reduce the friction coefficient and increase the anti-seizure load for Al-Si alloy [1]. Moreover, it is effective to reduce the susceptibility of stress-corrosion of the Al–Mg alloys with the addition of a small amount of Bi [2, 3]. The addition of Ti to Al alloys could substantially refine grains and increase the strength [4]. Cr and V are effective trace elements in Ti–Al alloys which could increase the bond energy of TiAl and TiAl$_3$ and enhance their stability, and hence significantly improve the mechanical performances of Ti-Al alloys [5-7].

The Bi–M (M = Ti, Cr, V) systems are several subsystems of multi-component Al alloys. To the best of our knowledge, thermodynamic descriptions for the Bi–M (M = Ti, Cr, V) systems are not available up to now. Since thermodynamic descriptions for binary subsystems are prerequisites for the development of a multi-component Al-base thermodynamic database [8-12], the present work is devoted to provide a set of self-consistent thermodynamic parameters for each of these binary systems by means of CALPHD method and first-principles calculations.

2. Literature Review
2.1 The Bi–Ti system

A number of groups of authors have made contributions to the identification of the Bi–Ti compounds. Nowotny *et al.* [13] and Auer *et al.* [14] firstly designated the BiTi$_4$ based on a structural similarity to PbTi$_4$ and observed BiTi$_2$ by X-ray diffraction (XRD) and density measurements. Then, Obinata *et al.* [15] confirmed the compound BiTi$_4$ to be BiTi$_3$ by XRD. After the work of Auer *et al.* [14] for the BiTi$_2$ phase, Shoemaker [16] also found this phase in sputtering thin films, and Richer and Jertschko [17] determined the crystal structure to be the space group of *I4/mmm*. A compound in the equiatomic region was described by Block [18] using indexing Guinier powder pattern with a tetragonal cell. Later, Richer and Jertschko [17] confirmed this compound which lied at about 50 at.% Bi and named by Bi$_9$Ti$_8$. Subsequently, Vassilev [19] confirmed the existence of the BiTi$_2$ phase and observed Bi$_3$Ti$_2$, Bi$_2$Ti and BiTi by means of electron probe microanalyses (EPMA) and wave disperse system (WDS) analysis on solid/liquid diffusion couples annealed at 400, 500, 600 and 700 °C. It is worth mentioning that Vassilev [19] considered that the BiTi phase was probably identical with Bi$_9$Ti$_8$ reported by Richer and Jertschko [17]. In general, only the crystallographic data for BiTi$_3$, BiTi$_2$ and Bi$_9$Ti$_8$ compounds were available, as shown in Table 1.

Obinata *et al.* [15] investigated the phase relationships in the composition range from 0 to 29.9 at.% Bi by means of microscopic observation, XRD and differential thermal analysis (DTA). According to the work by Obinata *et al.* [15], an eutectoid reaction (βTi) = (αTi) + BiTi$_3$ occurred at 725 °C ± 10 °C and 8.6 at.% Bi and a peritectic reaction liquid + (βTi) = BiTi$_3$ occurred at 1340°C ± 20 °C. The maximal solubility of Bi in (αTi) and (βTi) was 0.347 at.% Bi and 10.138 at.% Bi, respectively. The Bi-rich liquidus was measured by Weeks [23] using a sampling and chemical analysis technique. The compounds Bi$_2$Ti, Bi$_3$Ti$_2$, Bi$_9$Ti$_8$, BiTi$_2$ and BiTi$_3$ formed by the peritectic reactions [15, 19] were considered in the present work. There was no thermodynamic data available in this system.

Table 1. Crystallographic data of solid phases in the Bi–M (M = Ti, Cr, V) systems.

Phase / Temperature Range [°C]	Pearson Symbol / Space Group / Prototype	Lattice Parameters (nm)	Comments / References
(Bi)	hR2		25 °C / [20]
<271.4	$R\bar{3}m$	a=0.47460	
	αAs		
(αTi)	hP2	a=0.29503	25 °C / [20]
<881.8	P63/mmc	c=0.46836	
	Mg		
(βTi)	cI2		>881.84 °C / [21]
<1667.8	Im3m	—	
	W		
(Cr)	cI2		25 °C / [22]
<1906.8	$Im\bar{3}m$	a=0.2884	
	W		
(V)	cI2		25 °C / [22]
<1909.8	$Im\bar{3}m$	a=0.3025	
	W		
BiTi$_3$	Tetragonal	a=0.6020	[15]
<1336.0	—	c=0.8204	[13]
	—		
BiTi$_2$	tI12	a=0.408	[22]
<1289.5	I4/mmm	c=1.457	
	BiTi$_2$		
Bi$_9$Ti$_8$	tp34	a=1.0277	[22]
<997.8	P4/nmm	c=0.7375	
	V$_{7.46}$Sb$_9$		

2.2 The Bi–Cr system

The experimental data for the Bi–Cr system are limited. No intermetallic compound was reported in the system. Two reactions Liquid#1 = Liquid#2 + (Cr)

at 268 °C and Liquid#2 = (Cr) + (Bi) at 1553 °C were investigated by Williams [24] *via* continuous cooling of melting alloys of Bi and Cr. Johnson and Jesseman [25] and Weeks [26] measured the solubilities of Cr in liquid Bi by a sampling and chemical analysis technique.

2.3 The Bi–V system

The experimental information of the Bi–V system was extremely limited. The only one piece of experimental data is the liquidus on the Bi-rich side measured by Weeks [23]. Savitskii *et al.* [27] reported the existence of an intermediate phase BiV$_3$ with a prototype of Cr$_3$Si structure. However, the BiV$_3$ phase was not taken into account in the present modeling since the purity of raw material was low and the samples from Savitskii *et al.* [27] were contaminated by Si from quartz capsule during gas solid diffusion. Hence, the present assessment was based on the experimental data [23] mentioned above and the analogy of some other V-based binary systems adjacent to Bi–V, such as In–V [28] and Tl–V [29]. Smith [30] calculated all phase equilibria using a regular-solution approximation for the liquid alloys. The calculations from the present work will be compared with the results from Smith [30].

3. Thermodynamic modeling
3.1 Unary phase

The Gibbs energy function $^0G_i^\varphi(T) = G_i^\varphi(T) - H_i^{SER}$ for the element i (i = Bi, Ti, Cr and V) in the phase φ is expressed by the following equation:

$$^0G_i^\varphi(T) = a + b \cdot T + c \cdot T \cdot \ln T + d \cdot T^2 + e \cdot T^{-1} + f \cdot T^3 + g \cdot T^7 + h \cdot T^{-9} \quad \ldots(1)$$

where H_i^{SER} is the molar enthalpy of the element i at 298.15 K and 1 atm in its standard element reference (SER) state, and T is the absolute temperature. In the present work, the Gibbs energies of pure elements are taken from the SGTE compilation by Dinsdale [31].

3.2 Solution phases

The liquid, Bcc_A$_2$ ((βTi), (Cr), (V)), Hcp_A$_3$ (αTi) phases are treated as completely disordered solutions. The Gibbs energy is described by a Redlich-Kister polynomial [32]:

$$G_m^\varphi - H^{SER} = x_{Bi} \cdot {}^0G_{Bi}^\varphi + x_i \cdot {}^0G_i^\varphi + R \cdot T \cdot \left[x_{Bi} \cdot \ln(x_{Bi}) + x_i \cdot \ln(x_i) \right] + x_{Bi} \cdot x_i \sum_{j=0}^{n} L_{Bi,i}^{j,\varphi} (x_{Bi} - x_i)^j \quad \ldots(2)$$

where H^{SER} is the abbreviation of $x_{Bi} \cdot H_{Bi}^{SER} + x_i \cdot H_i^{SER}$, R is the gas constant, x_{Bi} and x_i are the mole fractions of

Bi and i (i = Ti, Cr, V), respectively. $L_{Bi,i}^{j,\varphi}$ is the jth interaction parameter of phase φ , and it is equal to $a_j + b_j \cdot T$. The a_j and b_j are the parameters to be optimized in this work.

3.3 Intermetallic compound

All the compounds (Bi_2Ti, Bi_3Ti_2, Bi_9Ti_8, $BiTi_2$ and $BiTi_3$) are treated as stoichiometric compounds. Taking Bi_2Ti as an example, its Gibbs energy per mole-atom is given by the following expression:

$$^0G_m^{TiBi_2} - 1/3 \cdot H_{Ti}^{SER} - 2/3 \cdot H_{Bi}^{SER}$$
$$= A + B \cdot T + 1/3 \cdot {}^0G_{Ti}^{Hcp\_A3} + 2/3 \cdot {}^0G_{Bi}^{Rhom\_A7} \quad ...(3)$$

where A and B are the parameters to be optimized in the present work. Analogous equations can be written for Gibbs energies of the other compounds.

3.4 Gas phase

The gas phase is described as an ideal gas mixture of the species Bi, Bi_2, Bi_3, Bi_4, Cr, Cr_2 and V. Its Gibbs energy per mol of species is given by the following expressions:

$$G^{Gas} - H^{Gas} = \sum y_i \left[G_i^{Gas} - H_i^{SER} + R \cdot T \cdot \ln(y_i) \right]$$
$$+ R \cdot T \cdot \ln\left(P/bar\right) \quad ...(4)$$

$$\left(n_{Bi}^0 + n_V^0\right)/n = y_{Bi} + 2 \cdot y_{Bi} + 3 \cdot y_{Bi} + 4 \cdot y_{Bi} + y_V \quad ...(5)$$

where n is the numbers of moles of the species in the gas in internal equilibrium, $\left(n_{Bi}^0 + n_V^0\right)$ is the number of moles of atoms in the gas, $y_i = n_i/n$ is the mole fraction of species i, R is the gas constant, $G_i^{gas} - H_i^{SER}$ is the Gibbs energy of species i and P is the pressure. The Gibbs energy functions of the individual gas species are taken from the SGTE substance database [33].

4. First-principles calculations

First-principles calculations have been demonstrated to be a powerful complement to CALPHAD modeling. Since no experimental thermodynamic properties about the Bi-Ti system were reported, the first-principles calculations method is utilized to calculate the enthalpy of formation (ΔH_f) for the full-occupied $BiTi_2$ phase in this system at 0 K. Density functional theory (DFT) calculations as implemented in the highly efficient Vienna ab initio simulation package (VASP) [34, 35] were utilized. The Perdew–Burke–Ernzerh of GGA was employed for the exchange-correlation potential, and the valence electrons were described by projector augmented plane-wave (PAW) [36, 37] potentials. A plane-wave cut off energy of 320 eV and an energy convergence criterion of 10^{-4} eV for electronic structure self-consistency were used in the

calculation. The k-points meshes for Brillouin zone (BZ) sampling were constructed using Monkhorst-Pack scheme [38], and at least 10, 000 per reciprocal atom were used.

The enthalpy of formation for the compound $BiTi_2$ is -13018.6 J/mol-atoms, which is evaluated by the following equation:

$$\nabla E^{eq}(BiTi_2) = E(BiTi_2) - [1/3E^{eq}(Bi) + 2/3E^{eq}(Ti)]...(6)$$

where $E(BiTi_2)$, $E^{eq}(Bi)$ and $E^{eq}(Ti)$ are static energies (per atom) at 0 K for compound $BiTi_2$ element, respectively.

5. Results and discussion

The optimization of the thermodynamic parameters in the Bi-M (M = Ti, Cr, V) systems were performed with the PARROT module of the Thermo-calc software [39], which works by minimizing the square sum of the differences between experimental and calculated values. The step-by-step optimization procedure described by Du *et al.* [40] was adopted in the present work. During the assessment procedure, each piece of experimental information was given a certain weight which was varied based on the uncertainties of experimental data.

Taking the Bi-Ti system as an example, the optimization began with the Bi-rich side. The experimental liquidus was firstly considered and the parameters a_0, b_0 and a_1 in Eq (2) were introduced in order to give a preliminary description of the liquid phase. Second, the intermetallic phases were considered in the optimization. In the case of the compounds, the compound $BiTi_2$ was taken into account first and the first-principles calculations enthalpy of formation was used as the starting value of the parameter A in the present modeling. Then the other intermetallic phases were introduced in the modeling one by one. Third, one regular parameter was employed for the (βTi) phase in order to account for the solubility data. Finally, the thermodynamic parameters for all the phases were optimized simultaneously. The optimizations of the other two systems were analogy with the Bi–Ti system.

The thermodynamic parameters obtained in the present work are listed in Table 2. Comparison of the calculated invariant equilibrium temperatures and compositions with regard to the experimental ones is listed in Table 3.

Fig.1 shows the calculated Bi–Ti phase diagram along with the experimental data [15, 23]. The calculated eutectoid point of reaction (βTi) = (αTi) + Ti_3Bi lies at 719.47 °C, 6.03 at.% Bi, while the experimental [15] one lies at 725 °C, 8.6 at.% Bi. It can be seen from Fig.1, most of experimental data can be well accounted for by the present modeling. The differences between the calculated and the measured

Table 2. *Summary of the thermodynamic parameters in the Bi–M (M = Ti, Cr, V) systems*.*

System	Phase	Sublattice model	Evaluated parameters
Bi-Ti	Liquid	(Bi,Ti)	$^0L_{Bi,Ti}^{Liquid} = -23067.8 + 19.0634 \cdot T$ $^1L_{Bi,Ti}^{Liquid} = 4440.1$ $^2L_{Bi,Ti}^{Liquid} = 5857.4$
	Bcc_A$_2$	$(Bi,Ti)_1(Va)_3$	$^0L_{Bi,Ti}^{Bcc\_A_2} = -48200.2 + 29.9955 \cdot T$ $^1L_{Bi,Ti}^{Bcc\_A_2} = 38739.8 - 29.6521 \cdot T$
	Bi$_2$Ti	$(Bi)_{2/3}(Ti)_{1/3}$	$^0G_{Bi:Ti}^{Bi_2Ti_1} = -11495.9 - 1.2653 \cdot T + 2/3 \cdot {}^0G_{Bi}^{Rhom\_A_7}$ $+ 1/3 \cdot {}^0G_{Ti}^{Hcp\_A_3}$
	Bi$_3$Ti$_2$	$(Bi)_{3/5}(Ti)_{2/5}$	$^0G_{Bi:Ti}^{Bi_3Ti_2} = -11829.4 - 1.7268 \cdot T + 3/5 \cdot {}^0G_{Bi}^{Rhom\_A_7}$ $+ 2/5 \cdot {}^0G_{Ti}^{Hcp\_A_3}$
	Bi$_9$Ti$_8$	$(Bi)_{9/17}(Ti)_{8/17}$	$^0G_{Bi:Ti}^{Bi_9Ti_8} = -12227.3 - 1.6671 \cdot T + 9/17 \cdot {}^0G_{Bi}^{Rhom\_A_7}$ $+ 8/17 \cdot {}^0G_{Ti}^{Hcp\_A_3}$
	BiTi$_2$	$(Bi)_{1/3}(Ti)_{2/3}$	$^0G_{Bi:Ti}^{BiTi_2} = -13286.6 + 1/3 \cdot {}^0G_{Bi}^{Rhom\_A_7}$ $+ 2/3 \cdot {}^0G_{Ti}^{Hcp\_A_3}$
	BiTi$_3$	$(Bi)_{1/4}(Ti)_{3/4}$	$^0G_{Bi:Ti}^{BiTi_3} = -13674.0 + 1.6161 \cdot T + 1/4 \cdot {}^0G_{Bi}^{Rhom\_A_7}$ $+ 3/4 \cdot {}^0G_{Ti}^{Hcp\_A_3}$
Bi-Cr	Liquid	(Bi,Cr)	$^0L_{Bi,Cr}^{Liquid} = 45521.5$ $^1L_{Bi,Cr}^{Liquid} = 13680.3$ $^2L_{Bi,Cr}^{Liquid} = -21422.4$
	Bcc_A$_2$	$(Bi,Cr)_1(Va)_3$	$^0L_{Bi,Cr}^{Bcc\_A2} = 124399.9$
	Gas	$(Bi,Bi_2,Bi_3,Bi_4,Cr,Cr_2)$	$^0G_{Bi}^{Gas} = F2272T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{Bi_2}^{Gas} = F2851T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{Bi_3}^{Gas} = F2879T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{Bi_4}^{Gas} = F2883T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{Cr}^{Gas} = F7638T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{Cr_2}^{Gas} = F7904T + R \cdot T \cdot \ln(10^{-5} \cdot P)$
Bi-V	Liquid	(Bi,V)	$^0L_{Bi,V}^{Liquid} = 78007.8 - 13 \cdot T$
	Bcc_A$_2$	$(Bi,V)_1(Va)_3$	$^0L_{Bi,V}^{Bcc\_A2} = 69861.8$
	Gas	(Bi,Bi_2,Bi_3,Bi_4,V)	$^0G_{Bi}^{Gas} = F2272T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{Bi_2}^{Gas} = F2851T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{Bi_3}^{Gas} = F2879T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{Bi_4}^{Gas} = F2883T + R \cdot T \cdot \ln(10^{-5} \cdot P)$ $^0G_{V}^{Gas} = F15914T + R \cdot T \cdot \ln(10^{-5} \cdot P)$

* Gibbs energy in J/ (mol-atoms), temperature (T) in Kelvin and pressure (P) in Pa. The Gibbs energies for pure elements are from the SGTE compilation [31], and the Gibbs energies for gas species are from [33].

temperatures are less than 6 °C.

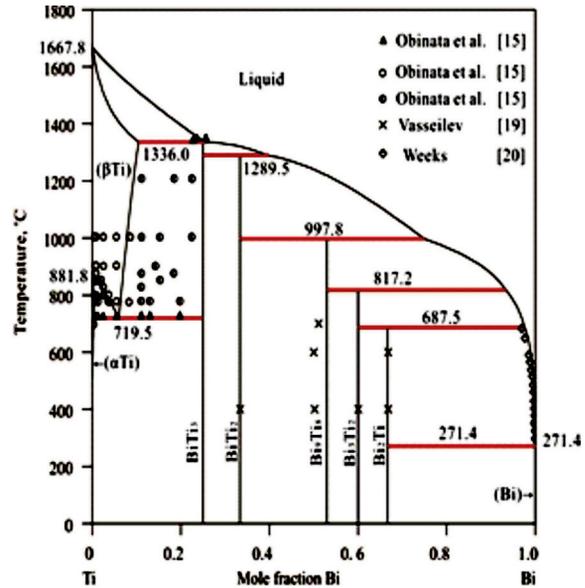   Fig.2 shows the calculated enthalpies of formation of the Bi–Ti system at 298 K along with the results from the first-principles calculations. As shown in Fig. 2, the calculated enthalpy of formation by CALPHAD method for the compound BiTi$_2$ is close

Table 3. *Calculated invariant equilibria in the Bi–M (M= Bi, Cr, V) systems compared with the literature data.*

system	Composition, at.% Bi			T (°C)	Ref.
Bi-Ti	Liquid=Bi$_2$Ti+(Bi)				
	—	0.667	1	271	[19]
	0.999	0.667	1	271.4	This work
	Liquid+Bi$_3$Ti$_2$=Bi$_2$Ti				
	—	0.6	0.6	687	[19]
	0.976	0.6	0.6	687.5	This work
	Liquid+Bi$_9$Ti$_8$=Bi$_3$Ti$_2$				
	—	0.529	0.6	817	[19]
	0.934	0.529	0.6	817.2	This work
	Liquid+BiTi$_2$=Bi$_9$Ti$_8$				
	—	0.333	0.529	997	[19]
	0.749	0.333	0.529	997.8	This work
	Liquid+BiTi$_3$=BiTi$_2$				
	—	0.25	0.333	1287	[19]
	0.397	0.25	0.333	1289..5	This work
	Liquid+Bcc_A$_2$=BiTi$_3$				
	0.26	0.1	0.25	1340±20	[15]
	0.255	0.105	0.25	1336	This work
	Bcc_A$_2$=BiTi$_3$+Hcp_A$_3$				
	0.086	0.25	0.003	725±10	[15]
	0.06	0.25	0.004	719.5	This work
Bi-Cr	Liquid#1+Gas=Liquid#2				
	—	—	—	—	—
	0.151	0.999	0.937	1567.8	This work
	Liquid#1=Liquid#2+(Cr)				
	—	0.91	0	1553	[24]
	0.15	0.938	0	1559	This work
	Liquid#2=(Cr)+(Bi)				
	1	0	1	271	[24]
	0.999	0	1	271.4	This work
Bi-V	Liquid#2=(Bi)+(V)				
	—	—	—	271.4	[30]
	1	1	0	271.4	This work
	Gas+(V)=Liquid#2				
	0.999	0.0035	0.989	1576	[30]
	0.999	0.0045	0.973	1558.4	This work
	Liquid#1=Gas+(V)				
	0.021	0.998	0.13	1877	[30]
	0.017	0.999	0.22	1884.8	This work

to that from the first-principles calculations. BiTi$_3$ has the most negative enthalpy of formation since its melting point is the highest among the existing compounds. The absolute values for the enthalpies of formation decrease with the increase of the content of Bi for the Bi–Ti compounds. Moreover, the tendency is consistent with these compounds stability.

Figs. 3 (a) and (b) shows the calculated Bi–Cr phase diagram with and without gas phase along with the experimental data [24, 26], respectively. The

Figure 1. *Calculated Bi–Ti phase diagram along with the experimental data [15, 23]. (○) Single phase region. (◉) Two phases region.*
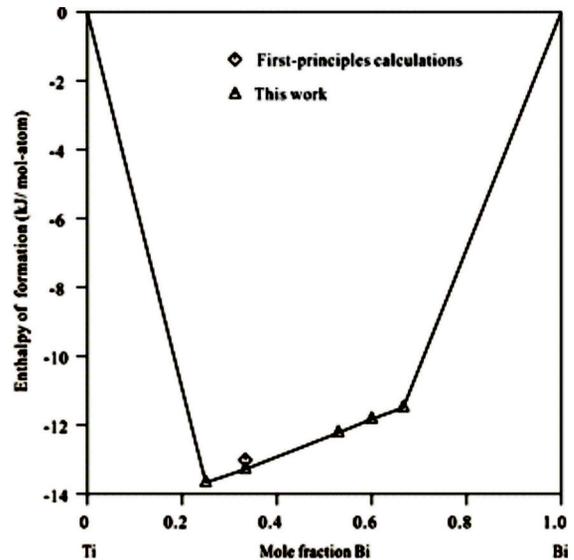
Figure 2. *Calculated enthalpy of formation of the Bi–Ti system at 298 K compared with the first-principles calculations data.*

monotectic reaction Liquid#1 = (Cr) + liquid#2 experimentally observed by Williams [24] is well reproduced.
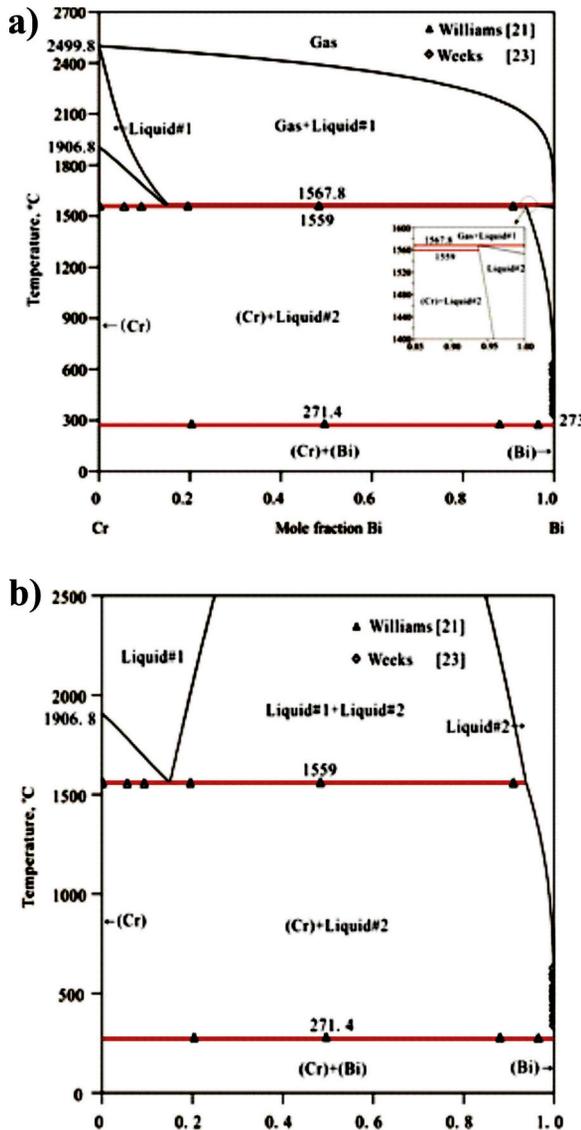

a)

b)

Figure 3. Calculated Bi–Cr phase diagram along with the experimental data [24, 26]; (a) with gas phase, (b) without gas phase.

Figs. 4 (a) and (b) presents the calculated Bi–V phase diagram with and without gas phase compared with the experimental data [23], respectively. The calculated temperatures and compositions of three invariant reactions for the Bi–V system are listed in Table 3. The comparisons of the present calculation and the extrapolated results [32] are listed in Table 3. According to this calculation, a miscibility gap of the liquid phase appears at 2359.7 °C.
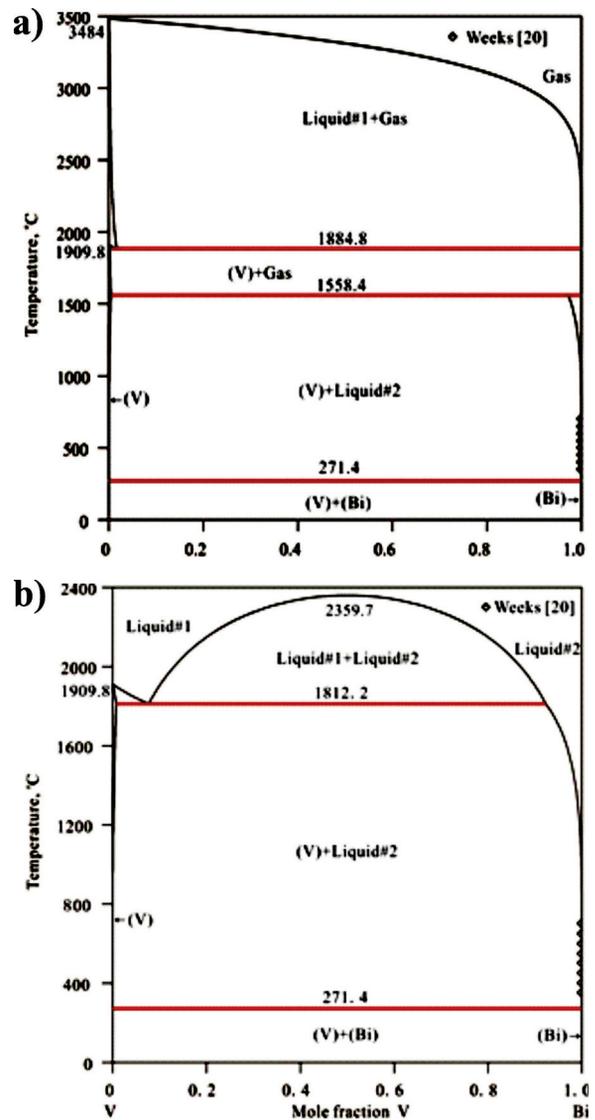

a)

b)

Figure 4. Calculated Bi–V phase diagram along with the experimental data [23]; (a) with gas phase, (b) without gas phase.

6. Conclusion

- The phase equilibrium data in the Bi–M (M = Ti, Cr, V) systems were critically reviewed. The enthalpy of formation for the $BiTi_2$ is computed via first-principles calculations.

- A set of self-consistent parameters for each of the Bi–M (M = Ti, Cr, V) systems has been obtained by the CALPHAD approach after considering the reliable experimental data in the literature and enthalpy of formation from the first-principles calculations. A comprehensive comparison shows that the calculated phase diagram and thermodynamic properties are in good agreement with experimental data and first-principles calculations.

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