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Thermodynamic Description of the Al-Mo and Al-Fe-Mo Systems

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The Al-Mo and Al-Fe-Mo systems were critically assessed using the CALPHAD technique. The solution phases (liquid, fcc and bcc) were described by a substitutional solution model. The nonstoichiometric compound $AlMo_3$ was described by a two-sublattice model $(Al,Mo)(Al,Mo)_3$ in the Al-Mo binary system and $(Al,Fe,Mo)(Al,Fe,Mo)_3$ in the Al-Fe-Mo ternary system. Other compounds $Al_{63}Mo_{37}$, Al_8Mo_3, Al_3Mo, Al_4Mo, $Al_{17}Mo_4$, $Al_{22}Mo_5$, $Al_{12}Mo$ and Al_5Mo in the Al-Mo system were treated as stoichiometric compounds in the binary system and as line compounds $Al_m(Fe,Mo)_n$ in the Al-Fe-Mo ternary system. The compounds μ and Fe_2Mo in the Fe-Mo system were treated as $(Al,Fe)_7Fe_2(Fe,Mo)_4$ and $(Fe,Mo)_2(Al,Mo)$ in the Al-Fe-Mo system, respectively. Compounds Al_5Fe_4, Al_2Fe, Al_5Fe_2 and $Al_{13}Fe_4$ in the Al-Fe system were treated as (Al,Fe,Mo), $Al_2(Fe,Mo)$, $(Al,Fe)_5(Al,Fe,Mo)_2$ and $(Fe,Mo)_{0.235}Al_{0.6275}(Al,Va)_{0.1375}$ in the Al-Fe-Mo system, respectively. Ternary compounds τ_1 and τ_2 were treated as $Al_8(Al,Fe)Mo_3$ and $(Al,Fe,Mo)(Va)_3$, respectively. A set of self-consistent thermodynamic parameters of the Al-Fe-Mo system was obtained.

Keywords Al-Fe-Mo system, aluminum alloys, CALPHAD technique, phase equilibria, thermodynamic properties

1. Introduction

The Al-Fe alloys with high Al contents are attractive for high-temperature applications because of their outstanding oxidation and hot-corrosion resistance.[1,2] However, insufficient strength and creep resistance have been identified as obstacles for the use of Fe-Al-based alloys at high temperatures. Molybdenum is one of the elements often added to improve the properties of Al-Fe alloys. The mechanical properties of Al-Fe-Mo alloys have been studied by many researchers, e.g. Eumann et al.[3,4] Knowledge of the Al-Fe-Mo phase diagram is significant for the development of Fe-Al-based alloys by providing information regarding the phases that are present at service temperatures, their compositions and volume fractions and so on.[5]

In the present work, thermodynamic modeling and optimization of the Al-Mo binary and the Al-Fe-Mo ternary systems are performed using the CALPHAD method on the basis of the experimental data reported in the literature.

2. Experimental Information

2.1 Al-Mo System

The Al-rich part of the phase diagram of the Al-Mo system was investigated by many researchers.[6-16] Yamaguchi and Simizu[8] measured the Al-rich liquidus compositions up to 1273 K. Roentgen and Koch,[7] Mondolfo[9] and Vigdorovich et al.[14] determined the solid solubility of Mo in fcc (Al). Based on the above experimental data, Walford[17] reviewed the Al-rich region of the Al-Mo system, and concluded that there were five intermediate phases, $Al_{12}Mo$, Al_6Mo, Al_5Mo, Al_4Mo and Al_8Mo_3.

The phase equilibria and the intermetallic compounds in the Al-Mo system were further investigated by many researchers.[18-26] The compound Al_2Mo[12,18,19] was not observed by Petzow and Rexer,[20] Hansen and Raman[21] and Rexer.[22] The compound Al_8Mo_3 was determined to melt congruently by Petzow and Rexer,[20] Rexer[22] and Shilo and Franzen.[23] In addition, Rexer[22] determined the phase equilibria related to the phases Al_8Mo_3, $Al_{63}Mo_{37}$, AlMo, $AlMo_3$ and bcc (Mo) in the temperature range of 1673 to 1873 K by light optical microscopy, thermal analysis, and XRD. Tendeloo et al.[24] determined the existence of compounds $Al_{17}Mo_4$ and $Al_{22}Mo_5$. Yeremenko et al.[25] and Malinovskii[26] measured the composition of the Al-rich liquidus. In addition, Ham,[10] Rexer[22] and Shilo and Franzen[23] determined the solubility of Al in bcc(Mo). Based on the assessed result of Walford[17] and the above experimental data (except for Shilo and Franzen[23] and Malinovskii[26]), Brewer and Lamoreaux[27] reviewed

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the Al-Mo phase diagram again. They included three solution phases (liquid, bcc (Mo) and fcc (Al)) and ten intermetallic phases: $Al_{12}Mo$, Al_6Mo, Al_5Mo, $Al_{17}Mo_4$, $Al_{22}Mo_5$, Al_4Mo, $Al_{63}Mo_{37}$, AlMo, Al_8Mo_3 and $AlMo_3$ in their equilibrium Al-Mo phase diagram.

Recently, Schuster and Ipser[28] reinvestigated the partial phase diagram between Al and Al_8Mo_3, and found ten intermetallic compounds, $Al_{12}Mo$, $Al_5Mo(h)$, $Al_5Mo(h')$, $Al_5Mo(r)$, $Al_3Mo(h)$, $Al_{3+x}Mo_{1-x}(h)$, $Al_{17}Mo_4$, $Al_{22}Mo_5$, $Al_4Mo(h)$, and Al_8Mo_3. The crystal structures of the phases $Al_5Mo(h')$, $Al_5Mo(r)$, $Al_3Mo(h)$, and $Al_{3+x}Mo_{1-x}(h)$ were reported. Eumann et al.[29] confirmed the phases and phase equilibria reported by Schuster and Ipser[28] with the exception of the phases $Al_{3+x}Mo_{1-x}(h)$ and $Al_5Mo(h')$ and determined the homogeneity ranges of the Al-rich intermetallic compounds. The work of Eumann et al.[29] was adopted in the present work.

Belyaeva et al.[18] determined the thermodynamic activities and derived partial free energies of Al in alloys between 8 and 75 at.% Mo using an electromotive force (EMF) method. Dubrovin et al.[30] measured the enthalpies of formation of the Al-Mo system by a calorimeter. Recently, Shilo and Franzen[23] determined the enthalpies of formation of alloys in the range from Mo to Al_8Mo_3. Sudsatsova et al.[31] measured the mixing enthalpies of liquid in the Al-rich region of Al-Mo system.

2.2 *Al-Fe-Mo System*

Markiv et al.[32] constructed the partial isothermal sections of the Al-rich part of the Al-Fe-Mo system at 1073 and 1323 K. Two ternary compounds "N-phase" and "S-phase" were observed at 1323 K. The compound "N-phase" was also designated as τ_1[33] with the formula $Al_8Fe_5Mo_3$.[34] Sokolovskaya et al.[35] investigated the phase equilibria in the Al-rich corner and constructed an isothermal section at 823 K and isopleths for Fe:Mo = 3:1 and $FeAl_3$-$MoAl_{12}$. Using five different alloys, Wang et al.[36] determined the phase equilibria between bcc (Al, Fe) and μ at 1073 K by both EDS and EPMA.

The effect of Mo on the AlFe ($D0_3$) ↔ AlFe (B2) and AlFe (B2) ↔ bcc (A2) transition temperatures was investigated by many researchers.[37-41] Stepien-Damm et al.[42] reported a ternary phase $Al_{0.25}Fe_{4.75}Mo_9$ formed at about 1923 K. During the process of studying mechanical properties of Al-Fe-Mo alloys,[3,4] an isothermal section at 1273 K was constructed. Based on the above experimental results, Raghavan[43] assessed the Al-Fe-Mo system.

Recently, Eumann et al.[44,45] systematically investigated three isothermal sections at 1073, 1273 and 1423 K in the Al-Fe-Mo system. The compound τ_1 reported by Markiv et al.[32] was confirmed by Eumann et al.[45] In addition, new ternary compounds τ_2 and ε^* were found.[45] The compound τ_2 with W-type structure was determined to have a large homogeneity range. And the compound ε^* has a hexagonal Al_8Cr_5-type structure and ranges in composition from $Al_{57.2}Fe_{39.0}Mo_{3.8}$ to $Al_{55}Fe_{30.9}Mo_{14.1}$. The μ phase in the Fe-Mo binary system had a high Al solubility.[44,45] From the established phase equilibria,[44,45] a reaction scheme in the temperature range 1073-1423 K was set up without any contradiction.

3. Thermodynamic Models

In order to maintain consistency with other thermodynamic assessments, the Gibbs energy of each pure element is taken from the SGTE compilation by Dinsdale.[46] The Gibbs energy function of element i is described by the following equation:

$$G_i^{\phi}(T) = a + bT + cT\ln T + dT^2 + eT^3 + fT^{-1} + gT^7 + hT^{-9} \qquad \text{(Eq 1)}$$

In a standard element reference (SER) state, it is denoted as $GHSER_i$, i.e.,

$$GHSER_i = {}^0G_i^{\phi}(T) - H_i^{SER}(298.15\ \text{K}) \qquad \text{(Eq 2)}$$

where $H_i^{SER}(298.15\ \text{K})$ is the molar enthalpy of the element i at 298.15 K in its SER state: fcc for Al, fcc for Fe and bcc for Mo.

3.1 *Solution Phases*

In the Al-Fe-Mo system, there are three solution phases: liquid, fcc, and bcc. Their molar Gibbs energies are described by the following expression:

$$G_m^{\phi} = x_{Al}G_{Al}^{\phi}(T) + x_{Fe}G_{Fe}^{\phi} + x_{Mo}G_{Mo}^{\phi}(T) + RT(x_{Al}\ln x_{Al} + x_{Fe}\ln x_{Fe} + x_{Mo}\ln x_{Mo}) + {}^{E}G_m^{\phi} + {}^{mg}G_m^{\phi} \qquad \text{(Eq 3)}$$

where R is the gas constant; x_{Al}, x_{Fe} and x_{Mo} are the mole fraction of Al, Fe and Mo, respectively; ${}^{E}G_m^{\phi}$ is the excess Gibbs energy and is expressed by the Redlich-Kister polynomial,

$$\begin{aligned} {}^{E}G_m^{\phi} = {} & x_{Al}x_{Fe}\sum_j {}^{j}L_{Al,Fe}^{\phi}(x_{Al} - x_{Fe})^j \\ & + x_{Fe}x_{Mo}\sum_j {}^{j}L_{Fe,Mo}^{\phi}(x_{Fe} - x_{Mo})^j \\ & + x_{Al}x_{Mo}\sum_j {}^{j}L_{Al,Mo}^{\phi}(x_{Al} - x_{Mo})^j + x_{Al}x_{Fe}x_{Mo}\,{}^{j}L_{Al,Fe,Mo}^{\phi} \end{aligned} \qquad \text{(Eq 4)}$$

where ${}^{j}L_{Al,Fe}^{\phi}$, ${}^{j}L_{Fe,Mo}^{\phi}$ and ${}^{j}L_{Al,Mo}^{\phi}$ are the interaction parameters between elements Al and Fe, Fe and Mo, and Al and Mo, respectively; ${}^{j}L_{Al,Fe,Mo}^{\phi}$ is the ternary interaction parameter; ${}^{j}L_{Al,Mo}^{\phi}$ and ${}^{j}L_{Al,Fe,Mo}^{\phi}$ are to be evaluated in the present work. The general form of the interaction parameters is

$$L^{\phi} = a + bT + cT\ln T + dT^2 + eT^3 + fT^{-1} \qquad \text{(Eq 5)}$$

In most cases, only the first one or two terms are used according to the temperature dependence on the experimental data. ${}^{mg}G_m^{\phi}$ is the magnetic contribution to the Gibbs energy.

3.2 *Intermetallic Compounds*

3.2.1 Al-Mo System. There are ten intermetallic compounds $Al_{12}Mo$, Al_3Mo, Al_5Mo, $Al_{17}Mo_4$, $Al_{22}Mo_5$, Al_4Mo, $Al_{63}Mo_{37}$, AlMo, Al_8Mo_3 and $AlMo_3$ in the Al-Mo binary system. The compound AlMo with A2 structure[22] was treated as the same phase as bcc (Mo), and its Gibbs energy function was similar to Eq 3. The $AlMo_3$ with a homogeneity range[22,23,29] was described by a two-sublattice model[47,48] (Al, Mo)(Al, Mo)$_3$. The Gibbs energy per mole of formula unit $AlMo_3$ is expressed as following:

$$\begin{aligned} G_{\mathrm{m}}^{\mathrm{AlMo_3}} = {} & y'_{\mathrm{Al}} y''_{\mathrm{Al}} G_{\mathrm{Al:Al}}^{\mathrm{AlMo_3}} + y'_{\mathrm{Al}} y''_{\mathrm{Mo}} G_{\mathrm{Al:Mo}}^{\mathrm{AlMo_3}} \\ & + y'_{\mathrm{Mo}} y''_{\mathrm{Al}} G_{\mathrm{Mo:Al}}^{\mathrm{AlMo_3}} + y'_{\mathrm{Mo}} y''_{\mathrm{Mo}} G_{\mathrm{Mo:Mo}}^{\mathrm{AlMo_3}} \\ & + RT\left(y'_{\mathrm{Al}} \ln y'_{\mathrm{Al}} + y'_{\mathrm{Mo}} \ln y'_{\mathrm{Mo}}\right) \\ & + 3RT\left(y''_{\mathrm{Al}} \ln y''_{\mathrm{Al}} + y''_{\mathrm{Mo}} \ln y''_{\mathrm{Mo}}\right) \\ & + y'_{\mathrm{Al}} y'_{\mathrm{Mo}} y''_{\mathrm{Al}} \sum_j {}^{j}L_{\mathrm{Al,Mo:Al}}^{\mathrm{AlMo_3}} \left(y'_{\mathrm{Al}} - y'_{\mathrm{Mo}}\right)^j \\ & + y'_{\mathrm{Al}} y'_{\mathrm{Mo}} y''_{\mathrm{Mo}} \sum_j {}^{j}L_{\mathrm{Al,Mo:Mo}}^{\mathrm{AlMo_3}} \left(y'_{\mathrm{Al}} - y'_{\mathrm{Mo}}\right)^j \\ & + y'_{\mathrm{Al}} y''_{\mathrm{Al}} y''_{\mathrm{Mo}} \sum_j {}^{j}L_{\mathrm{Al:Al,Mo}}^{\mathrm{AlMo_3}} \left(y''_{\mathrm{Al}} - y''_{\mathrm{Mo}}\right)^j \\ & + y'_{\mathrm{Mo}} y''_{\mathrm{Al}} y''_{\mathrm{Mo}} \sum_j {}^{j}L_{\mathrm{Mo:Al,Mo}}^{\mathrm{AlMo_3}} \left(y''_{\mathrm{Al}} - y''_{\mathrm{Mo}}\right)^j \end{aligned} \qquad \text{(Eq 6)}$$

where y'_* and y''_* are the site fractions of Al or Mo in the first and the second sublattices, respectively; $G_{*:*}^{\mathrm{AlMo_3}}$ represents the Gibbs energies of the compound $AlMo_3$ when the first and the second sublattices are occupied by only one element Al or Mo, which are related to the enthalpies of pure fcc for Al and bcc for Mo in their SER state; ${}^{j}L_{\mathrm{Al,Mo:*}}^{\mathrm{AlMo_3}}$ and ${}^{j}L_{\mathrm{*:Al,Mo}}^{\mathrm{AlMo_3}}$ represent the jth interaction parameters between the elements Al and Mo in the first and the second sublattices, respectively.

The homogeneity ranges of the other compounds in the Al-Mo system were determined to be within 0.1 to 0.4 at.% by Eumann et al.,[29] and thus these compounds were treated as stoichiometric compounds in the present work. The Gibbs energy per mole of formula unit Al_mMo_n, which presents compounds $Al_{12}Mo$, Al_3Mo, Al_5Mo, $Al_{17}Mo_4$, $Al_{22}Mo_5$, Al_4Mo, $Al_{63}Mo_{37}$ and Al_8Mo_3, is expressed as follows:

$$G_{\mathrm{m}}^{\mathrm{Al}_m\mathrm{Mo}_n} = m\mathrm{GHSER_{Al}} + n\mathrm{GHSER_{Mo}} + \Delta G_{\mathrm{f}}^{\mathrm{Al}_m\mathrm{Mo}_n} \qquad \text{(Eq 7)}$$

where $\Delta G_{\mathrm{f}}^{\mathrm{Al}_m\mathrm{Mo}_n}$ is the Gibbs energy of formation per mole of formula unit Al_mMo_n. Due to a lack of experimental measurements, it is assumed that the Neumann-Kopp rule applies to the heat capacity, i.e., $\Delta C_{pf} = 0$. Thus $\Delta G_{\mathrm{f}}^{\mathrm{Al}_m\mathrm{Mo}_n}$ can be given by the following expression:

$$\Delta G_{\mathrm{f}}^{\mathrm{Al}_m\mathrm{Mo}_n} = a + bT \qquad \text{(Eq 8)}$$

where the parameters a and b are to be evaluated in the present work.

3.2.2 Al-Fe-Mo System. The compound $AlMo_3$ in the Al-Mo system was treated as (Al,Fe,Mo)(Al,Fe,Mo)$_3$ in the Al-Fe-Mo system. The stoichiometric intermetallic compounds $Al_{12}Mo$, Al_3Mo, Al_5Mo, $Al_{17}Mo_4$, $Al_{22}Mo_5$, Al_4Mo, $Al_{63}Mo_{37}$ and Al_8Mo_3 in the Al-Mo system are treated as $Al_m(Fe,Mo)_n$ the Al-Fe-Mo ternary system with Al in the first sublattice and Fe and Mo in the second one. The Gibbs energy per mole of formula unit $Al_m(Fe,Mo)_n$ is expressed as follows:

$$\begin{aligned} G_{\mathrm{m}}^{\phi} = {} & y''_{\mathrm{Fe}} G_{\mathrm{Al:Fe}}^{\phi} + y''_{\mathrm{Mo}} G_{\mathrm{Al:Mo}}^{\phi} + nRT\left(y''_{\mathrm{Fe}} \ln y''_{\mathrm{Fe}} + y''_{\mathrm{Mo}} \ln y''_{\mathrm{Mo}}\right) \\ & + y''_{\mathrm{Fe}} y''_{\mathrm{Mo}} \sum_j {}^{j}L_{\mathrm{Al:Fe,Mo}}^{\phi} \left(y''_{\mathrm{Fe}} - y''_{\mathrm{Mo}}\right)^j \end{aligned} \qquad \text{(Eq 9)}$$

where y''_{Fe} and y''_{Mo} are the site fractions of Fe and Mo in the second sublattice, respectively; $G_{\mathrm{Al:Fe}}^{\phi}$ and $G_{\mathrm{Al:Mo}}^{\phi}$ represent the Gibbs energies of the compounds $Al_m(Fe,Mo)_n$ when the second sublattice is occupied by only one element Fe and Mo, respectively; ${}^{j}L_{\mathrm{Al:Fe,Mo}}^{\phi}$ represents the jth interaction parameter between the elements Fe and Mo in the second sublattice.

The compound Al_5Fe_2 in the Al-Fe binary system was treated as (Al,Fe)$_5$(Al,Fe)$_2$ by a two sublattice model according to the homogeneity range of Al_5Fe_2 determined by Eumann et al.[44,45] The compounds Al_5Fe_4, Al_5Fe_2 and $Al_{13}Fe_4$ in the Al-Fe system were treated as (Al,Fe,Mo), (Al,Fe)$_5$(Al,Fe,Mo)$_2$ and (Fe,Mo)$_{0.235}$Al$_{0.6275}$(Al,Va)$_{0.1375}$, respectively, in the Al-Fe-Mo ternary system considering the Mo solubility in these compounds.[44,45] The compound Al_2Fe in Al-Fe system was treated as a line compound Al_2(Fe,Mo) in the Al-Fe-Mo system.

The compounds μ and Fe_2Mo in the Fe-Mo system were treated as (Al,Fe)$_7$Fe$_2$(Fe,Mo)$_4$ and (Fe,Mo)$_2$(Al,Mo) in the Al-Fe-Mo system, respectively. The other compounds R and sigma (σ) were treated as binary compounds without Al solubility due to a lack of experimental data.

In the Al-Fe-Mo system, the intermetallic compound τ_1 is treated as Al_8(Al,Fe)Mo_3 with Al in the first sublattice, both Al and Fe in the second one and Mo in the third one according to the experimental data of Eumann et al.[45] The Gibbs energy per mole of formula unit τ_1 is expressed as following:

$$\begin{aligned} G_{\mathrm{m}}^{\tau_1} = {} & y''_{\mathrm{Al}} G_{\mathrm{Al:Al:Mo}}^{\tau_1} + y''_{\mathrm{Fe}} G_{\mathrm{Al:Fe:Mo}}^{\tau_1} + RT\left(y''_{\mathrm{Al}} \ln y''_{\mathrm{Al}} + y''_{\mathrm{Fe}} \ln y''_{\mathrm{Fe}}\right) \\ & + y''_{\mathrm{Al}} y''_{\mathrm{Fe}} \sum_j {}^{j}L_{\mathrm{Al:Al,Fe:Mo}}^{\tau_1} \left(y''_{\mathrm{Al}} - y''_{\mathrm{Fe}}\right)^j \end{aligned} \qquad \text{(Eq 10)}$$

The intermetallic compound τ_2 with an W-type structure[22] was treated as (Al,Fe,Mo)Va$_3$ according to the experimental data obtained by Eumann et al.[45] The expression of the Gibbs energy per mole of formula unit τ_2 is similar to Eq 3.

The ternary compound ε* in the Al-Fe-Mo system has a hexagonal Al_8Cr_5-type structure, and Al_5Fe_4 in the Al-Fe binary system has a cubic Cu_5Zn_8-type structure. Eumann et al.[45] thought that the transition from Al_5Fe_4 to ε* is a second order transition in the Al-Fe-Mo system. Since the composition where this transition takes place at 1423 K had not been established,[45] the ε* and Al_5Fe_4 were treated as one phase in the present work.

4. Assessment Procedure

In order to obtain a thermodynamic description of a multi-component system, it is necessary to have a thermodynamic description of each lower-order system. The thermodynamic descriptions of the Fe-Mo system optimized by Andersson[49] are adopted in the present work.

The Al-Fe system was optimized by Kaufman and Nesor,[50] Saunders and Rivlin[51] and Seierstein.[52] Saunders and Rivlin[51] did not consider the order-disorder transition between bcc-A2 and bcc-B2. Seierstein[52] calculated transformation temperature between bcc-A2 and bcc-B2,

Table 1 Thermodynamic parameters in the Al-Fe-Mo system (a)

Phase	Thermodynamic parameters		Reference
	$\mathrm{GHSER_{Al}}$ =		[46]
	298-700	$-7976.15 + 137.093038T - 24.3671976T \ln T$	
		$-1.884662\mathrm{E}\text{-}3T^2 - 0.877664\mathrm{E}\text{-}6T^3 + 74092T^{-1}$	
	700-933	$-11276.24 + 223.048446T - 38.5844296T \ln T$	
		$+18.531982\mathrm{E}\text{-}3T^2 - 5.764227\mathrm{E}\text{-}6T^3 + 74092\ T^{-1}$	
	933-2900	$-11278.378 + 188.684153T - 31.748192T \ln T - 1230.524\mathrm{E}25T^{-9}$	
	$\mathrm{GHSER_{Fe}}$ =		[46]
	298-1811	$+1225.7 + 124.134T - 23.5143T \ln T - 4.39752\mathrm{E}\text{-}3T^2$	
		$-0.058927\mathrm{E}\text{-}6T^3 + 77359T^{-1}$	
	1811-6000	$-25383.581 + 299.31255T - 46T \ln T + 2296.03\mathrm{E}28T^{-9}$	
	$\mathrm{GHSER_{Mo}}$ =		[46]
	130-2896	$-7746.302 + 131.9197T - 23.56414T \ln T$	
		$-0.0034433396T^2 + 5.66283\mathrm{E}\text{-}07T^3 + 65812T^{-1} - 1.30927\mathrm{E}\text{-}10T^4$	
	2896-5000	$-30556.41 + 283.559746T - 42.63829T \ln T - 4.849315\mathrm{E}{+}33T^{-9}$	
	GFCCFE =		
	298-1811	$-236.7 + 132.416T - 24.6643T \ln T$	
		$-0.00375752T^2 - 5.8927\mathrm{E}\text{-}08T^3 + 77359T^{-1}$	
	1811-6000	$-27097.3963 + 300.252559T - 46T \ln T + 2.78854\mathrm{E}{+}31T^{-9}$	
	GBCCAL =		
	298-700	$+2106.85 + 132.280038T - 24.3671976T \ln T$	
		$-0.001884662T^2 - 8.77664\mathrm{E}\text{-}07T^3 + 74092T^{-1}$	
	700-933	$-1193.24 + 218.235446T - 38.5844296T \ln T + 0.018531982T^2$	
		$-5.764227\mathrm{E}\text{-}06T^3 + 74092\ T^{-1}$	
	933-6000	$-1195.378 + 183.871153T - 31.748192T \ln T - 1.230524\mathrm{E}{+}28T^{-9}$	
liquid: $(\mathrm{Al,Fe,Mo})_1$	G(liquid,Fe) =		[46]
	298-1811	$+13265.87 + 117.57557T - 23.5143T \ln T$	
		$-0.00439752T^2 - 5.8927\mathrm{E}\text{-}08T^3 + 77359T^{-1} - 3.67516\mathrm{E}\text{-}21T^7$	
	1811-6000	$-10838.83 + 291.302T - 46T \ln T$	
	G(liquid,Al) =		[46]
	298-700	$+3028.879 + 125.251171T - 24.3671976T \ln T$	
		$-0.001884662T^2 - 8.77664\mathrm{E}\text{-}07T^3 + 74092T^{-1} + 7.9337\mathrm{E}\text{-}20T^7$	
	700-933	$-271.21 + 211.206579T - 38.5844296T \ln T$	
		$+0.018531982T^2 - 5.764227\mathrm{E}\text{-}06T^3 + 74092T^{-1} + 7.9337\mathrm{E}\text{-}20T^7$	
	933-2900	$-795.996 + 177.430178T - 31.748192T \ln T$	
	G(liquid,Mo) =		[46]
	130-2896	$+34085.045 + 117.224788T - 23.56414T \ln T$	
		$-0.0034433396T^2 + 5.66283\mathrm{E}\text{-}07T^3 + 65812T^{-1} - 1.30927\mathrm{E}\text{-}10T^4$	
		$+ 4.24519\mathrm{E}\text{-}22T^7$	
	2896-5000	$+3538.963 + 271.6697T - 42.63829T \ln T$	
	${}^0L^{\mathrm{liq.}}_{\mathrm{Al,Fe}} = -91976.5 + 22.1314T$		[52]
	${}^1L^{\mathrm{liq.}}_{\mathrm{Al,Fe}} = -7338.0 + 5.9149T$		This work
	${}^0L^{\mathrm{liq.}}_{\mathrm{Fe,Mo}} = -6973.0 - 0.3700T$		[49]
	${}^1L^{\mathrm{liq.}}_{\mathrm{Fe,Mo}} = -9424.0 + 4.5020T$		[49]
	${}^0L^{\mathrm{liq.}}_{\mathrm{Al,Mo}} = -96235.7 + 20.9416T$		This work
	${}^1L^{\mathrm{liq.}}_{\mathrm{Al,Mo}} = -4384.1 + 12.3636T$		This work
	${}^2L^{\mathrm{liq.}}_{\mathrm{Al,Mo}} = -25091.6$		This work
	${}^0L^{\mathrm{liq.}}_{\mathrm{Al,Fe,Mo}} = +81728.8$		This work
	${}^1L^{\mathrm{liq.}}_{\mathrm{Al,Fe,Mo}} = +5637.6$		This work
bcc (disordered part of B2):	G(bcc,Al:Va;0) =		[46]
$(\mathrm{Al,Fe,Mo})_1(\mathrm{Va})_3$	298-700	$+2106.85 + 132.280038T - 24.3671976T \ln T$	
		$-1.884662\mathrm{E}\text{-}3T^2 - 0.877664\mathrm{E}\text{-}6T^3 + 74092T^{-1}$	
	700-933	$-1193.24 + 218.235446T - 38.5844296T \ln T + 18.531982\mathrm{E}\text{-}3T^2$	
		$- 5.764227\mathrm{E}\text{-}6T^3 + 74092T^{-1}$	
	933-2900	$-1195.378 + 183.871153T - 31.748192T \ln T - 1230.524\mathrm{E}25T^{-9}$	

Table 1 Continued

Phase	Thermodynamic parameters	Reference
	G(bcc,Fe:Va;0) = $\mathrm{GHSER_{Fe}}$	[46]
	Tc(bcc,Fe:Va;0) = +1043.00	[46]
	Bm(bcc,Fe:Va;0) = +2.22	[46]
	G(bcc,Mo:Va;0) = $\mathrm{GHSER_{Mo}}$	[46]
	${}^{0}L^{\mathrm{bcc}}_{\mathrm{Al,Fe}} = -129691.8 + 35.8074T$	This work
	${}^{1}L^{\mathrm{bcc}}_{\mathrm{Al,Fe}} = +2907.1$	This work
	${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Al,Fe}} = +504$	[52]
	${}^{0}L^{\mathrm{bcc}}_{\mathrm{Fe,Mo}} = -36818.0 + 9.1410T$	[49]
	${}^{1}L^{\mathrm{bcc}}_{\mathrm{Fe,Mo}} = -362 - 5.7240T$	[49]
	${}^{0}T^{\mathrm{bcc}}_{c\mathrm{Fe,Mo}} = 335$	[49]
	${}^{1}T^{\mathrm{bcc}}_{c\mathrm{Fe,Mo}} = 526$	[49]
	${}^{0}L^{\mathrm{bcc}}_{\mathrm{Al,Mo}} = -75938.8 + 10.8187T$	This work
	${}^{1}L^{\mathrm{bcc.}}_{\mathrm{Al,Mo}} = -44502.8 + 21.6488T$	This work
	${}^{2}L^{\mathrm{bcc}}_{\mathrm{Al,Mo}} = -22927.1$	This work
	${}^{0}L^{\mathrm{bcc}}_{\mathrm{Al,Fe,Mo}} = -20873.3 + 61.9179T$	This work
	${}^{1}L^{\mathrm{bcc}}_{\mathrm{Al,Fe,Mo}} = -31675.6 + 10.3679T$	This work
	${}^{2}L^{\mathrm{bcc}}_{\mathrm{Al,Fe,Mo}} = -55074.3 + 14.7262T$	This work
fcc: $(\mathrm{Al,Fe,Mo})_1(\mathrm{Va})_1$	G(fcc,Al:Va;0) = $\mathrm{GHSER_{Al}}$	[46]
	G(fcc,Fe:Va;0) =	[46]
	298-1811 $-236.7 + 132.416T - 24.6643T \ln T$ $-0.00375752T^2 - 5.8927\mathrm{E}{-}08T^3 + 77359T^{-1}$	
	1811-6000 $-27097.3963 + 300.252559T - 46T \ln T + 2.78854\mathrm{E}{+}31T^{-9}$	
	$\mathrm{T_c}$(fcc,Fe:Va;0) = −201.00	[46]
	Bm(fcc,Fe:Va;0) = −2.10	[46]
	G(fcc,Mo:Va;0) =	[46]
	298-2896 $+7453.698 + 132.5497T - 23.56414T \ln T$ $-0.003443396T^2 + 5.66283\mathrm{E}{-}07\ T^3 + 65812T^{-1} - 1.30927\mathrm{E}{-}10T^4$	
	2896-5000 $-15356.41 + 284.189746T - 42.63829T \ln T - 4.849315\mathrm{E}{+}33T^{-9}$	
	${}^{0}L^{\mathrm{fcc}}_{\mathrm{Al,Fe}} = -76066.1 + 18.6758T$	[52]
	${}^{1}L^{\mathrm{fcc}}_{\mathrm{Al,Fe}} = +21167.4 + 1.3398T$	[52]
	${}^{0}L^{\mathrm{fcc}}_{\mathrm{Fe,Mo}} = +28347.0 - 17.6910T$	[49]
	${}^{0}L^{\mathrm{fcc}}_{\mathrm{Al,Mo}} = -85300.0 + 20.4000T$	[54]
	${}^{1}L^{\mathrm{fcc}}_{\mathrm{Al,Mo}} = -10000.0$	[54]
AlFe (ordered part of B2): $(\mathrm{Al,Fe,Mo})_{0.5}(\mathrm{Al,Fe,Mo})_{0.5}(\mathrm{Va})_3$	$G^{\mathrm{AlFe}}_{\mathrm{Al:Fe}} = -9000.0 - 2.7500T$	This work
	$G^{\mathrm{AlFe}}_{\mathrm{Fe:Al}} = -9000.0 - 2.7500T$	This work
	$L^{\mathrm{AlFe}}_{\mathrm{Fe:Al,Mo}} = L^{\mathrm{AlFe}}_{\mathrm{Al,Mo:Fe}} = -5250.0$	This work
$\mathrm{Al_5Fe_2}$: $(\mathrm{Al,Fe,Mo})_2(\mathrm{Al,Fe})_5$	$G^{\mathrm{Al_5Fe_2}}_{\mathrm{Al:Al}} = 7\mathrm{GHSER_{Al}} + 35000.0$	This work
	$G^{\mathrm{Al_5Fe_2}}_{\mathrm{Fe:Al}} = 5\mathrm{GHSER_{Al}} + 2\mathrm{GHSER_{Fe}} - 231624.1 + 51.7626T$	This work
	$G^{\mathrm{Al_5Fe_2}}_{\mathrm{Al:Fe}} = 2\mathrm{GHSER_{Al}} + 5\mathrm{GHSER_{Fe}} + 301624.1 - 51.7626T$	This work
	$G^{\mathrm{Al_5Fe_2}}_{\mathrm{Fe:Fe}} = 7\mathrm{GHSER_{Fe}} + 35000.0$	This work
	$G^{\mathrm{Al_5Fe_2}}_{\mathrm{Mo:Al}} = \frac{13}{21}G^{\mathrm{Al_8Mo_3}}_{\mathrm{Al:Mo}} + \frac{1}{21}G^{\mathrm{AlMo_3}}_{\mathrm{Al:Mo}} + 42000.0$	This work
	$G^{\mathrm{Al_5Fe_2}}_{\mathrm{Mo:Fe}} = 2\mathrm{GHSER_{Mo}} + 5\mathrm{GHSER_{Fe}} + 35000.0$	This work
	${}^{0}L^{\mathrm{Al_5Fe_2}}_{\mathrm{Al,Fe:Al}} = {}^{0}L^{\mathrm{Fe_2Al_5}}_{\mathrm{Al,Fe:Fe}} = -103529.0 + 45.0302T$	This work
	${}^{0}L^{\mathrm{Al_5Fe_2}}_{\mathrm{Al:Al,Fe}} = {}^{0}L^{\mathrm{Fe_2Al_5}}_{\mathrm{Fe:Al,Fe}} = -101095.0 + 44.9577T$	This work
$\mathrm{Al_2Fe}$: $(\mathrm{Fe,Mo})\mathrm{Al_2}$	$G^{\mathrm{Al_2Fe}}_{\mathrm{Fe:Al}} = 2\mathrm{GHSER_{Al}} + \mathrm{GHSER_{Fe}} - 100876.8 + 20.7349T$	This work
	$G^{\mathrm{Al_2Fe}}_{\mathrm{Mo:Al}} = \frac{5}{21}G^{\mathrm{Al_8Mo_3}}_{\mathrm{Al:Mo}} + \frac{2}{21}G^{\mathrm{AlMo_3}}_{\mathrm{Al:Mo}} + 24804.1$	This work
$\mathrm{Al_{13}Fe_4}$: $(\mathrm{Fe,Mo})_{0.235}\mathrm{Al}_{0.6275}(\mathrm{Al,Va})_{0.1375}$	$G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Al}} = 0.765\mathrm{GHSER_{Al}} + 0.235\mathrm{GHSER_{Fe}} - 31054.8 + 7.5963T$	This work
	$G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Va}} = 0.6275\mathrm{GHSER_{Al}} + 0.235\mathrm{GHSER_{Fe}} - 27466.6 + 7.2767T$	This work
	$G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Mo:Al:Al}} = \frac{1}{17}\left(\frac{7}{19}G^{\mathrm{Al_{17}Mo_4}}_{\mathrm{Al:Mo}} + \frac{16}{19}G^{\mathrm{Al_8Mo_3}}_{\mathrm{Al:Mo}}\right) + 5000.0$	This work
	$G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Mo:Al:Va}} = 0.6275\mathrm{GHSER_{Al}} + 0.235\mathrm{GHSER_{Mo}} + 5000.0$	This work
$\mathrm{Al_5Fe_4}$: $(\mathrm{Al,Fe,Mo})_1$	$G^{\mathrm{Al_5Fe_4}}_{\mathrm{Al}} = \mathrm{GHSER_{Al}} + 9285.7 - 5.1818T$	This work
	$G^{\mathrm{Al_5Fe_4}}_{\mathrm{Fe}} = \mathrm{GHSER_{Fe}} + 60675.0$	This work
	$G^{\mathrm{Al_5Fe_4}}_{\mathrm{Mo}} = \mathrm{GHSER_{Mo}} + 29106.1$	This work

Table 1 Continued

Phase	Thermodynamic parameters	Reference
	${}^{0}L^{\mathrm{Al_5Fe_4}}_{\mathrm{Al,Fe}} = -213741.0 + 15.6364T$	This work
	${}^{1}L^{\mathrm{Al_5Fe_4}}_{\mathrm{Al,Fe}} = -41619.0 + 76.9227T$	This work
	${}^{0}L^{\mathrm{Al_5Fe_4}}_{\mathrm{Fe,Mo}} = +5000.0$	This work
	${}^{0}L^{\mathrm{Al_5Fe_4}}_{\mathrm{Al,Fe,Mo}} = -693184.5 - 44.1504T$	This work
	${}^{1}L^{\mathrm{Al_5Fe_4}}_{\mathrm{Al,Fe,Mo}} = +375088.2$	This work
	${}^{2}L^{\mathrm{Al_5Fe_4}}_{\mathrm{Al,Fe,Mo}} = -888547.6 - 27.6887T$	This work
Fe_2Mo: $(Fe,Mo)_2(Al,Mo)$	$G^{\mathrm{Fe_2Mo}}_{\mathrm{Fe:Mo}} = 2\mathrm{GFCCFE} + \mathrm{GHSER_{Mo}} - 10797.9 - 0.132T$	[49]
	$G^{\mathrm{Fe_2Mo}}_{\mathrm{Mo:Mo}} = 3\mathrm{GHSER_{Mo}} + 15000.0$	[49]
	$G^{\mathrm{Fe_2Mo}}_{\mathrm{Fe:Al}} = 1.5\mathrm{GHSER_{Fe}} + 0.5G^{\mathrm{Al_2Fe}}_{\mathrm{Fe:Al}} + 15000.0$	This work
	$G^{\mathrm{Fe_2Mo}}_{\mathrm{Mo:Al}} = \frac{1}{21}G^{\mathrm{Al_8Mo_3}}_{\mathrm{Al:Mo}} + \frac{13}{21}G^{\mathrm{AlMo_3}}_{\mathrm{Al:Mo}} + 15000.0$	This work
	$L^{\mathrm{Fe_2Mo}}_{\mathrm{Fe,Mo:Mo}} = +200000.0$	[49]
μ:$(Al,Fe)_7Mo_2(Fe,Mo)_4$	$G^{\mu}_{\mathrm{Al:Mo:Fe}} = 7\mathrm{GHSER_{Al}} + 2\mathrm{GHSER_{Mo}} + 4\mathrm{GHSER_{Fe}} + 835282.0 + 71.6587T$	This work
	$G^{\mu}_{\mathrm{Fe:Mo:Fe}} = 7\mathrm{GFCCFE} + 2\mathrm{GHSER_{Mo}} + 4\mathrm{GHSER_{Fe}} + 39475.0 - 6.0320T$	[49]
	$G^{\mu}_{\mathrm{Al:Mo:Mo}} = \frac{5}{7}G^{\mathrm{Al_8Mo_3}}_{\mathrm{Al:Mo}} + \frac{9}{7}G^{\mathrm{AlMo_3}}_{\mathrm{Al:Mo}} + 117666.5 + 15.6431T$	This work
	$G^{\mu}_{\mathrm{Fe:Mo:Mo}} = 7\mathrm{GFCCFE} + 6\mathrm{GHSER_{Mo}} - 46663.0 - 5.8910T$	[49]
	${}^{0}L^{\mu}_{\mathrm{Al:Mo:Fe,Mo}} = -2580495.1 - 21.1903T$	This work
	${}^{1}L^{\mu}_{\mathrm{Al:Mo:Fe,Mo}} = -1425536.5$	This work
	${}^{0}L^{\mu}_{\mathrm{Al,Fe:Mo:Mo}} = -308534.9 + 11.9578T$	This work
	${}^{1}L^{\mu}_{\mathrm{Al,Fe:Mo:Mo}} = +128862.5$	This work
R:$Fe_{27}Mo_{14}(Fe,Mo)_{12}$	$G^{\mathrm{R}}_{\mathrm{Fe:Mo:Fe}} = 27\mathrm{GFCCFE} + 14\mathrm{GHSER_{Mo}} + 12\mathrm{GHSER_{Fe}} - 77487.0 - 50.4860T$	[49]
	$G^{\mathrm{R}}_{\mathrm{Fe:Mo:Mo}} = 27\mathrm{GFCCFE} + 26\mathrm{GHSER_{Mo}} + 313474.0 - 289.4720T$	[49]
σ: $Fe_8Mo_4(Fe,Mo)_{18}$	$G^{\sigma}_{\mathrm{Fe:Mo:Fe}} = 8\mathrm{GFCCFE} + 4\mathrm{GHSER_{Mo}} + 18\mathrm{GHSER_{Fe}} - 1813.0 - 27.2720T$	[49]
	$G^{\sigma}_{\mathrm{Fe:Mo:Mo}} = 8\mathrm{GFCCFE} + 22\mathrm{GHSER_{Mo}} + 83326.0 - 69.6180T$	[49]
	${}^{0}L^{\sigma}_{\mathrm{Fe:Mo:Fe,Mo}} = +222909.0$	[49]
$Al_{12}Mo$:$Al_{12}(Fe,Mo)$	$G^{\mathrm{Al_{12}Mo}}_{\mathrm{Al:Mo}} = 12\mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mo}} - 146766.8 + 23.1256T$	This work
	$G^{\mathrm{Al_{12}Mo}}_{\mathrm{Al:Fe}} = \frac{17}{4}G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Al}} + \frac{35}{4}\mathrm{GHSER_{Al}} + 65000.0$	This work
Al_5Mo: $Al_5(Fe,Mo)$	$G^{\mathrm{Al_5Mo}}_{\mathrm{Al:Mo}} = 5\mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mo}} - 144819.3 + 25.4357T$	This work
	$G^{\mathrm{Al_5Mo}}_{\mathrm{Al:Fe}} = \frac{17}{4}G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Al}} + \frac{7}{4}\mathrm{GHSER_{Al}} + 30000.0$	This work
$Al_{22}Mo_5$: $Al_{22}(Fe,Mo)_5$	$G^{\mathrm{Al_{22}Mo_5}}_{\mathrm{Al:Mo}} = 22\mathrm{GHSER_{Al}} + 5\mathrm{GHSER_{Mo}} - 723273.3 + 132.3154T$	This work
	$G^{\mathrm{Al_{22}Mo_5}}_{\mathrm{Al:Fe}} = \frac{85}{4}G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Al}} + \frac{23}{4}\mathrm{GHSER_{Al}} + 441068.3$	This work
$Al_{17}Mo_4$: $Al_{17}(Fe,Mo)_4$	$G^{\mathrm{Al_{17}Mo_4}}_{\mathrm{Al:Mo}} = 17\mathrm{GHSER_{Al}} + 4\mathrm{GHSER_{Mo}} - 578455.4 + 107.4145T$	This work
	$G^{\mathrm{Al_{17}Mo_4}}_{\mathrm{Al:Fe}} = 17G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Al}} + 4\mathrm{GHSER_{Al}} + 172925.6$	This work
Al_4Mo: $Al_4(Fe,Mo)$	$G^{\mathrm{Al_4Mo}}_{\mathrm{Al:Mo}} = 4\mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mo}} - 138851.8 + 23.1120T$	This work
	$G^{\mathrm{Al_4Mo}}_{\mathrm{Al:Fe}} = \frac{17}{4}G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Al}} + \frac{3}{4}\mathrm{GHSER_{Al}} + 15778.2$	This work
Al_3Mo: $Al_3(Fe,Mo)$	$G^{\mathrm{Al_3Mo}}_{\mathrm{Al:Mo}} = 3\mathrm{GHSER_{Al}} + \mathrm{GHSER_{Mo}} - 143196.7 + 30.6912T$	This work
	$G^{\mathrm{Al_3Mo}}_{\mathrm{Al:Fe}} = \frac{1}{6}G^{\mathrm{Al_5Fe_2}}_{\mathrm{Fe:Al}} + \frac{17}{6}G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Al}} + 35000.0$	This work
Al_8Mo_3: $Al_8(Fe,Mo)_3$	$G^{\mathrm{Al_8Mo_3}}_{\mathrm{Al:Mo}} = 8\mathrm{GHSER_{Al}} + 3\mathrm{GHSER_{Mo}} - 432556.9 + 99.1737T$	This work
	$G^{\mathrm{Al_8Mo_3}}_{\mathrm{Al:Fe}} = \frac{7}{6}G^{\mathrm{Al_5Fe_2}}_{\mathrm{Fe:Al}} + \frac{17}{6}G^{\mathrm{Al_{13}Fe_4}}_{\mathrm{Fe:Al:Al}} + 496161.3$	This work
$Al_{63}Mo_{37}$: $Al_{63}(Fe,Mo)_{37}$	$G^{\mathrm{Al_{63}Mo_{37}}}_{\mathrm{Al:Mo}} = 63\mathrm{GHSER_{Al}} + 37\mathrm{GHSER_{Mo}} - 1638310.2 - 403.7604T$	This work
	$G^{\mathrm{Al_{63}Mo_{37}}}_{\mathrm{Al:Fe}} = \frac{63}{2}G^{\mathrm{Al_2Fe}}_{\mathrm{Fe:Al}} + \frac{11}{2}\mathrm{GHSER_{Fe}} + 500000.0$	This work
$AlMo_3$: $(Al,Fe,Mo)(Al,Fe,Mo)_3$	$G^{\mathrm{AlMo_3}}_{\mathrm{Al:Al}} = 4\mathrm{GHSER_{Al}} + 20000.0$	This work
	$G^{\mathrm{AlMo_3}}_{\mathrm{Fe:Al}} = \mathrm{GHSER_{Fe}} + 3\mathrm{GHSER_{Al}} + 20000.0$	This work
	$G^{\mathrm{AlMo_3}}_{\mathrm{Mo:Al}} = \mathrm{GHSER_{Mo}} + 3\mathrm{GHSER_{Al}} + 135830.9 - 2.0081T$	This work
	$G^{\mathrm{AlMo_3}}_{\mathrm{Al:Fe}} = \mathrm{GHSER_{Al}} + 3\mathrm{GHSER_{Fe}} + 50000.0$	This work
	$G^{\mathrm{AlMo_3}}_{\mathrm{Fe:Fe}} = 4\mathrm{GHSER_{Fe}} + 20000.0$	This work
	$G^{\mathrm{AlMo_3}}_{\mathrm{Mo:Fe}} = \mathrm{GHSER_{Mo}} + 3\mathrm{GHSER_{Fe}} + 20000.0$	This work
	$G^{\mathrm{AlMo_3}}_{\mathrm{Al:Mo}} = \mathrm{GHSER_{Al}} + 3\mathrm{GHSER_{Mo}} - 95830.9 + 2.0081T$	This work

Table 1 Continued

Phase	Thermodynamic parameters	Reference
	$G^{AlMo_3}_{Fe:Mo} = GHSER_{Fe} + 3GHSER_{Mo} + 10000.0$	This work
	$G^{AlMo_3}_{Mo:Mo} = 4GHSER_{Mo} + 20000.0$	This work
	${}^0L^{AlMo_3}_{Al,Mo:Al} = {}^0L^{AlMo_3}_{Al,Mo:Al} = +11628.1$	This work
	${}^0L^{AlMo_3}_{Al:Al,Mo} = {}^0L^{AlMo_3}_{Mo:Al,Mo} = +52100.0$	This work
	${}^0L^{AlMo_3}_{Fe:Fe,Mo} = {}^0L^{AlMo_3}_{Mo:Fe,Mo} = +50000.0$	This work
	${}^0L^{AlMo_3}_{Fe,Mo:Fe} = {}^0L^{AlMo_3}_{Fe,Mo:Mo} = +50000.0$	This work
τ_1: $Al_8(Al,Fe)Mo_3$	$G^{\tau_1}_{Al:Al:Mo} = 3G^{Al_3Mo}_{Al:Mo} + 10000.0$	This work
	$G^{\tau_1}_{Al:Fe:Mo} = 8GHSER_{Al} + GHSER_{Fe} + 3GHSER_{Mo} - 397772.5 + 67.2088T$	This work
	${}^0L^{\tau_1}_{Al:Al,Fe:Mo} = -90500.0$	This work
τ_2: $(Al,Fe,Mo)_1(Va)_3$	$G^{\tau_2}_{Al:Va} = GBCCAL$	This work
	$G^{\tau_2}_{Fe:Va} = GHSER_{Fe}$	This work
	$G^{\tau_2}_{Mo:Va} = GHSER_{Mo}$	This work
	${}^0L^{\tau_2}_{Al,Fe:Va} = -129000.0 + 35.8074T$	This work
	${}^1L^{\tau_2}_{Al,Fe:Va} = +2907.1$	This work
	${}^0L^{\tau_2}_{Al,Mo:Va} = -74000.0 + 10.8187T$	This work
	${}^1L^{\tau_2}_{Al,Mo:Va} = -44502.8 + 21.6488T$	This work
	${}^0L^{\tau_2}_{Fe,Mo:Va} = +36818.0 - 9.1410T$	This work
	${}^1L^{\tau_2}_{Fe,Mo:Va} = -362.0 - 5.7240T$	This work
	${}^0L^{\tau_2}_{Al,Fe,Mo:Va} = -40194.6 + 17.7874T$	This work
	${}^1L^{\tau_2}_{Al,Fe,Mo:Va} = +114371.2 - 68.9163T$	This work
	${}^2L^{\tau_2}_{Al,Fe,Mo:Va} = -113794.9 + 82.5891T$	This work

(a) In SI units (Joule, mole of the formula units and Kelvin)

Table 2 Invariant reactions in the Al-Mo system

	Present work				Ref 29			
Reaction	***T*, K**	***x* (Mo)**			***T* , K**	***x* (Mo)**		
liq. + bcc(Mo) → $AlMo_3$	2423	0.7155	0.7767	0.7520	2423	…	0.810	0.755
liq. + $AlMo_3$ → AlMo	1993	0.4378	0.7315	0.5523	1993	0.450	0.740	0.540
liq. + AlMo → $Al_{63}Mo_{37}$	1843	0.3546	0.4802	…	1843	0.350	0.475	…
liq. → Al_8Mo_3 + $Al_{63}Mo_{37}$	1814	0.3083	…	…	1808	0.320	…	…
$Al_{63}Mo_{37}$ → Al_8Mo_3 + AlMo	1763	…	…	0.4818	1763	…	…	0.490
AlMo → Al_8Mo_3 + $AlMo_3$	1743	0.4914	…	0.7331	1743	0.500	…	0.740
liq. → Al_8Mo_3	1819	…	…	…	1819	…	…	…
liq. → Al_8Mo_3 + Al_3Mo	1495	0.0582	…	…	1495	0.055	…	…
liq. + Al_3Mo → Al_4Mo	1425	…	0.0227	…	1425	…	0.035	…
liq. + Al_4Mo → $Al_{17}Mo_4$	1267	0.0227	…	…	<1273	0.030	…	…
liq. + $Al_{17}Mo_4$ → $Al_{22}Mo_5$	1218	0.0168	…	…	<1223	0.020	…	…
Al_4Mo → Al_3Mo + $Al_{17}Mo_4$	1215	…	…	…	1215	…	…	…
liq. + $Al_{22}Mo_5$ → Al_5Mo	1119	0.0079	…	…	1119	0.010	…	…
Al_3Mo → Al_8Mo_3 + $Al_{17}Mo_4$	1017	…	…	…	<1073	…	…	…
liq. + Al_5Mo → $Al_{12}Mo$	985	0.0018	…	…	985	0.005	…	…
liq. → $Al_{12}Mo$ + fcc	933	0.0005	…	…	933	0.002	…	…

but his result was higher than the experimental temperature.[53] Considering the availability of new experimental data,[44,45,53] the thermodynamic parameters of the Al-Fe system were re-optimized while adopting the Seierstein's thermodynamic parameters of liquid and fcc.[52]

The Al-Mo system was optimized by Kaufman and Nesor[50] and Saunders.[54] Kaufman and Nesor[50] optimized the partial phase diagram between Al_8Mo_3 and bcc(Mo) including four compounds $AlMo_3$, AlMo, Al_3Mo_2, and Al_8Mo_3. Since the work of Saunders[54] was submitted in 1989, the experimental data of Schuster and Ipser[28] published in 1991 was not included in his work. In the assessed phase diagram of Saunders,[54] five intermetallic compounds $Al_{12}Mo$, Al_5Mo, Al_4Mo and Al_8Mo_3 were

Table 3 Predicted invariant reactions in the Al-Fe-Mo system

		Present work				
			Composition in liquid			
Reaction	Type	*T*, K	*x* (Al)	*x* (Fe)	*x* (Mo)	Ref 45 *T*, K
liq. $\to Al_5Fe_4 + AlMo_3$	C_1	1862	0.4739	0.2485	0.2776	…
liq. $\to \tau_1 + Al_8Mo_3$	C_2	1803	0.7210	0.0221	0.2569	…
liq. $\to \tau_1 + AlMo_3$	C_3	1779	0.3046	0.4791	0.2163	
liq. $\to \tau_1 + Al_5Fe_4$	C_4	1742	0.6180	0.1610	0.2210	…
liq. $+ Al_8Mo_3 \to Al_{63}Mo_{37} + \tau_1$	U_1	1794	0.6717	0.0234	0.3049	…
liq. $+ Al_{63}Mo_{37} \to \tau_1 + AlMo$	U_2	1786	0.6439	0.0395	0.3166	…
liq. $+ AlMo_3 \to Al_5Fe_4 + AlMo$	U_3	1785	0.5627	0.1533	0.2840	…
liq. $+ AlMo_3 \to \tau_2 +$ bcc	U_4	1778	0.2649	0.5063	0.2288	…
liq. $+ Al_5Fe_4 + AlMo_3 \to \tau_2$	U_5	1769	0.4102	0.3895	0.2003	…
liq. $+ \sigma \to$ bcc + R	U_6	1751	0.0140	0.6898	0.2962	…
liq. $\to Al_5Fe_4 + AlMo + \tau_1$	E_1	1740	0.5992	0.1394	0.2614	…
liq.$+ \tau_2 \to Al_5Fe_4 + AlFe$	U_7	1544	0.5703	0.4048	0.0249	…
liq. $+ Al_5Fe_4 + \tau_1 \to Al_5Fe_2$	P_1	1447	0.6928	0.2938	0.0134	…
liq. $+ Al_8Mo_3 \to \tau_1 + Al_3Mo$	U_8	1435	0.8981	0.0709	0.0310	…
liq. $+ Al_5Fe_2 \to Al_{13}Fe_4 + \tau_1$	U_9	1400	0.8132	0.1758	0.0110	…
liq. $+ \tau_1 \to Al_{13}Fe_4 + Al_3Mo$	U_{10}	1339	0.8746	0.1141	0.0113	…
liq. $+ Al_3Mo \to Al_{13}Fe_4 + Al_4Mo$	U_{11}	1329	0.8811	0.1079	0.0110	…
liq. $+ Al_{17}Mo_4 \to Al_{22}Mo_5 + Al_4Mo$	U_{12}	1167	0.9669	0.0252	0.0079	…
liq. $+ Al_{22}Mo_5 \to Al_5Mo + Al_4Mo$	U_{13}	1114	0.9660	0.0296	0.0044	…
liq. $+ Al_4Mo \to Al_{13}Fe_4 + Al_5Mo$	U_{14}	1100	0.9647	0.0317	0.0036	…
liq. $+ Al_5Mo \to Al_{13}Fe_4 + Al_{12}Mo$	U_{15}	972	0.9860	0.0130	0.0010	…
liq. $\to Al_{12}Mo + Al_{13}Fe_4 +$ fcc	E_2	927	0.9909	0.0087	0.0004	…
$Al_{63}Mo_{37} + \tau_1 \to Al_8Mo_3 + AlMo$	U_{16}	1764				…
bcc $+ \sigma \to$ R + mu	U_{17}	1736				…
$AlMo + Al_8Mo_3 \to \tau_1 + AlMo_3$	U_{18}	1725				…
$AlMo \to Al_5Fe_4 + \tau_1 + AlMo_3$	E_3	1700				…
$Al_5Fe_4 + AlMo_3 \to \tau_1 + \tau_2$	U_{19}	1431				…
$Al_5Fe_4 + \tau_2 \to AlFe + \tau_1$	U_{20}	1421				…
$Al_5Fe_2 + Al_5Fe_4 \to Al_2Fe + \tau_1$	U_{21}	1378				…
$Al_5Fe_4 \to Al_2Fe + \tau_1 + AlFe$	E_4	1353				1358-1368
$\tau_2 \to AlFe + AlMo_3 + \tau_1$	E_5	1350				1344-1368
$Al_3Mo + \tau_1 \to Al_8Mo_3 + Al_{13}Fe_4$	U_{22}	1317				…
$Al_{13}Fe_4 + \tau_1 \to Al_5Fe_2 + Al_8Mo_3$	U_{23}	1275				…
$\tau_1 + Al_5Fe_2 \to Al_2Fe + Al_8Mo_3$	U_{24}	1174				…
$AlMo_3 + \tau_1 \to Al_8Mo_3 + AlFe$	U_{25}	1139				…
$\tau_1 \to Al_2Fe + Al_8Mo_3 + AlFe$	E_6	1120				~1120[32]
$Al_4Mo + Al_5Mo \to Al_{13}Fe_4 + Al_{22}Mo_5$	U_{26}	1080				…
$Al_4Mo + Al_{22}Mo_5 \to Al_{13}Fe_4 + Al_{17}Mo_4$	U_{27}	1066				…
$Al_4Mo \to Al_3Mo + Al_{13}Fe_4 + Al_{17}Mo_4$	E_7	1030				…
$Al_3Mo \to Al_8Mo_3 + Al_{13}Fe_4 + Al_{17}Mo_4$	E_8	958				…

optimized in the Al-rich region. Schuster and Ipser[28] and Eumann et al.[29] re-measured the Al-Mo phase diagram, and found more compounds in the Al-rich region. In the present work, the Al-Mo system is re-optimized according to the experimental data of Eumann et al.[28,29]

The optimization is carried out by means of the optimization module PARROT of the thermodynamic software Thermo-Calc.[55] The program works by minimizing a squared error sum where each of the selected values is given a certain weight. The weight is chosen by our personal judgment and changed by trial and error during the work until most of the selected experimental information is reproduced within the expected uncertainty limits.

4.1 Al-Mo System

The phase relations and the transformation temperatures are optimized on the basis of the Al-Mo phase diagram determined by Eumann et al.[29]

The optimization is carried out in two steps. In the first treatment, $Al_{12}Mo$, Al_3Mo, Al_5Mo, $Al_{17}Mo_4$, $Al_{22}Mo_5$, Al_4Mo, $Al_{63}Mo_{37}$, Al_8Mo_3 and $AlMo_3$ are assumed to be

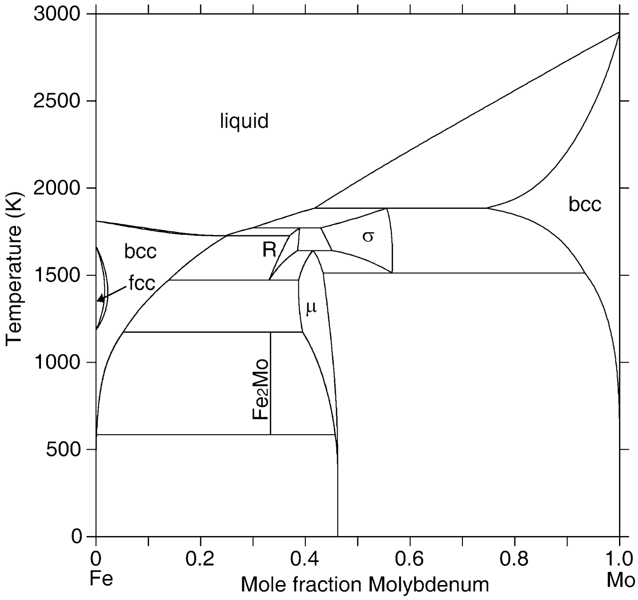

Fig. 1 Calculated Fe-Mo phase diagram using the thermodynamic parameters from Ref 49

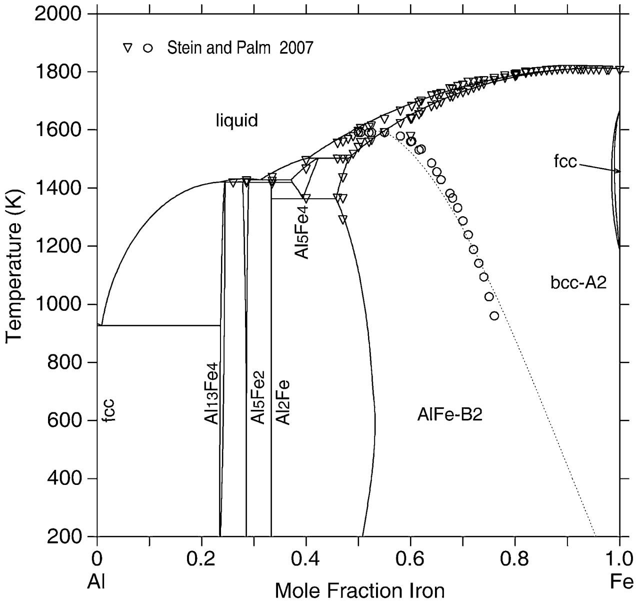

Fig. 2 Calculated Al-Fe phase diagram using the present thermodynamic parameters, in which the thermodynamic parameters of fcc are from Ref 52

stoichiometric compounds; in the second step, $AlMo_3$ is treated as the formula $(Al,Mo)(Al,Mo)_3$. The thermodynamic parameters obtained from the first step are the starting values for the second step.

4.2 Al-Fe-Mo System

The thermodynamic parameters for the Al-Fe-Mo system are optimized on the basis of the experimental results.[44,45] As a rule, only those coefficients that can be optimized from experimental data should be adjusted.[56] When there are insufficient experimental data to adjust a particular parameter, a reasonable estimate has to be made. This kind of estimation is mainly used to reduce the number of thermodynamic parameters of each compound.

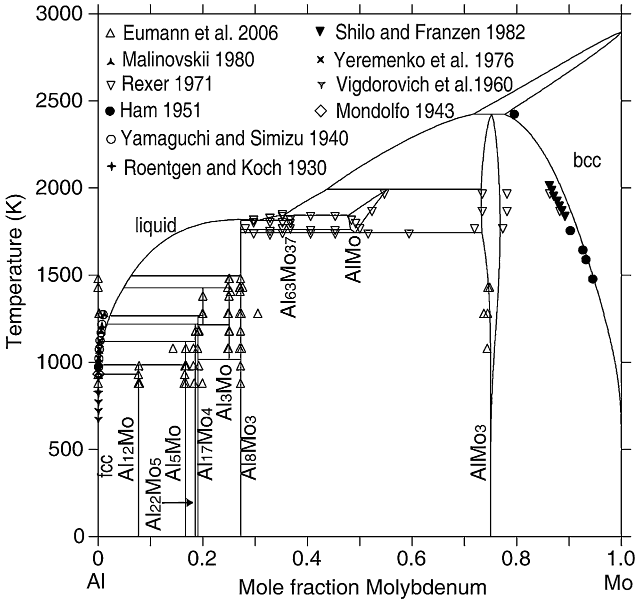

Fig. 3 Calculated Al-Mo phase diagram by the present thermodynamic description

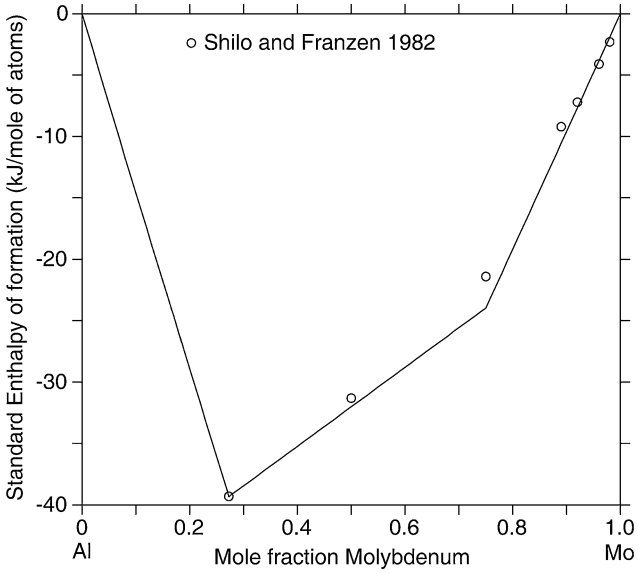

Fig. 4 Calculated standard enthalpy of formation at 298 K of the Al-Mo system in comparison with the experimental data from Ref 23

5. Results and Discussion

The thermodynamic description of the Al-Fe-Mo system obtained in the present work is shown in Table 1. The

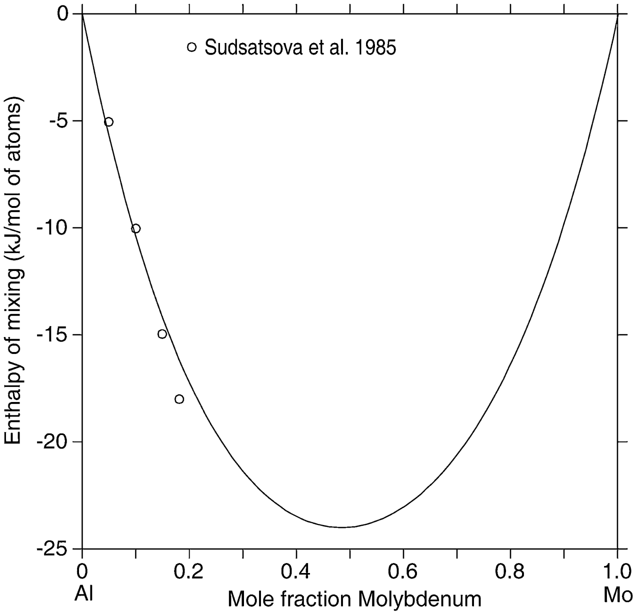

Fig. 5 Calculated enthalpy of mixing at 3000 K of the Al-Mo system in comparison with the experimental data from Ref 31

calculated invariant reaction temperatures and phase compositions of the Al-Mo system are listed in Table 2 showing satisfactory agreement between the calculated and the experimental data with the largest discrepancy of about 6 K in the temperature of the invariant reaction liq. $\rightarrow$ $Al_8Mo_3 + Al_{63}Mo_{37}$. All experimental invariant reaction compositions determined by Eumann et al.[29] in the Al-Mo system are well reproduced within 1-2 at.%. Table 3 presents the predicted temperatures and the liquid compositions for the invariant reactions in the Al-Fe-Mo system. The decomposition temperatures of τ_1, τ_2 and $\varepsilon^*(Al_5Fe_4)$ are 1120, 1350 and 1353 K, respectively, which are basically in agreement with the experimental temperatures 1120,[32] 1344-1368[45] and 1358-1368 K.[45]

The calculated phase diagram of the Fe-Mo system by means of the thermodynamic parameters optimized by Andersson[49] is shown in Fig. 1.

Figure 2 is the calculated phase diagrams of the Al-Fe system using the present thermodynamic descriptions, in which the thermodynamic parameters of liquid and fcc are adopted from Seierstein.[52] The optimized phase diagram is in good agreement with the experimental data.[53]

The Al-Mo phase diagram calculated using the present thermodynamic parameters is presented in Fig. 3. The phase Al_5Mo(r) is not considered due to the uncertainty in the transition temperature between Al_5Mo(r) and Al_5Mo(h). The optimized phase diagram is nearly identical to the one determined by Eumann et al.,[29] as shown in Fig. 3.

Figure 4 is the calculated standard enthalpies of formation at 298 K in the Al-Mo system in comparison with the experimental data.[23] Figure 5 compares the calculated mixing enthalpies of liquid at 3000 K in the Al-Mo system with the experimental data.[31] It can be seen that the calculated mixing enthalpies and the standard enthalpies of formation are in good agreement with the experimental data of Sudsatsova et al.[31] and Shilo and Franzen.[23]

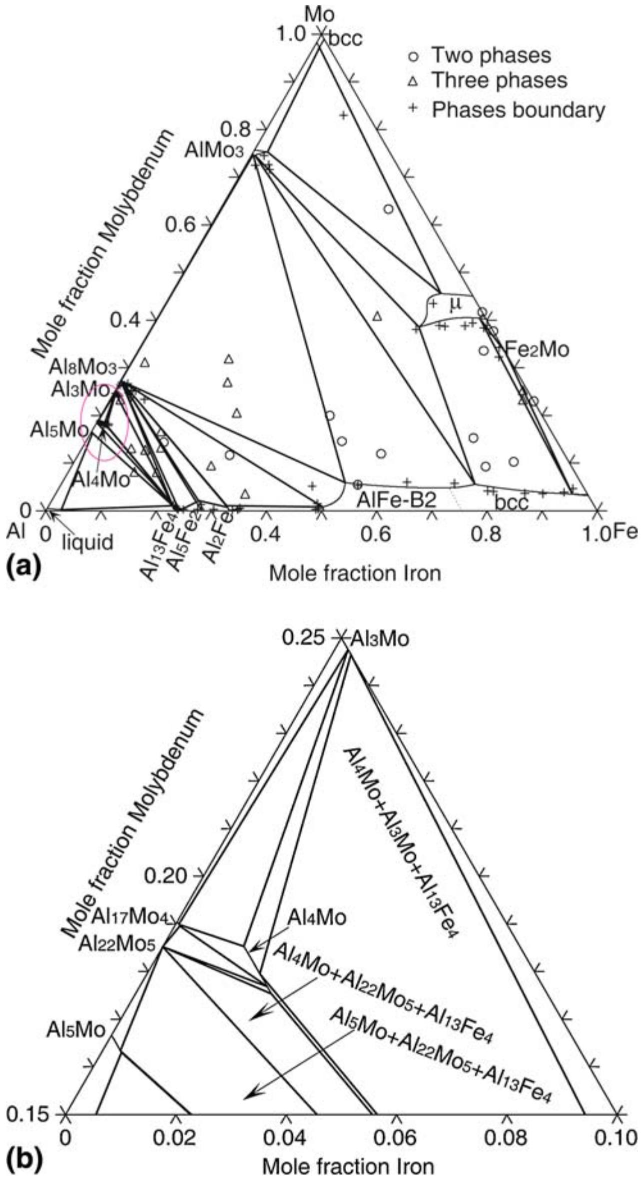

Fig. 6 (a) Calculated isothermal section of the Al-Fe-Mo system at 1073 K using the present thermodynamic description in comparison with the experimental data from Ref 44. (b) Enlarged section of (a)

Figures 6-8 present the calculated isothermal sections of the Al-Fe-Mo system at 1073, 1273 and 1423 K using the present thermodynamic descriptions. Satisfactory agreement is obtained between the calculated and the experimental results.[44,45] Figure 6(b) is the enlarged section of the isothermal section at 1073 K in the Al-Fe-Mo system, and agrees well with the second sketch (Fig. 4b in Ref 44) of three cases proposed by Eumann et al.[44] There is appreciable difference in the Al-rich corner of the Al-Fe-Mo isothermal section at 1073 K between the calculated one and that determined by Markiv et al.[32] This is partly due to

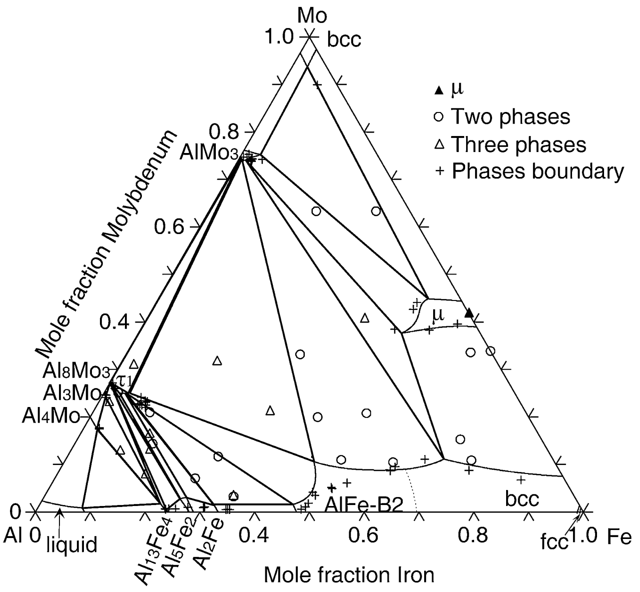

Fig. 7 Calculated isothermal section of the Al-Fe-Mo system at 1273 K using the present thermodynamic description in comparison with the experimental data from Ref 45

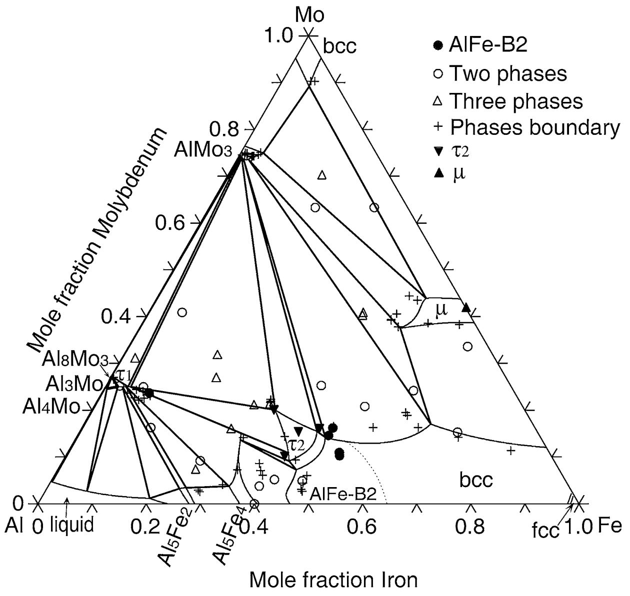

Fig. 8 Calculated isothermal section of the Al-Fe-Mo system at 1423 K using the present thermodynamic description in comparison with the experimental data from Ref 45

the confirmation of the existence of $Al_{22}Mo_5$, $Al_{17}Mo_4$ and the change of the stability temperature range of Al_4Mo. In the Al-Mo system presented by Markiv et al.,[32] there is no existence of $Al_{22}Mo_5$ and $Al_{17}Mo_4$, and the compound Al_4Mo is still stable at room temperature, which is different from the experimental results by Eumann et al.[29] that the stability temperature range of Al_4Mo is 1215-1425 K. In the present work, the isothermal section of the Al-Fe-Mo at

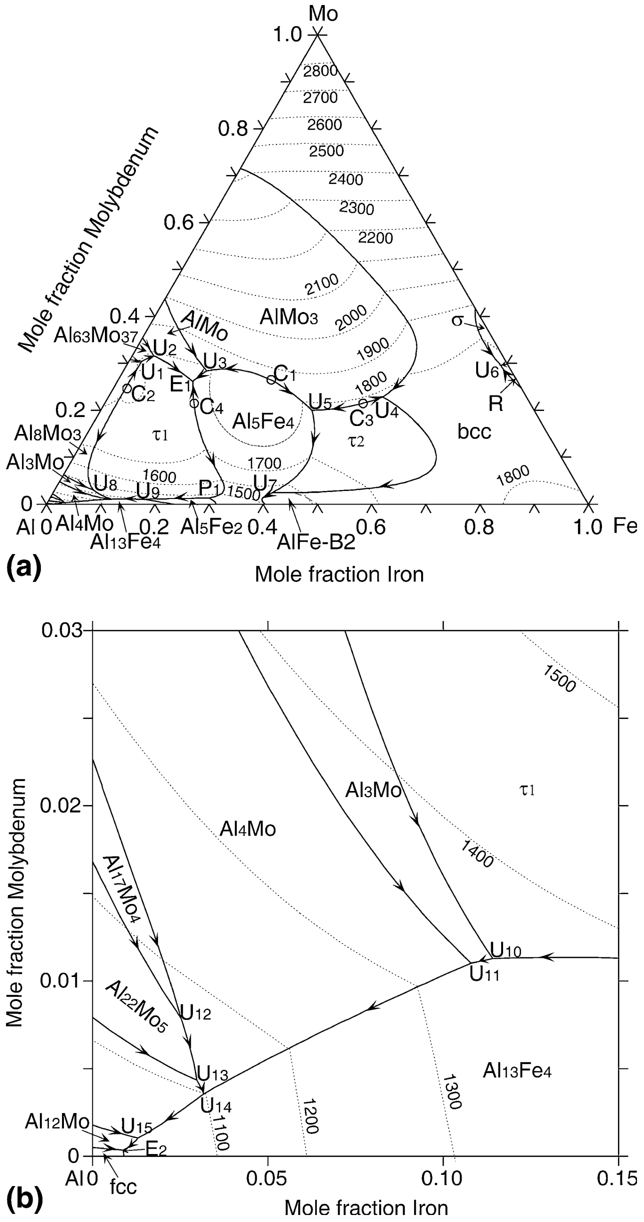

Fig. 9 (a) Predicted the projection of liquidus surface in the Al-Fe-Mo system using the present thermodynamic description. (b) Enlarged section of (a)

1073 K determined by Eumann et al.[44] is adopted as a basis of optimization.

The alloy with 60 at.% Al and 40 at.% Fe at 1423 K was determined to have AlFe and Al_2Fe phases by Eumann et al.[45]; but according to the binary Al-Fe phase diagram determined by Stein and Palm,[53] this alloy should be in the single phase region of Al_5Fe_4.[45] The alloy with 48.7 at.% Al, and 46.4 at.% Fe was reported to have three different phases at 1423 K in the experimental results of Eumann et al.,[45] thus the phase equilibria at this composition had not reached equilibrium and are not considered in the present work. The contradiction exists between the calculated decomposition temperature of Al_5Fe_4 and solid

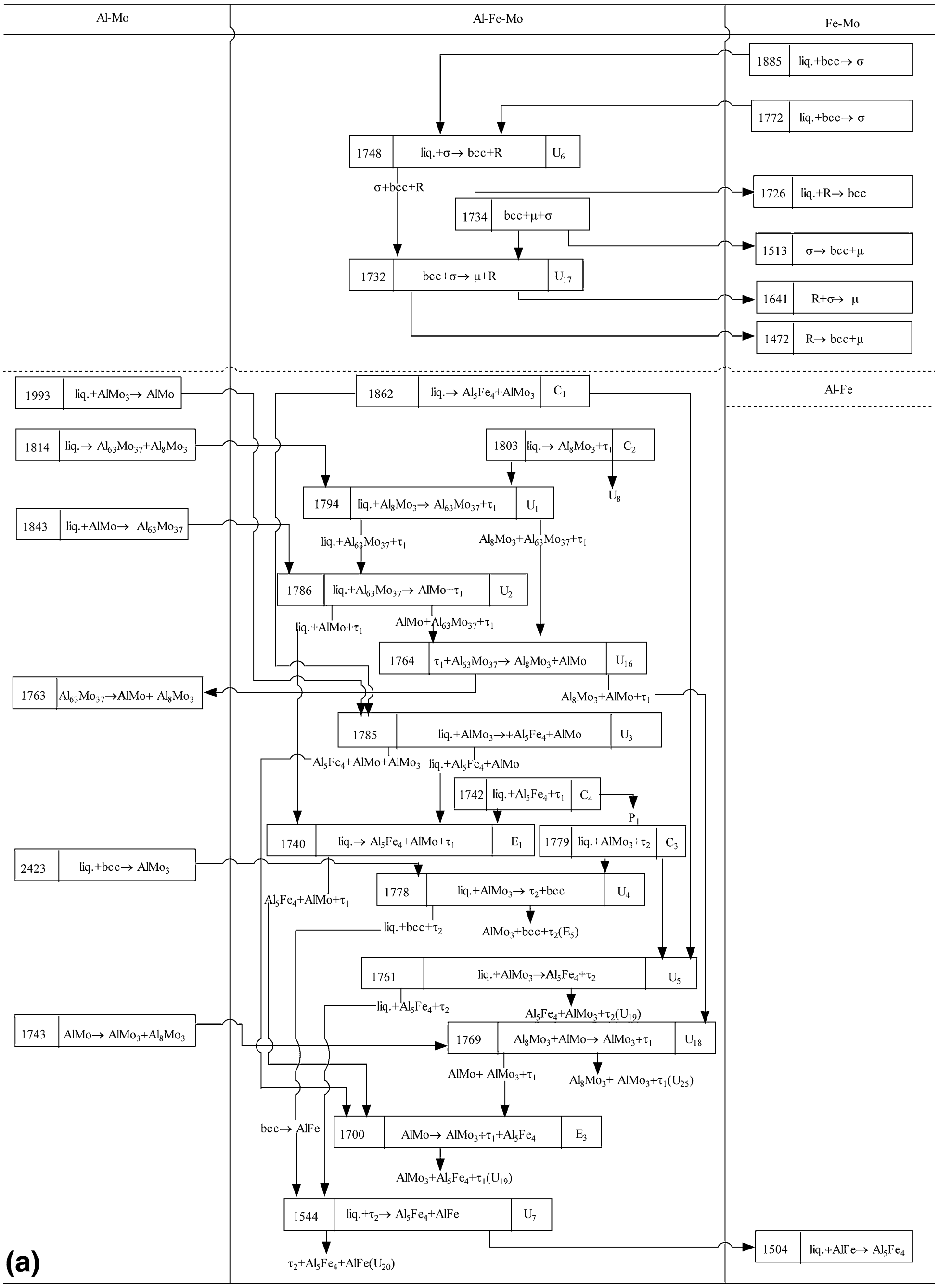

Fig. 10 Computed reaction scheme in the Al-Fe-Mo system

solubilities of AlFe-B2 and AlFe-A2. If the solid solubility of AlFe-B2 at 1423 K agrees well with the experimental data,[45] the decomposition temperature of Al_5Fe_4 is 1309 K and the discrepancy is about 50 K. So the present calculated results of the discrepancy 5 K on the decomposition temperature of Al_5Fe_4 and the phase boundary of AlFe-B2 related to Al_5Fe_4 were accepted as a final result of this work.

Figure 9 shows the computed liquidus surface projection of the Al-Fe-Mo system. Figure 10 is the predicted reaction scheme which is divided into three sections and shown in Fig. 10(a)-(c). Comparing with the established reaction scheme,[45] the calculated three-phase regions at 1073, 1273 and 1423 K are similar to the experimental data, but the calculated reaction scheme is different from the established reaction scheme[45] between 1273 and 1423 K in the Al-rich corner. The difference is mainly caused by one key invariant reaction liq. + τ_1 → Al_5Fe_2 + Al_3Mo proposed by Ref 45 which is substituted by the present invariant reaction liq. + Al_5Fe_2 → $Al_{13}Fe_4$ + τ_1 at 1400 K. Attempts to reproduce the invariant reaction liq. + τ_1 → Al_5Fe_2 + Al_3Mo

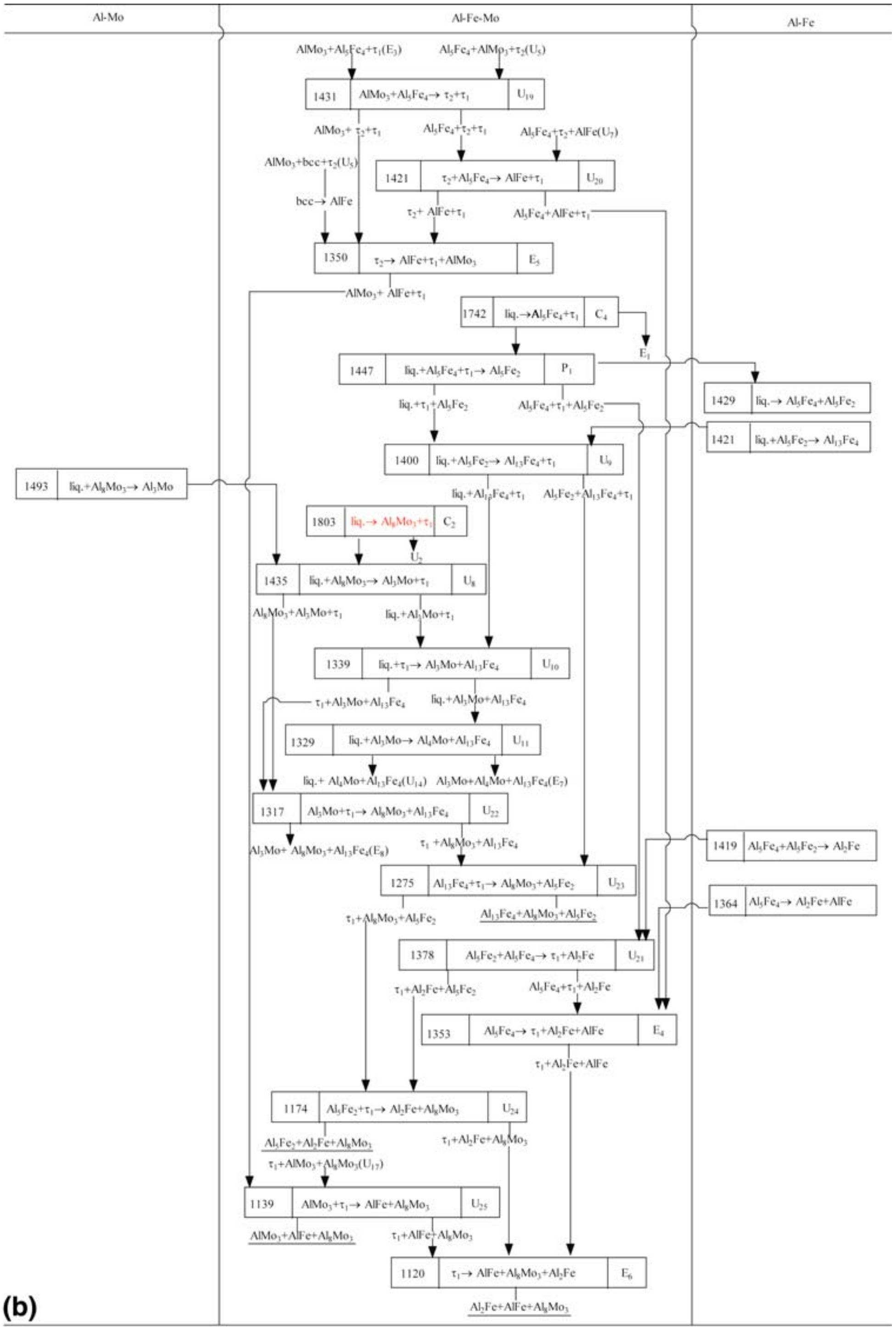

Fig. 10 Continued

was unsuccessful. If the liquidus surface of Al_3Mo is forced to contact with the one of Al_5Fe_2, the phase relationships[45] among Al_8Mo_3, $AlMo_3$, $Al_{13}Fe_4$ and τ_1 at 1273 K can not to be reproduced. So the calculated invariant reaction liq. + $Al_5Fe_2 \rightarrow Al_{13}Fe_4 + \tau_1$ at 1400 K is accepted in the present work.

6. Conclusions

The phase relations and the thermodynamic properties in the Al-Mo binary and the Al-Fe-Mo ternary systems are optimized from the experimental information available in

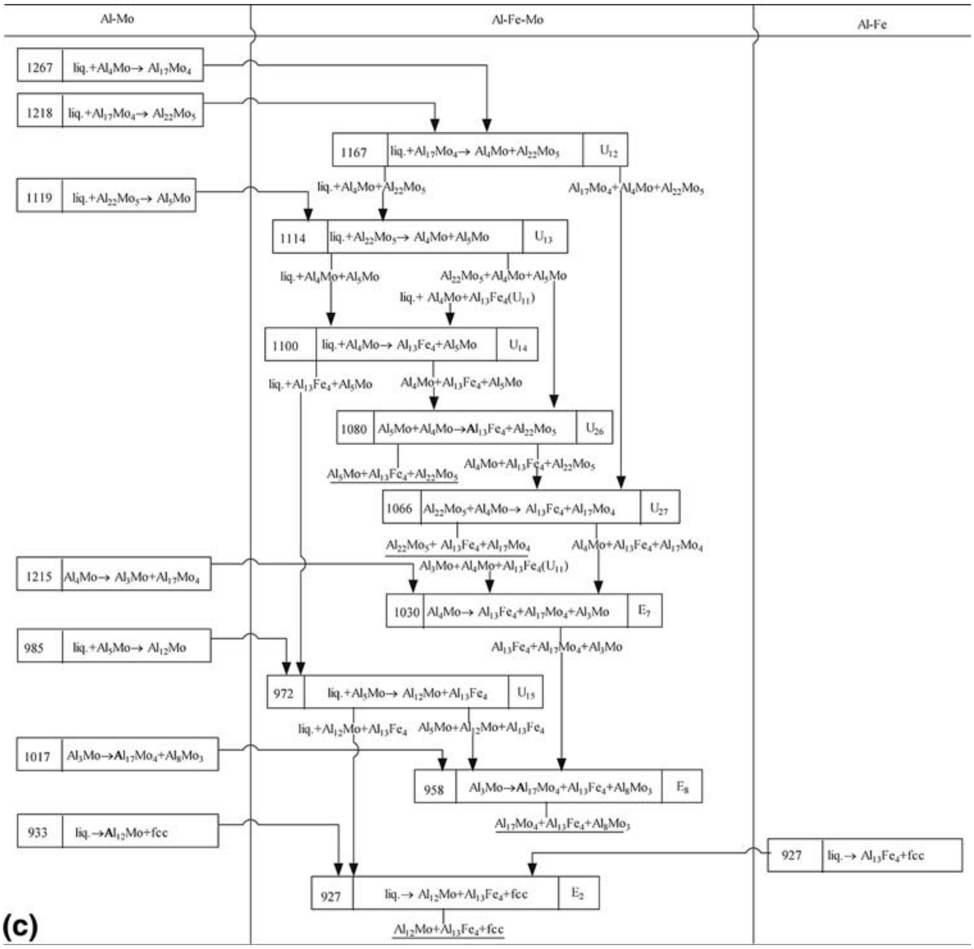

Fig. 10 Continued

the literature. A set of self-consistent thermodynamic parameters describing the Gibbs energies of individual phases as functions of composition and temperature is obtained. With the present optimized parameters, various thermodynamic calculations of practical interest can be made.

Acknowledgment

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References

1. J. Klöwer, High Temperature Corrosion Behaviour of Iron Aluminides and Iron–Aluminium–Chromium Alloys, *Werkst. Korros.*, 1996, **47**, p 685-694
2. P.F. Tortorelli and K. Natesan, Critical Factors Affecting the High-Temperature Corrosion Performance of Iron Aluminides, *Mater. Sci. Eng. A*, 1998, **258**, p 115-125
3. M. Eumann, M. Palm, and G. Sauthoff, Iron-Rich Iron-Aluminium-Molybdenum Alloys with Strengthening Intermetallic μ Phase and R Phase Precipitates, *Steel Res. Int.*, 2004, **75**, p 62-73
4. M. Eumann, M. Palm, and G. Sauthoff, Alloys Based on Fe_3Al or FeAl with Strengthening Mo_3Al Precipitates, *Intermetallics*, 2004, **12**, p 625-633
5. M. Palm, Concepts Derived from Phase Diagram Studies for the Strengthening of Fe–Al-Based Alloys, *Intermetallics*, 2005, **13**, p 1286-1295
6. H. Reimann, Al–Mo Alloys, *Z. Metallkd.*, 1922, **14**, p 119-123
7. P. Roentgen and W. Koch, The Influence of Heavy Metals on Al Alloys, *Z. Metallkd.*, 1930, **25**, p 182-185
8. K. Yamaguchi and K. Simizu, The Equilibrium Diagram of the Al–Mo System, *Nippon Kinzoku Gakkai-Shi*, 1940, **4**, p 390-392
9. L.F. Mondolfo, *The Al–Mo System*, Metallography of Aluminum Alloys, John Wiley & Sons, 1943, p 30-31
10. J.L. Ham, First and Second Annual Reports on Project NR 031-331, Climax Molybdenum Co. 1950 and 1951, respectively; see also J.L. Ham, *Trans. Am. Soc. Mech. Eng.*, 1951, **73**, p 727-728
11. R.L. Wachtell, Some Preliminary Comments on the System Mo–Al, *Power Met. Bull.*, 1952, **6**, p 99-104
12. F. Sperner, The Binary System Al–Mo, *Z. Metallkd.*, 1959, **50**, p 588-591

13. J.W.H. Clare, Compounds Present in Aluminium Alloys of the Al–Mo System, *J. Inst. Met.*, 1960-61, **89**, p 232-234
14. V.N. Vigdorovich, V.M. Glazov, and N.N. Glagoleva, An Investigation of the Solubility of Cr, Mo and W in Al by the Microhardness Method, *Izv. VUZ, Tsvetnaya Met.*, 1960, **2**, p 143-146
15. J.B. Forsyth and G. Gran, The Structure of the Intermetallic Phase (Mo–Al)–Al_8Mo_3, *Acta Crystallogr.*, 1962, **15**, p 100-104
16. M. Potzschke and K. Schubert, Towards the Synthesis of Several T_4-B^3 Homologous and Quasi-Homologous System. II. The Systems Ti–Al, Zr–Al, Hf–Al, Mo–Al and Several Ternary Systems, *Z. Metallkd.*, 1962, **53**, p 548-561
17. L.K. Walford, The Phase Diagram of the Al–Mo System, *Philos. Mag.*, 1964, **9**, p 513-516
18. G.I. Belyaeva, N.G. Ilyuhchenko, and A.I. Anfinogenov, Thermodynamics of Solid Alloys of the Mo–Al System, *Tr. Inst. Elektrokhim., Akad. Nauk. SSSR, Ural. Filial*, 1967, **10**, p 85-95
19. K. Kamei, T. Ninomiya, and S. Terauchi, Al–Mo Binary Phase Diagram, *Tech. Rep. Kansai Univ., Osaka*, 1972, **13**, p 93-106
20. G. Petzow and J. Rexer, Melting Equilibria in the System U–UAl_2–Al_8Mo_3–Mo, *Z. Metallkd.*, 1969, **60**, p 449-453
21. R.C. Hansen and A. Raman, Alloy Chemistry of σ Related Phases III. σ Phases with Non-Transition Metals, *Z. Metallkd.*, 1970, **61**, p 115-120
22. J. Rexer, The Phase Equilibria in the Al–Mo System at Temperatures Above 1400°C, *Z. Metallkd.*, 1971, **62**, p 844-848
23. I. Shilo and H.F. Franzen, High Temperature Thermodynamic Study of the Mo-Rich Regions of the Mo–Al Systems, *J. Electrochem. Soc.*, 1982, **129**, p 2613-2617
24. G. Van Tendeloo, J. Van Landuyt, and S. Amelinckx, The Defect Structure of Aluminium Rich Al–Mo Alloys, *Mater. Res. Bull.*, 1975, **10**, p 941-948
25. V. Yeremenko, Ya.V. Natanzon, and V.I. Dybkov, Interaction of the Refractory Metals with Liquid Al, *J. Less-Common Met.*, 1976, **50**, p 29-48
26. R.R. Malinovskii, Position of the Liquidus in the Al–Mo System, *Teknol. Legk. Splavov*, 1980, (1), p 60-61
27. L. Brewer and R.H. Lamoreaux, The Mo–Al System, *Bull. Alloy Phase Diagram*, 1980, **1**, p 71-75
28. J.C. Schuster and H. Ipser, The Al–Al_8Mo_3 Section of the Binary System Aluminum-Molybdenum, *Metall. Trans. A*, 1991, **22**, p 1729-1736
29. M. Eumann, G. Sauthoff, and M. Palm, Re-Evaluation of Phase Equilibria in the Al–Mo System, *Int. J. Mater. Res.*, 2006, **97**, p 1502-1511
30. A.S. Dubrovin, O.S. Gorelkin, Yu.Ya. Demidov, N.A. Chirkov, L.S. Kostylev, and O.D. Kolesnikova, Calorimetric Study of Heats of Solution of Si and Al in Aluminothermic Alloys, *Metalloterm. Protsessy Khim. Metall. Mater: Konf.*, A.T. Dogvinenko, Ed., Nauk. Sib. Otd. Novosibirsk, 1971, p 121
31. V.S. Sudsatsova, G.I. Batalin, and V.S. Tutevich, Thermodynamic Properties of Molten Binary Alloys in Systems Al–(Zr,Nb,Mo), *Russ. Metall.*, 1985, (5), p 183-185
32. V.Ya. Markiv, V.V. Burnashova, and V.P. Ryabov, Investigation of Al-Rich Part of the Mo–Fe–Al System, *Dopov. Akad. Nauk Ukr. RSR, Ser. A*, 1970, **1**, p 69-72
33. V. Raghavan, *Phase Diagrams of Ternary Iron Alloys, Part 6A*, Indian Institute of Metals, 1992, p 135
34. P. Villars, A. Prince, and H. Okamoto, *Handbook of Ternary Alloy Phase Diagrams*, Vol 3, ASM International, Metals Park, 1995, p 3514
35. E.M. Sokolovskaya, G.M. Chel'dieva, E.F. Kazakova, and N.I. Kaloev, An Investigation of Alloys in the Al–Al_3Fe–$Al_{12}Mo$ System, *Moscow Univ. Chem. Bull.*, 1987, **42**, p 108-109
36. G. Wang, D.L. Douglass, and F. Gesmundo, High-temperature Sulfidation of Fe-30Mo Alloys Containing Ternary Additions of Al, *Oxid. Met.*, 1991, **35**, p 349-373
37. N.A. Birun and Y.P. Selisskii, Effect of Molybolenum on Transformations in an Ordering Alloy Fe3Al, *Phys. Met. Metallogr.*, 1969, **27**, p 1060-1066
38. Y.P. Selisskiy and M.N. Tolocko, *Ukr. Fiz. Zh.,* 1969, **14**, p 1692 (cited from Ref 44)
39. M.G. Mendiratta and H.A. Lipsitt, $D0_3$-Domain Structures in Fe_3Al-X Alloys, High-Temperature Ordered Intermetallic Alloys, *Materials Research Society Symposium Proceedings*, C.C. Koch, C.T. Liu, and N.S. Stoloff, Ed., 1985, Vol 39, p 155
40. R.T. Fortnum and D.E. Mikkola, Effects of Molybdenum, Titanium and Silicon Additions on the $D0_3 \rightarrow B2$ Transition Temperature, *Mater. Sci. Eng*, 1987, **91**, p 223
41. U. Prakash, R.A. Buckley, and H. Jones, Effect of Molybdenum Substitution on Crystal Structure of Ordered Fe–Al Alloys, *Mater. Sci. Technol.*, 1993, **9**, p 16-20
42. J. Stepien-Damm, P. Salamakha, K. Wochowski, and W. Suski, Crystal Structure of $Mo_9Fe_{4.75}Al_{0.25}$, *J. Alloys Compd.*, 1999, **282**, p 182-183
43. V. Raghavan, Al–Fe–Mo (Aluminum-Iron-Molybdenum), *J. Phase Equilib. Diffus.*, 2005, **26**, p 68-69
44. M. Eumann, G. Sauthoff, and M. Palm, Phase Equilibria in the Fe–Al–Mo System—Part I: Stability of the Laves Phase Fe_2Mo and Isothermal Section at 800°C, *Intermetallics*, 2008, **16**, p 706-716
45. M. Eumann, G. Sauthoff, and M. Palm, Phase Equilibria in the Fe–Al–Mo System—Part II: Isothermal Sections at 1000 and 1150°C, *Intermetallics*, 2008, **16**, p 834-846
46. A.T. Dinsdale, *SGTE Pure Element (Unary) Database*, Version 4.5, 2006 (private communication)
47. M. Hillert and L.I. Staffansson, The Regular Solution Model for Stoichiometric Phase and Ionic Melts, *Acta Chem. Scand.*, 1970, **24**, p 3618-3626
48. B. Sundman and J. Agren, Regular Solution Model for Phases with Several Components and Sublattices, Suitable for Computer Applications, *J. Phys. Chem. Solids*, 1981, **42**, p 297-301
49. J.-O. Andersson, A Thermodynamic Evaluation of the Fe-Mo-C System, *CALPHAD*, 1988, **12**, p 9-23
50. L. Kaufman and H. Nesor, Coupled Phase Diagrams and Thermodynamical Data for Transition Metal Binary Systems, *CALPHAD*, 1978, **2**, p 325-348
51. N. Saunders and V.G. Rivlin, A Critical Review and Thermodynamic Calculations for the Al-Rich Portion of the Al–Cr–Fe Phase Diagram, *Z. Metallkd.*, 1987, **78**, p 795-801
52. M. Seierstein, System Al–Fe. COST507, *Thermochemical Database for Light Metal Alloys*, Vol 2, I. Ansara, A.T. Dinsdale, and M.H. Rand, Ed., European Commission, Luxembourg, 1998, p 234
53. F. Stein and M. Palm, Re-determination of Transition Temperatures in the Fe–Al System by Differential Thermal Analysis, *Int. J. Mater. Res.*, 2007, **98**, p 580-588
54. N. Saunders, The Al–Mo System, *J. Phase Equilib.*, 1997, **18**, p 370-378
55. B. Sundman, B. Jansson, and J.-O. Andersson, The Thermo-Calc Databank System, *CALPHAD*, 1985, **9**, p 153-190
56. H.L. Lukas and S.G. Fries, Demonstration of the Use of "BINGSS" with the Mg–Zn System as Example, *J. Phase Equilib.*, 1992, **13**, p 532-542