Phase Equilibria in Al-Ca-Li System: a Thermodynamic Description

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Abstract   Relations of equilibrium phases in the Al-Ca-Li system were calculated by means of the CALPHAD (calculation of phase diagram) method. The reported thermodynamic model parameters for all the constituent binary systems were directly used in the present calculation. A novel thermodynamic description for the three ternary intermetallic compounds(τ_1, τ_2 and τ_3) was made on the basis of experimental phase equilibria in the Al-Ca-Li system. Comparison between the calculated and experimental phase equilibria shows that we have successfully derived a set of self-consistent thermodynamic parameters for the Al-Ca-Li system. These parameters were then used for the prediction of the selected isothermal and isopleth sections and projected liquidus surface of this ternary system over the entire composition range.

Keywords   Phase diagram; Thermodynamics; Alloy

1   Introduction

Al-Li based alloys have been extensively investigated as a family of structure materials for application in the aerospace, automotive and marine industries. Most recently, much more attention has also been paid to the significant hydrogen storage capacity involved in the Al-Li based hydride systems[1—5]. Therefore, the phase equilibria of the Al-Li based multi-component systems are of actual interest, which can help the investigators improve the design of new structure materials or hydrogen storage materials, and understand the relationship between microstructure on the one hand and properties on the other hand.

The systematic experimental approach for obtaining the phase diagram and thermodynamics of a multicomponent system seems very costly and time consuming and hence irrealistic. Thanks to the great development of the advanced CALPHAD method, various types of phase diagrams and thermodynamic properties of interest can now be easily calculated *via* mathematical models involving empirical parameters for the Gibbs energy of the individual phases, and only limited experimental information or other theoretical data(if lack of experimental data) are needed to obtain these empirical parameters.

Many efforts have been made to perform the thermodynamic descriptions of the Al-Li based ternary system, such as the Al-Li-Mg system[6], Al-Li-Zn system[7] etc, while, until now, no such investigations have been conducted on the Al-Ca-Li ternary system. The present work is to apply the CALPHAD-type thermodynamic calculation to reasonably predicting various types of phase diagrams of interest for the ternary Al-Ca-Li system.

2   Literature Review

Phase equilibrium researches based on the CALPHAD method require the complete and detailed review of the relative information reported in the literature including the analysis and selection of the experimental data, the reproduction and improvement of the previous thermodynamic assessment, and measuring and theoretically predicting critical data points unavailable.

2.1   Al-Li Binary System

There are three groups of researchers[7—9] who have performed the thermodynamic descriptions of the Al-Li binary system. The differences among these investigations only existed in the thermodynamic modeling of AlLi phase with B32-type structure. It was once described by Saunders[8] as a two sublattice model of (Al, Li)(Li, V_a). Recently, Hallstedt *et al.*[9] have treated it as the formula (Al, Li)$_{0.25}$(Al, Li)$_{0.25}$(Al, Li)$_{0.25}$(Al, Li)$_{0.25}$ by a four sublattice model in order to cope with the order-disorder transition between B32(AlLi) and body-centered cubic solution(bcc-A2). At latest, Guo *et al.*[7] simplified the description of the order-disorder transition by a two-sublattice model (Al,Li)$_{0.5}$(Al, Li)$_{0.5}$ instead.

2.2   Ca-Li Binary System

The phase equilibrium information on the Ca-Li system has firstly been reviewed by Bale *et al.*[10]. Later on, an

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exclusive evaluation on the literature has also been conducted by Gröbner et al.[11] in consideration of the formation enthalpy of CaLi$_2$ determined via a drop solution calorimetric measurement in order to give a Calphad-type thermodynamic modeling of this system.

2.3   Al-Ca Binary System

The experimental information concerning phase equilibria in the Al-Ca system was reported in several phase diagram compilations[12—14]. On the basis of all the reported literature information, Hansen et al.[15] constructed the first phase diagram labeled by two binary compounds CaAl$_2$ and CaAl$_4$ which is fundamental to the earlier thermodynamic investigations of this system. Recent thermodynamic assessments[16—18] have been modified to include another two binary compounds Ca$_{13}$Al$_{14}$ and Ca$_8$Al$_3$ in the Al-Ca binary system. Of these assessments, most investigators[16,17] were apt to simply treat these intermetallic phases as stoichiometric compound due to their limited homogeneity range, and only Ozturk et al.[18] used the formula (Al, Ca)$_2$(Al, Ca)$_1$ to define the Gibbs free energy of the Laves C15 compound CaAl$_2$.

The phase relations and thermodynamics of the ternary Al-Ca-Li system are poorly known due to the limited and even self-contradictory experimental data in the literature. The first investigation on the ternary Al-Ca-Li system was performed by Lee et al.[19] who aimed at calculating the vapor pressures over ternary melts on the basis of thermodynamic data of binary Al and Li liquid alloys. Miller et al.[20] reported, in the form of an abstract, that the two binary Laves phases CaAl$_2$(Cu$_2$Mg structure type) and CaLi$_2$(MgZn$_2$ structure type) unlikely reach the direct equilibrium. Instead, a ternary Laves phase with the MgNi$_2$ structure was considered to keep in direct equilibrium with both the two binary Laves phases. Miller et al.[21] reported crystal structure of a ternary phase Al$_3$Ca$_{8-x}$Li$_x$ which was later confirmed by Kevorkov et al.[22] to be the binary phase Al$_3$Ca$_8$. Two plausible ternary compounds Al$_{2-x}$CaLi$_x$ were synthesized by Nesper et al.[23] in a Mo crucible and later structurally characterized in the forms of MgNi$_2$ type(τ_1, $0.80 \leqslant x \leqslant 1.0$) and MgZn$_2$ type(τ_2, $0.25 \leqslant x \leqslant 0.75$), respectively. Another ternary phase Al$_{12}$Ca$_6$Li$_{11}$ was reported and also structurally determined later in detail by Haeussermann et al.[24]. For the further phase with the composition Al$_{7-x}$Ca$_8$Li$_x$, no information has been available in the text. Phase equilibria in the Al-Ca-Li system were studied by the same group of researchers[25—27] via X-ray phase and differential thermal analyses. Ganieva et al.[26] proposed a partial isothermal section up to 33%(molar fraction) Ca at 150 °C, and soon after they[27] presented additionally six vertical sections and a constructed partial liquidus surface. In these investigations, there was absolutely no evidence for the existence of a large solubility range of the Laves phase and the earlier reported ternary phases. In contrast, recent experimental work from Janz[28] confirmed clearly the stability of the ternary Laves phase of the Ni$_2$Mg structure and the phase Al$_{12}$Ca$_6$Li$_{11}$(τ_3), while the phase Li$_2$Ca$_6$Al$_2$ reported by Nesper et al.[23] was not confirmed. With the critical review of all the existed phase equilibrium information, Gröbner[29] proposed an

evaluated isothermal section of the Al-Ca-Li system at room temperature. However, there has been no thermodynamic modeling of the Al-Ca-Li ternary system up to now, leastways no one we have known of.

3   Thermodynamic Models

The Gibbs energy functions of pure elements Al, Li and Ca were taken from the SGTE compilation by Dinsdale[30], which are referred to the enthalpy for their stable state at 298.15 K, namely H^{SER}. The Gibbs free energy of pure elements(^0G) is described as

$$^0G = G(T) - H^{SER} = a + bT + \ln T + dT^2 + eT^3 + f/T + \sum_n g_n T^n \quad (1)$$

where a to f and g_n are coefficients and n stands for a set of integers and T refers to the absolute temperature(K).

There exist a total of 14 phases in the Al-Ca-Li system. They are liquid, Fcc, Bcc, B32, Al$_2$Li$_3$, Al$_4$Li$_9$, CaLi$_2$, Al$_4$Ca, Al$_2$Ca, Al$_{14}$Ca$_{13}$, Al$_3$Ca$_8$, τ_1, τ_2 and τ_3. Their crystal structures and thermodynamic models are listed in Table 1. Among the 14 phases in the ternary system, only 6 phases are the ternary phase of which Gibbs energy should be modeled in the present work. The Gibbs energy of the other binary phases was directly adopted from the previous assessments.

Table 1   Phases in the Al-Ca-Li system

Phase symbol	Pearson symbol	Thermodynamic model	Phase description
L	N/A	(Al, Ca, Li)	Ternary liquid phase
Fcc	cF4	(Al, Ca, Li)	Ternary solid solution
Bcc	cI2	(Al, Ca, Li)	Ternary solid solution
CaLi$_2$	hP12	(Ca)(Li)$_2$	Binary phase
Al$_4$Li$_9$	mC26	(Al)$_4$(Li)$_9$	Binary phase
Al$_2$Li$_3$	hR15	(Al)$_2$(Li)$_3$	Binary phase
B32	cF16	(Al, Li)$_{0.5}$(Al, Li)$_{0.5}$	Binary phase
Al$_4$Ca	tI10	(Al)$_4$(Ca)	Binary phase
Al$_2$Ca	cF24	(Al)$_2$(Ca)	Binary phase
Al$_{14}$Ca$_{13}$	mC54	(Al)$_{14}$(Ca)$_{13}$	Binary phase
Al$_3$Ca$_8$	aP22	(Al)$_3$(Ca)$_8$	Binary phase
τ_1	hP12	(Al)(Ca)(Li)	Ternary intermetallic phase
τ_2	hP24	(Al)$_3$(Ca)$_2$(Li)	Ternary intermetallic phase
τ_3	cF116	(Al)$_{12}$(Ca)$_6$(Li)$_{11}$	Ternary intermetallic phase

The liquid, Fcc and Bcc solution phases are described by one sublattice(Al, Ca, Li) with the molar Gibbs energy G_m^ϕ expressed in the following expression:

$$G_m^\phi = \sum_i x_i {}^0G_i^\phi + RT \sum_i x_i \ln x_i + {}^{xs}G_m^\phi \quad (2)$$

where $^0G_i^\phi$ is the molar Gibbs energy of the pure element i with the structure ϕ from Dinsdale[30], x_i is the molar fraction of element i, R is the gas constant; T is temperature, $^{xs}G_m^\phi$ is the excess Gibbs energy, expressed in the Redlich-Kister polynomial[31] as follows:

$$^{xs}G_m^\phi = \sum_i \sum_{j>i} x_i x_j \sum_{k=0} {}^kL_{i,j}^\phi (x_i - x_j)^k + x_i x_j x_k I_{i,j,k}^\phi \quad (3)$$

where $^kL_{i,j}^\phi$ is the kth binary interaction parameter between i and j, may depend on temperature in the form of $A+BT$, where A and B are model parameters to be evaluated. The ternary interaction parameter $I_{i,j,k}^\phi$ is assumed to be zero due to the

lack of experimental data in the ternary system.

The existence of limited homogeneity regions in the τ_1 and τ_2 phases was once reported but not verified in the subsequent investigations. Therefore, both the two phases are described by the stoichiometric compound model with formulae AlCaLi and Al_3Ca_2Li, respectively. It is noteworthy that such simplified treatment should not affect the phase equilibria in the Al-Ca-Li ternary system. The τ_3 phase with formula $Ca_6Al_{12}Li_{11}$ is also modeled as a stoichiometric compound in this ternary system. Based on the Kopp-Neumann rule[32], the Gibbs energy of formation of stoichiometric compound $Al_pCa_qLi_n$ can be described by

$$G_{Al_pCa_qLi_n} = p\,{}^0G_{Al}^{Fcc} + q\,{}^0G_{Ca}^{Fcc} + n\,{}^0G_{Li}^{Fcc} + \Delta H_f - \Delta S_f T \quad (4)$$

with formation enthalpy ΔH_f and formation entropy ΔS_f to be optimized *via* experimental phase equilibria information and ${}^0G_{Al}^{Fcc}$, ${}^0G_{Ca}^{Fcc}$, ${}^0G_{Li}^{Fcc}$ referred to the Gibbs free energies of pure elements Al, Ca and Li in stable Fcc phase, respectively.

4　Results and Discussion

In this section, several calculated results are first compared with the original experimental information to demonstrate the fine accuracy of the present calculation, and then other interesting results are also calculated in order to provide some instructions for researchers in the process of material design for the Al-Ca-Li system. All the calculations were carried out with the Pandat software[33].

Figs.1—3 present the calculated Ca-Li, Al-Li and Al-Ca phase diagrams *via* the thermodynamic descriptions of Gröbner *et al.*[11], Guo *et al.*[7] and Koray *et al.*[18] along with experimental data, respectively. The well consistency between calculated result and experimental point shows that the selected sets of thermodynamic parameters from these literatures are credible which can be safely extrapolated to the ternary Al-Ca-Li system.
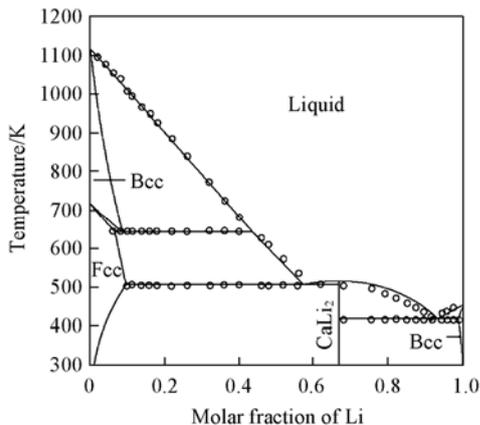

Fig.1　Ca-Li phase diagram calculated *via* the thermodynamic description from literature [11] along with experimental data

The thermodynamic optimization performed in this work is mainly focused on determining the formation enthalpies and entropies of the three ternary intermetallic phases(TTTIP), which are used to obtain their Gibbs free energies according to
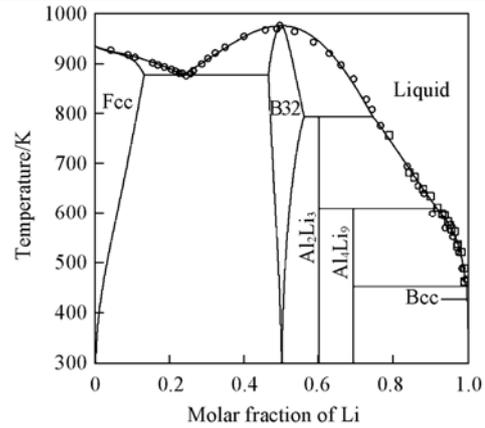

Fig.2　Al-Li phase diagram calculated *via* the thermodynamic description from literature [7] along with experimental data
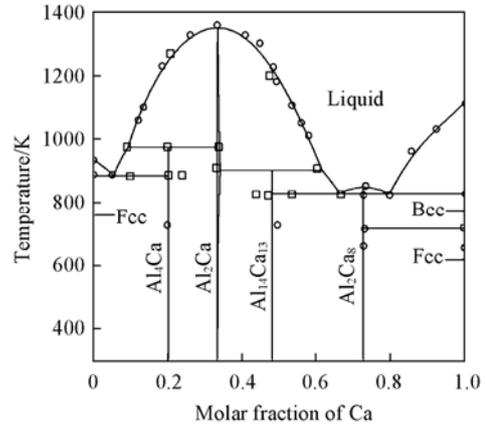

Fig.3　Al-Ca phase diagram calculated *via* the thermodynamic description from literature [18] along with experimental data

Eq.(4) in Section 3. The thermochemical data concerning TTTIP have been unavailable from the literature till now. Therefore, the formation enthalpies and entropies of TTTIP can only be optimized in terms of the reported phase equilibria in the Al-Ca-Li system. Fig.4 displays the isothermal section of the Al-Ca-Li system at room temperature constructed by Gröbner[29] with the critical review of all the reported experimental information. To completely calculate the phase relationships reflected in Fig.4, the thermodynamic database(tdb file) of this ternary system should be initially constructed. The model parameters of all the binary phases were directly introduced in the tdb file, and the three ternary solutions were thermodynamically modeled from immediate extrapolation of constituent binaries, then much attention has been paid to the thermodynamic optimization of TTTIP. The detailed optimization procedure by trials and errors can be conducted as follows: firstly the formation enthalpy of τ_3 phase was determined in order to keep it in direct equilibria with Li_2Ca, Li_9Al_4, Li_3Al_2 and $CaAl_2$ phases; secondly, the formation enthalpy of τ_1 phase was confirmed in order to reach the equilibria between τ_2 phase with τ_1, Li_2Ca and $Ca_{13}Al_{14}$ phases; thirdly, the similar parameter of τ_2 phase was also adjusted in order to form equilibria relationships between τ_2 phase with τ_1, τ_3, $CaAl_2$ and $Ca_{13}Al_{14}$ phases. Finally, for the purpose of keeping TTTIP instable

above 150 °C observed experimentally from Ganiev *et al.*[25—27], the formation entropy of them was assigned to −11.0 J·mol⁻¹·K⁻¹ per mole atom due to lack of additional experimental data. Table 2 lists the thermodynamic parameters assessed in this work.

calculated diagram(Fig.6), which is well consistent with the experimental observations[25—27] that no such phases were detected at that temperature.
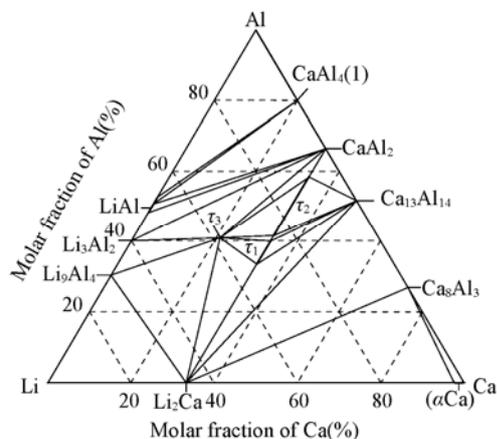

Fig.4   Isothermal sections of the Al-Ca-Li system at room temperature proposed by Gröbner[29]

Table 2   Enthalpy(J/mol) and entropy(J·mol⁻¹·K⁻¹) of formation of TTTIP obtained in the present work

AlCaLi(τ_1)		Al₃Ca₂Li(τ_2)		Al₁₂Ca₆Li₁₁(τ_3)	
$\Delta H_f^{\tau_1}$	$\Delta S_f^{\tau_1}$	$\Delta H_f^{\tau_2}$	$\Delta S_f^{\tau_2}$	$\Delta H_f^{\tau_3}$	$\Delta S_f^{\tau_3}$
−62150	−33.0	−165800	−66	−670700	−319

Based on the established thermodynamic database, the isothermal section of the Al-Ca-Li system at 300 K was calculated, as shown in Fig.5. It can be seen from Fig.5 that the calculated phase equilibria have shown noticeable agreement with the isothermal section reviewed by Gröbner[29] when the negligible homogeneity range was neglected in TTTIP. It should be noted that the model parameters have to be confirmed within an accuracy range of ±50 J per mole atom so as to keep the phase relationships in Fig.5 the same as those in Fig.4, otherwise the phase equilibria will be fragilely broken. It thus can reasonably explain the much discrepancy existed in most of the experiments carried out for the investigation of the phase equilibria because the accuracy range seems difficult to be reached in the course of practical measurement. With the temperature increasing to 423 K(150 °C), TTTIP disappeared in view of the
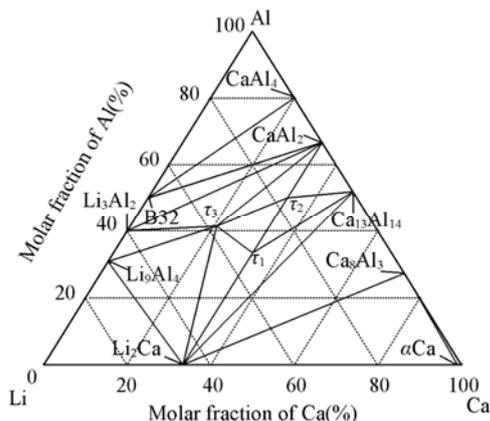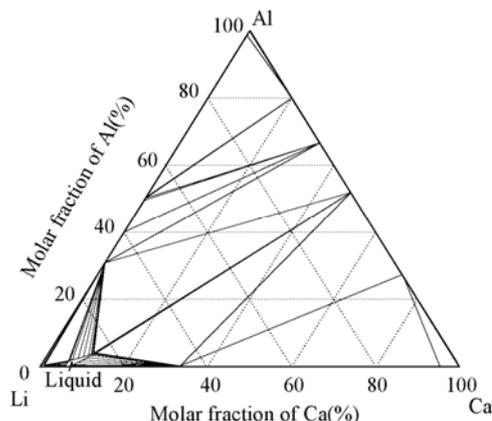

Fig.6   Isothermal sections of the Al-Ca-Li system at 423 K calculated in the present work

The calculated liquidus projection of the Al-Ca-Li ternary system is presented in Figs.7—9 with the primary phases formed from the liquid phase in the process of solidification. The dotted lines in Fig.7 are isotherms, with the numbers indicating the temperature in degree Kelvin. Fig.8 and Fig.9 show the liquidus projection of the Al-rich corner and Li-rich corner, respectively. It can be seen from these Figs. that there are a total of ten invariant reactions on the liquidus surface, with the phase compositions, temperatures and reaction types listed in Table 3. Of these ten reactions, three are eutectic reactions and the other seven are transition reactions labeled by capital E and U symbols in Table 3, respectively. An interesting isopleth section of the Al-Ca-Li system with the composition of 33%(molar fraction) Ca was also calculated *via* the present thermodynamic database, as shown in Fig.10. It is obvious that two compounds CaAl₂ and CaLi₂ cannot form a pseudo-binary phase diagram according to the phase rule in this Figure. Although there are no credible experimental data available to validate the calculated liquidus projection and isopleth section, the calculated diagrams can also serve as a guide to smartly design material compositions for future experimental investigation.
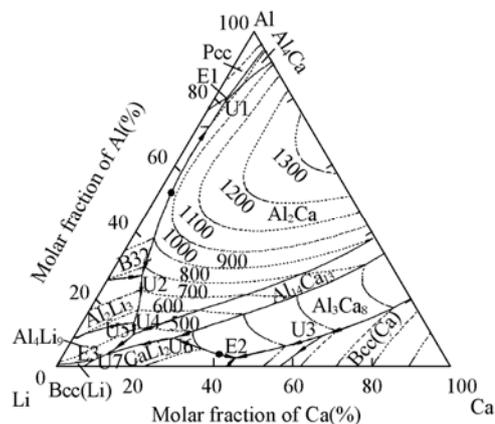

Fig.5   Isothermal sections of Al-Ca-Li system at 300 K calculated in the present work

Fig.7   Liquidus projection to the composition triangle in the Al-Ca-Li system with isotherms(dotted lines) superimposed and their temperatures
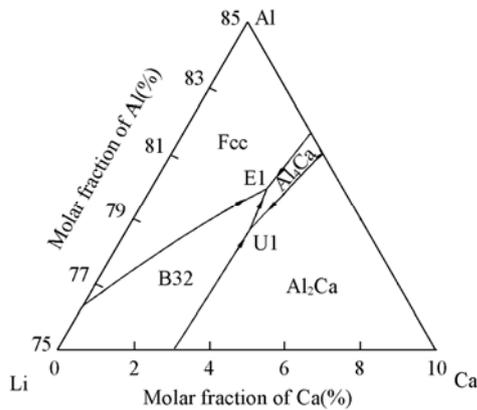The solid circles indicate the saddle points.
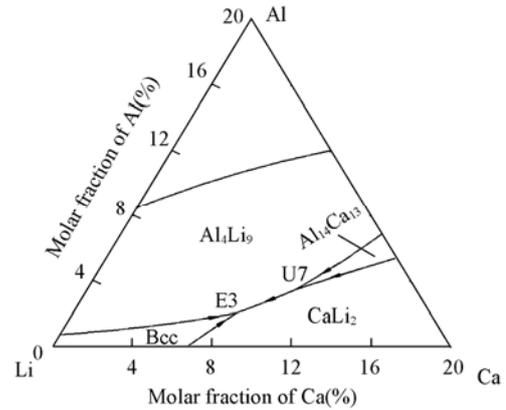
Fig.8 Liquidus projection of Al-rich corner

Fig.9 Liquidus projection of Li-rich corner

Table 3 Invariant reactions in the Al-Ca-Li system predicted in the present work

Reaction	Type	Temperature/K	Molar fraction of Li and Ca(%)							
			Phase 1		Phase 2		Phase 3		Phase 4	
Liquid+Al$_2$Ca⟶B32+Al$_4$Ca	U1	865.81	18.11	3.23	0	33.33	46.69	0	0	20
Liquid⟶B32+Al$_4$Ca+Fcc	E1	857.63	17.03	3.05	46.57	0	0	20	12.65	0
Liquid+B32⟶Al$_2$Ca+Al$_2$Li$_3$	U2	760.36	64.91	7.99	54.91	0	0	33.33	60.00	0
Liquid+Fcc⟶Bcc+Al$_3$Ca$_8$	U3	671.34	28.06	62.77	3.92	96.08	5.03	94.97	0	72.73
Liquid+Al$_2$Li$_3$⟶Al$_4$Li$_9$+ Al$_2$Ca	U4	535.05	73.94	12.98	60.00	0	69.23	0	0	33.33
Liquid⟶Fcc+Al$_3$Ca$_8$+CaLi$_2$	E2	499.27	53.45	44.02	9.10	90.90	0	72.73	66.67	33.33
Liquid+Al$_2$Ca⟶Al$_{14}$Ca$_{13}$+Al$_4$Li$_9$	U5	471.42	75.94	14.62	0	33.33	0	48.15	69.23	0
Liquid+Al$_3$Ca$_8$⟶CaLi$_2$+Al$_{14}$Ca$_{13}$	U6	468.17	66.04	25.47	0	72.73	66.67	33.33	0	48.15
Liquid+Al$_{14}$Ca$_{13}$⟶CaLi$_2$+ Al$_4$Li$_9$	U7	419.76	10.53	86.05	0	48.15	66.67	33.33	69.23	0
Liquid⟶CaLi$_2$+Al$_4$Li$_9$+Bcc	E3	412.54	89.78	8.23	66.67	33.33	69.23	0	98.62	1.15
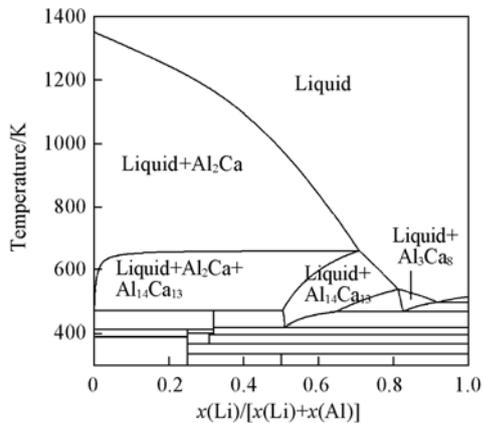
Fig.10 Calculated isopleth section along a composition of 33% Ca

functions of composition and temperature. With the present optimized parameters, the isopleth section along a composition of 33%(molar fraction) Ca and liquidus projection were predicted which can guide researchers to smartly design material compositions of practical interest.

5 Conclusions

In this work, the literature information regarding the three constituent binary systems was concisely reviewed in order to compile the optimum binary interaction parameters into the Al-Ca-Li ternary thermodynamic database. A tentative thermodynamic modeling has been applied to the three ternary intermetallic phases based upon the phase relations in the Al-Ca-Li system critically evaluated from the experimental information available in the literature. Such thermodynamic modeling has proved to be effective on the satisfactory consistency between the calculated phase diagram and the experimental information. Thus, a set of self-consistent thermodynamic parameters have been derived for describing the Gibbs energies of individual phases in the Al-Ca-Li system as the

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