

# Thermodynamic description of the Lu–Pb binary system

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**Abstract** The thermodynamic modeling of the Lu–Pb binary system was carried out with the help of CALPHAD (Calculation of PHase Diagram) method. The liquid phase has been described with the association solution model with “Lu<sub>5</sub>Pb<sub>3</sub>” as an associated complex. Lu<sub>5</sub>Pb<sub>3</sub>,  $\alpha$ -Lu<sub>5</sub>Pb<sub>4</sub>,  $\beta$ -Lu<sub>5</sub>Pb<sub>4</sub>, Lu<sub>6</sub>Pb<sub>5</sub>, and LuPb<sub>2</sub> have been treated as stoichiometric compounds, while a sublattice model has been used for the description of the HCP phase. The calculations based on the thermodynamic modeling are in good agreement with the phase diagram data and experimental thermodynamic values.

**Keywords** Lu–Pb system · Phase diagram · Thermodynamic description · Calphad method

## Introduction

This study is a part of a thermodynamic investigation of M–Pb systems (M = Yb [1], Ca [2], Ba [3]) already calculated in our laboratory which is intended to give a better understanding of the constitutional properties and potential technological applications of these alloys.

This study deals with an assessment of the thermodynamic description of the Lu–Pb system using the CALPHAD technique [4]. The thermodynamic parameters involved in the models are optimized from the experimental thermodynamic and phase diagram data.

## Review of experimental data

The assessed Lu–Pb phase diagram by Massalski [5] is based on the work of McMasters and Gschneidner [6] according to this assessment, four intermetallic compounds were reported (Lu<sub>5</sub>Pb<sub>3</sub>, Lu<sub>5</sub>Pb<sub>4</sub>, Lu<sub>6</sub>Pb<sub>5</sub>, and LuPb<sub>2</sub>). For the Lu<sub>5</sub>Pb<sub>3</sub> compound, a congruent melting was estimated at 1,968 K, while the LuPb<sub>2</sub>, Lu<sub>6</sub>Pb<sub>5</sub>, and Lu<sub>5</sub>Pb<sub>4</sub> ( $\alpha$  and  $\beta$ ) compounds, a peritectic formation was reported, respectively, at 843, 1443, and 1773 K. A polymorphic transition ( $\alpha \leftrightarrow \beta$ ) was determined at 1,748 K for Lu<sub>5</sub>Pb<sub>4</sub> (Fig. 1). The crystal structures of various phases are reported in Table 1.

Borzzone et al. [7] measured the standard enthalpy of formation of LuPb<sub>2</sub> using the differential calorimetry method. Colinet et al. [8] calculated the enthalpies of formation for three intermetallic compounds: LuPb<sub>2</sub>, Lu<sub>5</sub>Pb<sub>4</sub>, and Lu<sub>5</sub>Pb<sub>3</sub>. Borzzone et al. [7] measured also the molar heat capacities of the intermetallic compounds Lu<sub>5</sub>Pb<sub>3</sub> and Lu<sub>6</sub>Pb<sub>5</sub> in the range 523–823 K using the differential calorimetry method.

## Thermodynamic models

Pure elements

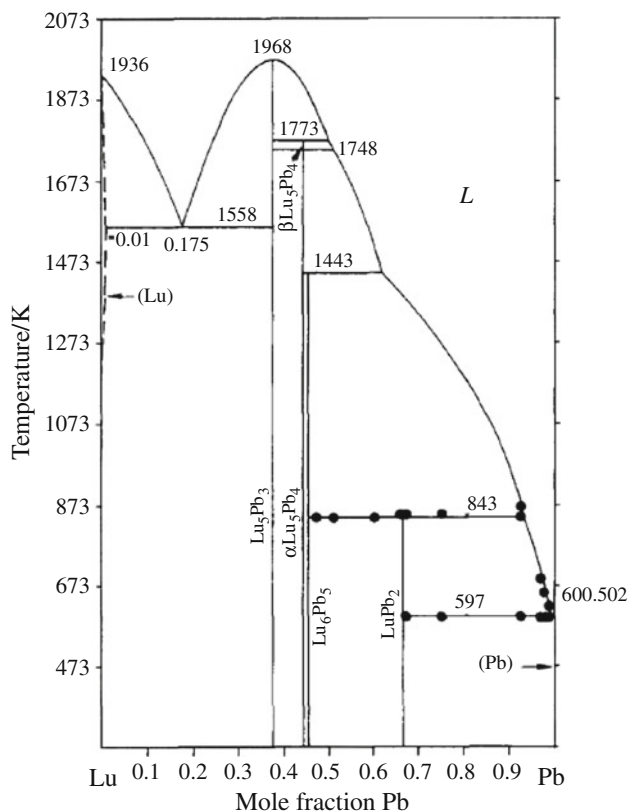
The Gibbs energy function

$$G_i^\varphi(T) = {}^0G_i^\varphi - H_i^{\text{SER}}(298.15\text{K}) \quad (1)$$

(298.15) for the element  $i$  ( $i = \text{Lu}, \text{Pb}$ ) in the phase  $\varphi$  ( $\varphi = \text{Liquid}, \text{HCP\_A3}, \text{or FCC\_A1}$ ) is described by an equation of the following form:

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

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**Fig. 1** Experimental Lu–Pb phase diagram previously published by McMasters et al. [6] (experimental data (solid circle) by Borzone et al. [7])

**Table 1** Symbols and crystal structures of the stable solid phases in the Lu–Pb system

Diagram symbol	Composition at.% Pb	Pearson symbol	Symbol used in thermo-calc data file	Prototype
Lu	0	hP2	HCP_A3	Mg
Lu <sub>5</sub> Pb <sub>3</sub>	37.5	hP16	Lu <sub>5</sub> Pb <sub>3</sub>	Mn <sub>5</sub> Si <sub>3</sub>
β-Lu <sub>5</sub> Pb <sub>4</sub>	44.4	–	Lu <sub>5</sub> Pb <sub>4</sub> -HT	–
α-Lu <sub>5</sub> Pb <sub>4</sub>	44.4	oP*	α-Lu <sub>5</sub> Pb <sub>4</sub> -BT	–
Lu <sub>6</sub> Pb <sub>5</sub>	45.4	oI44	Lu <sub>6</sub> Pb <sub>5</sub>	Ti <sub>6</sub> Ge <sub>5</sub>
LuPb <sub>2</sub>	66.7	tI6	LuPb <sub>2</sub>	MoSi <sub>2</sub>
LuPb <sub>3</sub>	75.0	cP4	–	AuCu <sub>3</sub>
Pb	100	cF4	FCC_A1	Cu

where  $H_i^{SER}(298.15\text{ K})$  is the molar enthalpy of the element  $i$  at 298.15 K in its standard element reference (SER) state, HCP\_A3 for Lu, and FCC\_A1 for Pb.

In this article, The Gibbs energy functions are taken from the SGTE compilation of Dinsdale [9].

### Liquid phase

The liquid phase has been described by the association model by Sommer [10]. The association model is based on the hypothesis that a C complex is formed in the liquid phase (where A and B are pure elements initially present in the mixing) as follows:  $pA + qB \leftrightarrow A_pB_q$  ( $A_pB_q$  corresponds to the C complex with  $p$  and  $q$ , the stoichiometric coefficients). Such a formation of C complex in the liquid phase can be suggested by the experimental enthalpies of formation of intermetallic phases which show a nearly triangular-shaped concentration dependence. As in the Yb–Pb [1] and Ca–Pb [2] systems, the compound which presents the highest melting point has been taken as the associated complex. In the Lu–Pb system, The Lu<sub>5</sub>Pb<sub>3</sub> is the most probable liquid-associated complex (C).

Therefore, the Gibbs energy of one mole of formula unit is expressed as the sum of four terms:

$$G^{Liq} - H^{SER} = {}^{ref}G^{Liq} + {}^{form}G^{Liq} + {}^{id}G^{Liq} + {}^{ex}G^{Liq} \quad (3)$$

In the following, we give briefly the equivalence between the formalism described by Sommer [10] and the different terms of Eq. 3 involved in thermocalc software.

$${}^{ref}G^{Liq} = \{x_{Lu} [{}^0G_{Lu}^{Liq}(T) - H_{Lu}^{SER}] + x_{Pb} [{}^0G_{Pb}^{Liq}(T) - H_{Pb}^{SER}]\} \times (y_{Lu} + (p + q)y_C + y_{Pb}) \quad (4)$$

$${}^{ref}G^{Liq} = \{x_{Lu} [{}^0G_{Lu}^{Liq}(T) - H_{Lu}^{SER}] + x_{Pb} [{}^0G_{Pb}^{Liq}(T) - H_{Pb}^{SER}]\} \times (1 + 7y_C)$$

$${}^{for}G_C^{Liq} = (y_{Lu} {}^0G_{Lu}^{Liq}(T)) + (y_{Pb} {}^0G_{Pb}^{Liq}(T)) + (y_C {}^0G_C^{Liq}(T)) \quad (5)$$

$${}^{id}G^{Liq} = RT(y_{Lu} \ln y_{Lu} + y_{Pb} \ln y_{Pb} + y_C \ln y_C) \quad (6)$$

where  $R$  is the perfect gas constant;  $T$  is the temperature.

The three species A, B, C in the liquid phase have  $y_{Lu}$ ,  $y_{Pb}$  and  $y_C$  as mole fractions, normalized to  $y_{Lu} + y_{Pb} + y_C = 1$ .  $x_A$  and  $x_B$  are the absolute mole fractions of two components A and B of the liquid, without considering the associated species, normalized to

$$x_A + x_B = 1.$$

For a regular liquid solution  $C_{Lu,Pb}^{reg}$ ,  $C_{Lu,Lu_5Pb_3}^{reg}$ , and  $C_{Pb,Lu_5Pb_3}^{reg}$  are, respectively, equal to the  ${}^0L_{Lu,Pb}^{Liq}$ ,  ${}^0L_{Lu,Lu_5Pb_3}^{Liq}$  and  ${}^0L_{Pb,Lu_5Pb_3}^{Liq}$  terms of the Redlich–Kister polynomial [11] of the  ${}^{ex}G^{Liq}$  energy part in Eq. 3:

$${}^{ex}G^{Liq} = y_i y_j \sum_{v=0}^v L_{ij}^{Liq} (y_i - y_j)^v \quad (7)$$

where  $i$  and  $j$  are indices which correspond to the three species Lu, Pb, and Lu<sub>5</sub>Pb<sub>3</sub>.

The binary interaction parameters of the  ${}^0L_{ij}^{\text{Liq}}$  type, evaluated in the present work, were temperature dependent as follows:

$${}^0L_{ij}^{\text{Liq}} = a_0 + b_0T \tag{8}$$

$a_0$  and  $b_0$  are the coefficients to be optimized.

**Stoichiometric compounds**

The Gibbs energy of the stoichiometric compounds  $A_pB_q$  is expressed as follows:

$${}^0G_{A_pB_q} = \frac{p}{p+q} {}^0G_A + \frac{q}{p+q} {}^0G_B + a + bT \tag{9}$$

where  ${}^0G_A$  and  ${}^0G_B$  are the Gibbs energy of the pure elements Lu and Pb, respectively,  $a$  and  $b$  are parameters to be determined.

**Solid solution**

The solution phase (HCP\_A3) was modeled as substitution solution. The Gibbs energy of 1 mol of formula unit of phase  $\varphi$  is expressed as the sum of the reference part  ${}^{\text{ref}}G^\varphi$ , the ideal part  ${}^{\text{id}}G^\varphi$ , and the excess part  ${}^{\text{exc}}G^\varphi$ :

$$G_m^\varphi = {}^{\text{ref}}G^\varphi + {}^{\text{id}}G^\varphi + {}^{\text{exc}}G^\varphi \tag{10}$$

As used in the thermo-calc software [12]:

$${}^{\text{ref}}G^\varphi(T) = ({}^0G_{\text{Lu}}^\varphi(T) - H_{\text{Lu}}^{\text{SER}}(298.15\text{ K}))x_{\text{Lu}} + ({}^0G_{\text{Pb}}^\varphi(T) - H_{\text{Pb}}^{\text{SER}}(298.15\text{ K}))x_{\text{Pb}} \tag{11}$$

$${}^{\text{id}}G^\varphi = RT(x_{\text{Lu}}\ln x_{\text{Lu}} + x_{\text{Pb}}\ln x_{\text{Pb}}) \tag{12}$$

where  $R$  is the gas constant,  $T$  the temperature, in Kelvin,  $x_{\text{Lu}}$  and  $x_{\text{Pb}}$  are the fraction of elements Lu and Pb, respectively.

The excess terms of all the solution phases were modeled by the Redlich–Kister [11] formula:

$${}^{\text{exc}}G_m^\varphi(T) = x_{\text{Lu}}x_{\text{Pb}}[{}^0L_{\text{Lu,Pb}}^\varphi(T) + {}^1L_{\text{Lu,Pb}}^\varphi(T)(x_{\text{Lu}} - x_{\text{Pb}}) + {}^2L_{\text{Lu,Pb}}^\varphi(T)(x_{\text{Lu}} - x_{\text{Pb}})^2 + \dots] \tag{13}$$

$${}^iL_{\text{Lu,Pb}}^\varphi(T) = a_i + b_iT \tag{14}$$

where  ${}^iL_{\text{Lu,Pb}}^\varphi(T)$  is the interaction parameter between the elements Lu and Pb, which is evaluated in the presented work,  $a_i$  and  $b_i$  are the coefficients to be optimized.

**Results and discussions**

The thermodynamic parameters for different phases were evaluated with the PARROT [13] module in Thermo-Calc software [12], which is based on the minimization of the error norm formed by the discrepancy between the calculated and experimentally measured quantities. Many kinds of experimental data can be taken into one optimization,

**Table 2** The optimized thermodynamic parameters of the Lu–Pb system

Phase	Thermodynamic models	Parameters in Pb
Liquid	(Lu, Pb, Lu <sub>5</sub> Pb <sub>3</sub> ) <sub>1</sub>	${}^0G_{\text{Lu}_5\text{Pb}_3}^{\text{Liq}} - 3{}^{298}H_{\text{Pb}}^{\text{FCC}_A1} - 5{}^{298}H_{\text{Lu}}^{\text{HCP}} = 17544179.5 + 218.347405T$ $+ 5G_{\text{Lu}}^{\text{Liq}} + 3G_{\text{Pb}}^{\text{Liq}}$ ${}^0L_{\text{Pb,Lu}}^{\text{Liq}} = -60990.839 - 25.9125471T$ ${}^0L_{\text{Lu,Lu}_5\text{Pb}_3}^{\text{Liq}} = 15498123 - 88.99091T$ ${}^0L_{\text{Pb,Lu}_5\text{Pb}_3}^{\text{Liq}} = -412088.971 + 917.48740T$
FCC_A1	(Lu, Pb)1(Va) <sub>1</sub>	No excess term
HCP_A3	(Lu, Pb)1(Va) <sub>5</sub>	${}^0L^{\text{HCP}_A3} = -56540.1798 + 0.776823002T$
Lu <sub>5</sub> Pb <sub>3</sub>	(Lu) <sub>0.625</sub> :(Pb) <sub>0.375</sub>	$G_{\text{Lu:Pb}}^{\text{Lu}_5\text{Pb}_3} - 0.375{}^{298}H_{\text{Pb}}^{\text{FCC}_A1} - 0.625{}^{298}H_{\text{Lu}}^{\text{HCP}_A3}$ $= 0.375{}^{298}G_{\text{Pb}}^{\text{FCC}_A1} + 0.625{}^{298}G_{\text{Lu}}^{\text{HCP}_A3} - 40636.333 - 0.38140463$
$\alpha$ Lu <sub>5</sub> Pb <sub>4</sub>	(Lu) <sub>0.555</sub> :(Pb) <sub>0.445</sub>	$G_{\text{Lu:Pb}}^{\alpha\text{Lu}_5\text{Pb}_4} - 0.445{}^{298}H_{\text{Pb}}^{\text{FCC}_A1} - 0.555{}^{298}H_{\text{Lu}}^{\text{HCP}_A3}$ $= 0.445{}^{298}G_{\text{Pb}}^{\text{FCC}_A1} + 0.555{}^{298}G_{\text{Lu}}^{\text{HCP}_A3} - 47455.3241 + 3.52126569T$
$\beta$ Lu <sub>5</sub> Pb <sub>4</sub>	(Lu) <sub>0.555</sub> :(Pb) <sub>0.445</sub>	$G_{\text{Lu:Pb}}^{\beta\text{Lu}_5\text{Pb}_4} - 0.445{}^{298}H_{\text{Pb}}^{\text{FCC}_A1} - 0.555{}^{298}H_{\text{Lu}}^{\text{HCP}_A3}$ $= 0.445{}^{298}G_{\text{Pb}}^{\text{FCC}_A1} + 0.555{}^{298}G_{\text{Lu}}^{\text{HCP}_A3} - 46211.1586 + 2.81012884T$
Lu <sub>6</sub> Pb <sub>5</sub>	(Lu) <sub>0.545</sub> :(Pb) <sub>0.455</sub>	$G_{\text{Lu:Pb}}^{\text{Lu}_6\text{Pb}_5} - 0.455{}^{298}H_{\text{Pb}}^{\text{FCC}_A1} - 0.545{}^{298}H_{\text{Lu}}^{\text{HCP}_A3}$ $= 0.455{}^{298}G_{\text{Pb}}^{\text{FCC}_A1} + 0.545{}^{298}G_{\text{Lu}}^{\text{HCP}_A3} - 47864.3233 + 4.10175426T$
LuPb <sub>2</sub>	(Lu) <sub>0.333</sub> :(Pb) <sub>0.667</sub>	$G_{\text{Lu:Pb}}^{\text{LuPb}_2} - 0.667{}^{298}H_{\text{Pb}}^{\text{FCC}_A1} - 0.333{}^{298}H_{\text{Lu}}^{\text{HCP}_A3}$ $= 0.667{}^{298}G_{\text{Pb}}^{\text{FCC}_A1} + 0.333{}^{298}G_{\text{Lu}}^{\text{HCP}_A3} - 34448.9925 + 7.24254526T$

where different weight can be assigned to different data from the uncertainties in the original publications and upon the user’s judgment. The optimization results strongly depend on the model selected for a certain phase and the number of parameters used for that phase. In the present parameter optimization procedure, we first imposed the conditions  $d^2G/dx^2 > 0$  for modeling the liquid phase using the phase boundary data reported by Massalski [5] and

thermodynamic data. The optimization procedure was the following steps. The thermodynamic parameters of the associate liquid complex are optimized first.

In the second step, we determine the excess terms  ${}^0L_{Lu,Pb}^{Liq}$ ,  ${}^0L_{Lu,Lu_5Pb_3}^{Liq}$ , and  ${}^0L_{Pb,Lu_5Pb_3}^{Liq}$  which describe the interaction of the free atoms Lu and Pb with the  $Lu_5Pb_3$  associates. For all the intermetallic compounds ( $Lu_5Pb_3$ ,  $\alpha-Lu_5Pb_4$ ,  $\beta-Lu_5Pb_4$ ,  $Lu_6Pb_5$ , and  $LuPb_2$ ), the coefficients  $a$  and  $b$  in Eq. 9, were adjusted according to the enthalpies of formation evaluated by [7] and calculated in [8]. Finally, the ( $\alpha \leftrightarrow \beta$ ) polymorphic transformation of  $Lu_5Pb_4$  was the last to be optimized. All the calculated parameters are listed in Table 2.

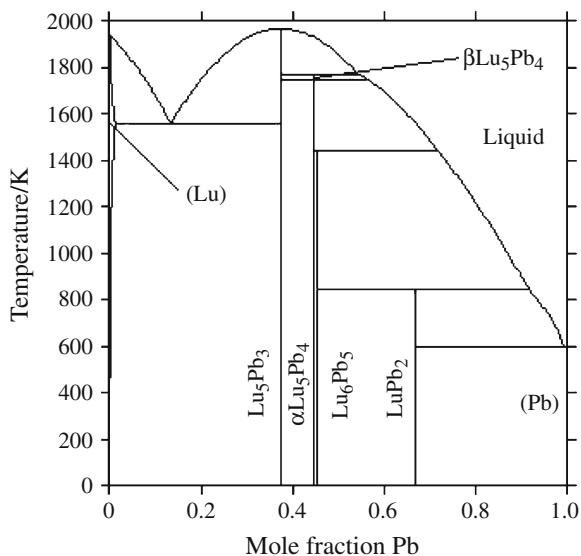


Fig. 2 Calculated Lu–Pb phase diagram

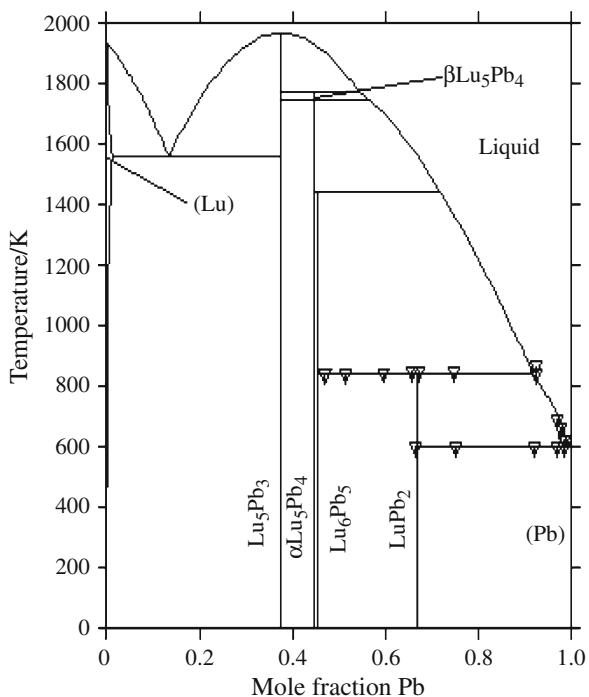


Fig. 3 Comparison of the calculated phase boundaries with reported experimental data (open inverted triangle) by Borzone et al. [7]

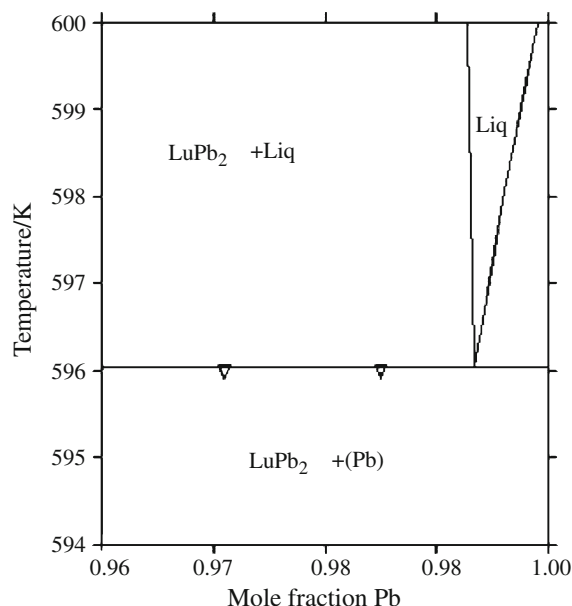
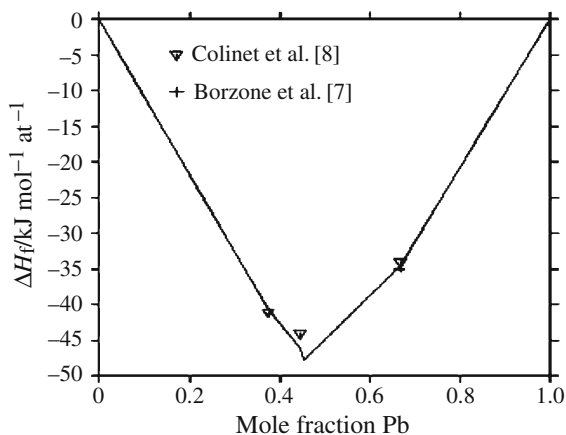


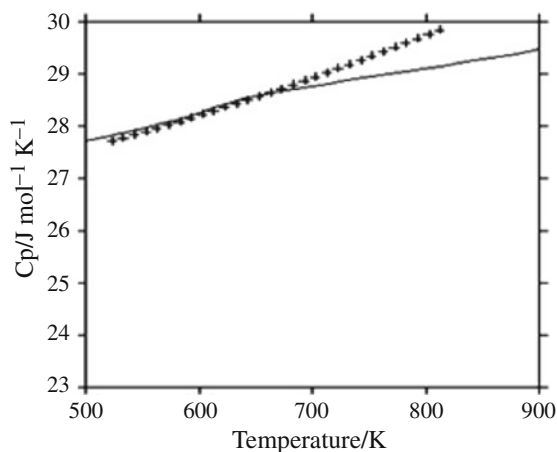
Fig. 4 Enlarged part on the Pb-rich Lu–Pb eutectic region (open inverted triangle), Experimental data of Borzone et al. [7]

Table 3 Invariant reactions in the Lu–Pb system

Reaction	McMasters et al. [6]		This work	
	T/K	$x_{liq}/at.\% Pb$	T/K	$x_{liq}/at.\% Pb$
Liq $\leftrightarrow$ $Lu_5Pb_3$ + (Lu)	1558	Liq 0.175	1558	Liq 0.134
Liq $\leftrightarrow$ $Lu_5Pb_3$	1968	(Lu) 0.01	1967	(Lu) 0.011
Liq + $Lu_5Pb_3 \leftrightarrow \beta-Lu_5Pb_4$	1773	Liq 0.49	1773	Liq 0.544
$\alpha-Lu_5Pb_4 \leftrightarrow \beta-Lu_5Pb_4$	1748	Liq 0.51	1750	Liq 0.563
Liq + $Lu_5Pb_3 \leftrightarrow \alpha-Lu_5Pb_4$	1748	Liq 0.62	1750	Liq 0.718
Liq + $\alpha-Lu_5Pb_4 \leftrightarrow Lu_6Pb_5$	1443	Liq 0.92	1443	Liq 0.918
Liq + $Lu_6Pb_5 \leftrightarrow LuPb_2$	843	Liq 0.995	843	Liq 0.993
Liq $\leftrightarrow$ $LuPb_2$ + (pb)	597	(Pb) 0.999	596	(Pb) 1



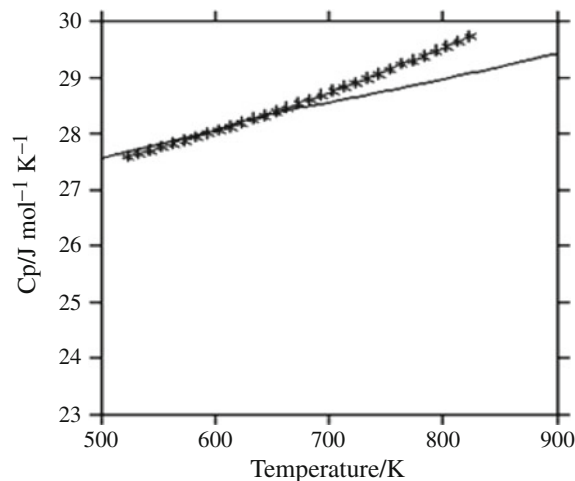
**Fig. 5** Calculated and measured enthalpies of formation of the intermetallic compounds



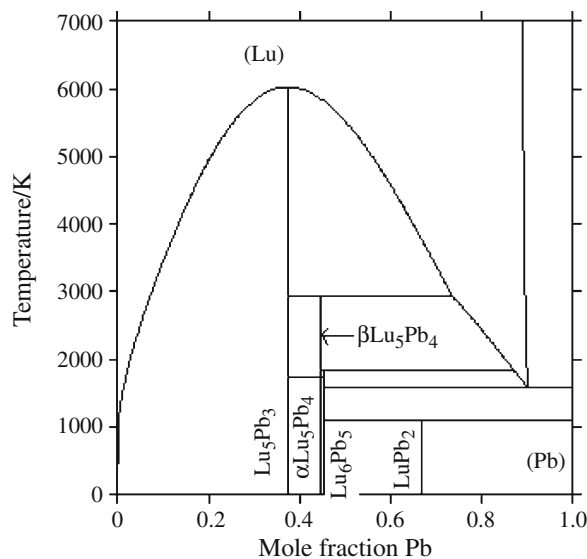
**Fig. 6** Calculated molar heat capacity of  $\text{Lu}_5\text{Pb}_3$  compared with the experimental data of Borzone et al. [8]

The Lu–Pb phase diagram calculated from our optimized thermodynamic parameters is plotted in Fig. 2. It is compared with the numerous experimental data in Fig. 3. A satisfactory agreement is noted. The Pb-Rich Lu–Pb eutectic region is drawn in Fig. 4. The temperature of this  $\text{Liq} \leftrightarrow \text{LuPb}_2 + \text{Pb}$  eutectic reaction is found to occur at 596 K, and is therefore, in very good agreement with that of [7]. The calculated invariant reactions of the Lu–Pb system are listed in Table 3 and compared with the experimental results by [6].

The optimized temperature of the polymorphic transition  $\text{Lu}_5\text{Pb}_4$  is in agreement with the experimental data of [6]. The enthalpies of formation of the two polytypes,  $\alpha\text{-Lu}_5\text{Pb}_4$  and  $\beta\text{-Lu}_5\text{Pb}_4$ , are very similar and confirm the conclusion by Stein et al. [14] concerning the small structural energies of the different laves phases polytypes. The measured and calculated enthalpies of formation of the intermetallic compounds are collected in Fig. 5. They are in reasonable agreement. Figures 6 and 7 show the



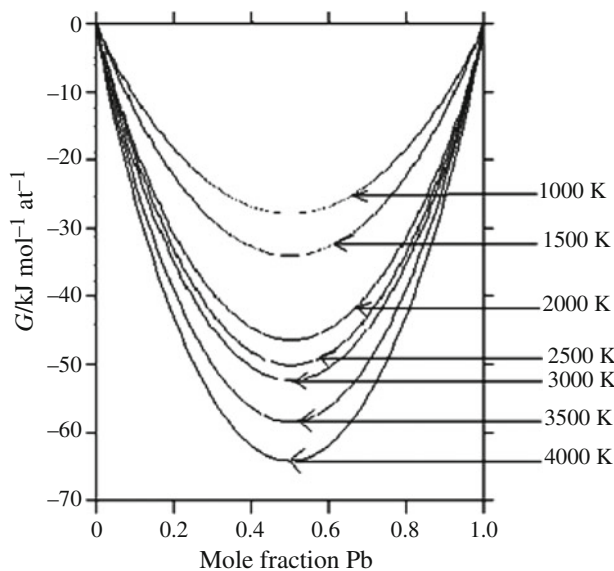
**Fig. 7** Calculated molar heat capacity of  $\text{Lu}_6\text{Pb}_5$  compared with the experimental data of Borzone et al. [8]



**Fig. 8** Calculated Lu–Pb phase diagram when the liquid phase is suspended

calculated molar heat capacity of  $\text{Lu}_5\text{Pb}_3$  and  $\text{Lu}_6\text{Pb}_5$  as function of temperature with data from the literature [7]. The calculated values are in good agreement with the experimental results in the range 523–663 K but deviate at about 2% from the measured values [7] in the range 663–823 K.

As mentioned by [15], in order to check that the optimized thermodynamic parameters of the intermetallic compounds are satisfactory, we verified that, when the liquid phase is suspended during the calculation of the Lu–Pb phase diagram, the stoichiometric phases disappear at high temperatures. A terminal solid solutions and a two-phase domain existing between them are found to be stable (Fig. 8). The calculated entropies of formation are



**Fig. 9** Gibbs energy of mixing of the liquid phase at different temperature. The reference states were Lu and Pb liquids

reasonable and negative for  $\text{Lu}_5\text{Pb}_4$ ,  $\text{Lu}_6\text{Pb}_5$ , and  $\text{LuPb}_2$  and is positive but low for  $\text{Lu}_5\text{Pb}_3$ .

The evolutions of Gibbs energy for the liquid phase as a function of temperature ( $T$ ) are shown in Fig. 9. With our optimization, when  $T$  is increasing up to 4,000 K, the Gibbs energy for the liquid phase decreases.

## Conclusions

The phase diagram of the Lu–Pb binary system has been optimized based on the experimental data and phase diagram data from literature. A set of self-consistent thermodynamic parameters have been obtained, which can reasonably reproduce the experimental and thermodynamic data.

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