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Thermodynamic description of the binary Ag–Ga system

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ABSTRACT

The $AgGaSe_2$ as well as $AgGaS_2$ has been showed to be efficient frequency doubling crystals for infrared radiation such as the 10.6 μm CO_2 laser. The production of these crystals needs good knowledge of the phase relationship. The thermodynamic description of the binary Ag–Ga system has been chosen as a first step for the description of the Ag–Ga–Se and Ag–Ga–S systems. The Calphad approach has been used for this modeling. Good agreement between experimental data and calculated values has been found.

1. Introduction

The $AgGaSe_2$ as well as $AgGaS_2$ has been showed to be efficient frequency doubling crystals for infrared radiation such as the 10.6 μm CO_2 laser [1]. The production of these crystals needs a good knowledge about the phase relationship. For the description of the phase equilibrium in both cases: Ag–Ga–Se and Ag–Ga–S it is necessary to know the phase diagram of the Ag–Ga binary system. In this case, the optimization of thermodynamic parameters of the binary Ag–Ga phase diagram has been choosing as a first step of the thermodynamic evaluation of the Ag–Ga–Se and the Ag–Ga–S systems.

2. Literature information

The thermodynamic properties of the liquid phase using electromotive force (EMF) measurement have been investigated by Danilin and Yatsenko [2] at 980 K, Predel and Schallner [3] at 1000 K and Jendrzejczyk-Handzlik and Fitzner [4] at 973 K. Besides EMF measurements, the activities of silver and gallium were measured by Qi et al. [5] at 1200 K by Knudsen effusion method. The experimental data sets described activities of the elements are in good agreement with one another. The enthalpy of mixing of the liquid phase was investigated by Predel and Stein [6] at 1323 K, Itagaki and Yazawa [7] at 1243 K, Jendrzejczyk-Handzlik and Fitzner [4] at 1128 and 925 K, Beja [8] at 980 and Beja and Laffite [9] 773 K. The enthalpy of mixing of the liquid phase is strong dependent on temperature. The information about enthalpy of mixing agrees well one another except Itagaki and Yazawa [7] data which seems to be not negative enough. The liquidus and the solidus were measured by Hume-Rothery and Andrews [10], Hume-Rothery et al. [11], Predel and Stein [12], Weibke and Wiegles [13], Gunneas et al. [14], Zhang et al. [15], Feschotte and Bass [16], Muller and Merl [17]. All the information provided by these references agrees well one another. Besides the solidus–liquidus information, phase equilibria in solid state were measured by Hume-Rothery and Andrews [10,18], Predel and Stein [12], Feschotte and Bass [16], Zhang et al. [15]. The invariant reactions temperatures were measured by Predel and Stein [12], Feschotte and Brass [16], Owen and Rowlands [19] and Weibke and Wiegles [13]. The investigations of the thermodynamic properties of the solid phases are very rare. Enthalpy of formation of the HCP_A3 and ζ′ (ordered HCP) phases were measured by calorimetric method at 864 and at 746 K, respectively, by Predel and Stein [12]. The chemical potential of Ga in the FCC_A1 phase was determined by Predel and Schallner [20] at 1000 K and Danilin and Yatsenko [2] at 980 K. The available data do not agree each other and the difference between them is equal 40,000 [J] for concentration of Ga equal 0.1 mole fraction. The information about the crystal structures of the phases in the Ag–Ga binary system is gathered in Table 1. The literature information reveals some inconsistency about ζ′ (ordered HCP) and Ag_2Ga_3 phases. The phase ζ′ (ordered HCP) has been described at the beginning as an isostructural with ζ AgZn phase (space group $P\overline{3}$) by Hume-Rothery and Andrews [10] and Moeller [21]. However, recent investigation by XRD technique done by Gunneas et al. [14] and Zhang et al. [15] sug-

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Table 1
Crystal structures of the phases in the Ag–Ga binary system.

Phase	Strukturbericht designation	Pearson symbol	Space group
FCC_A1 (Ag)	A1	cF4	$Fm\bar{3}m$
HCP_A3	A3	hP2	$P6_3/mmc$
ζ' (HCP_ORD)	C22	hP9	$P\bar{6}2m$
Ag_3Ga_2	...	...	...
Orthorhombic_Ga (Ga)	A11	oC8	$Cmca$

gests the space group $P\bar{6}2m$. The difference between these works is that Gunneas et al. [14] explained the homogeneity range of this phase by anti-site Ag atoms and vacancies on the Ga sublattice when Zhang et al. [15] used only anti-site atoms on the Ga sublattice. The intermetallic compound which exists between ζ' (ordered HCP) and Ga has been described as AgGa by Feschotte and Bass [16] what was adopted by Okamoto [22] in his evaluation of the phase diagram of the Ag–Ga binary system. The crystal structure of the AgGa was reported as $Im\bar{3}m$ (BCC_A2). The latest work done by Zhang et al. [23] described this intermetallic compound as Ag_3Ga_2 with a hexagonal structure. There is no further information about a space group in that work [23]. Thermodynamic optimization of the system Ag–Ga has been done by Zhang et al. [24]. They used an associated liquid solution model [25] for describing the liquid phase and two-sublattice compound energy model (Ag)2:(Ga,Ag)1 for describing ζ' phase. The available literature information about the Ag–Ga system is collected in Landolt–Bornstein database [26].

3. Thermodynamic models

The binary Ag-Ga system includes 5 phases: FCC_A1 (Ag), Orthorhombic_GA (Ga), ζ (HCP_A3), ζ' (ordered HCP), Ag_3Ga_2 and liquid. The description of the crystal structures is given in Table 1. The system shows 3 invariant reactions: eutectic reaction between liquid, solid Ga and intermetallic compound Ag_3Ga_2 at temperature 299 K and 2 peritectic reactions: one between Ag, liquid and ζ phase at 886 K and another between liquid, Ag_3Ga_2 and ζ' at 575 K. The temperature of the order–disorder transformation of the HCP phase is 708 K [27].

The Gibbs free energies of pure elements with respect to temperature ${}^0G_i(T) = G_i(T) - H_i^{SER}$ are represented by Eq. (1):

$$ {}^0G_i(T) = a + bT + cT\ \ln(T) + dT^2 + eT^{-1} + fT^3 + iT^4 + jT^7 + kT^{-9} \quad (1) $$

The ${}^0G_i(T)$ data are referred to the constant enthalpy value of the standard element reference H_i^{SER} at 298.15 K and 1 bar as recommended by Scientific Group Thermodata Europe (SGTE) [28]. The reference states are FCC_A1 (Ag) and Orthorhombic_GA (Ga). The ${}^0G_i(T)$ expression may be given for several temperature ranges, where the coefficients $a, b, c, d, e, f, i, j, k$ have different values. The ${}^0G_i(T)$ functions are taken from SGTE Unary (Pure elements) TDB v.4 [28].

The solid Ga was treated as a pure component because there is no information about solubility of Ag in solid gallium. In this case, the Gibbs energy of Ga in Orthorhombic_GA structure was directly taken from the SGTE Unary database [28].

3.1. Intermetallic compound Ag_3Ga_2

The Ag_3Ga_2 phase was treated as the line compound because the homogeneity range of it is negligible. In this case, the Gibbs energy is described as follows:

$$ G^0_{Ag_3Ga_2} = a + bT + 3 \cdot \mathrm{GHSERAG} + 2 \cdot \mathrm{GHSERGA} \quad (2) $$

where GHSERAG and GHSERGA are Gibbs energies of silver and gallium in FCC_A1 and Orthorhombic_GA structures, respectively.

3.2. Substitutional solutions

Solid and liquid solution phases (Liquid, FCC_A1 (Ag), ζ (HCP_A3)) were described by the substitutional solution model [29]:

$$ G_m(T) = \sum_i x_i {}^0G_i(T) + RT \sum_i x_i\ \ln(x_i) + \sum_i \sum_{j>i} x_i x_j \left(\sum_\nu {}^\nu L_{ij} (x_i - x_j)^\nu \right) \quad (3) $$

where the $\sum_i \sum_{j>i} x_i x_j \left(\sum_\nu {}^\nu L_{ij} (x_i - x_j)^\nu \right)$ part is the Redlich–Kister polynomial for excess Gibbs free energy.

3.3. ζ' (ordered HCP_A3)

The crystal structure of the ζ' has been described by Gunneas et al. [14] and Zhang et al. [15]. In agreement with the Gunneas description of ζ' phase, the Ga sublattice can be occupied by Ga and Ag atoms as well as by vacancies. In this case the two-sublatice model (Ag)2:(Ga,Ag,Va)1 has been applied in this optimization. The Gibbs energy of the ζ' (HCP_A3) is described as follows:

$$ G_m^{HCP\_ORD}(T) = Y^I_{Ag} Y^{II}_{Ga} {}^\circ G^\gamma_{Ag:Ga} + Y^I_{Ag} Y^{II}_{Ag} {}^\circ G^\gamma_{Ag:Ag} + Y^I_{Ag} Y^{II}_{Va} {}^\circ G^\gamma_{Ag:Va} + RT(Y^{II}_{Ga}\ \ln Y^{II}_{Ga} + Y^{II}_{Ag}\ \ln Y^{II}_{Ag} + Y^{II}_{Va}\ \ln Y^{II}_{Va}) + {}^{xs}G^\gamma_m \quad (4) $$

where ${}^{xs}G_m^{HCP\_ORD}$ represents excess Gibbs free energy:

$$ {}^{xs}G_m^{HCP\_ORD} = Y^I_{Ag} Y^{II}_{Ga} Y^{II}_{Ag} L^{HCP\_ORD}_{Ag:Ga,Ag} + Y^I_{Ag} Y^{II}_{Ga} Y^{II}_{Va} L^{HCP\_ORD}_{Ag:Ga,Va} + Y^I_{Ag} Y^{II}_{Ag} Y^{II}_{Va} L^{HCP\_ORD}_{Ag:Ag,Va} \quad (5) $$

in which Y_i^N denotes the site fraction of element i on sublattice N, symbol ":" indicates separation of elements on the different sublattices, and "," indicates separation of elements on the same sublattice.

4. Optimization procedure

The thermodynamic parameters for all phases in the system were optimized using ThermoCalc software [30]. For this optimization, thermodynamic data for the liquid phase, invariant reactions and phase equilibrium data were used. To each piece of the selected information was given a certain weight based on personal judgment. The optimization was carried out step by step in agreement with Schmid-Fetzer et al.'s [31] guideline. First, the optimization of the liquid phase was performed, and then the solid phases were assessed. All parameters were finally evaluated together to provide the best description of the system. The calculated interaction parameters are shown in Table 2. For checking of the results of optimization the system was also calculated using Pandat software [32].

5. Results and discussion

The set of parameters obtained during the optimization is collected in Table 2. The calculated phase diagram superimposed with experimental data obtained by Feschotte and Bass [16], Hume-Rothery and Andrews [10,18], Predel and Stein [12], Weibke and Wiegles [13], Muller and Merl [17] and Zhang et al. [15] is shown in Fig. 1. As can be seen from this figure calculated phase diagram is in very good agreement with the experimental data. However,

Table 2
Gibbs free energies of the phases in the A–Ga binary system.

Phase	T	Function
Liquid	$298.15 < T < 1234.93$	$G_{\mathrm{Ag}}^{\mathrm{Liquid}} = +3815.564 + 109.310993 \ast T - 23.8463314 \ast T \ast LN(T) - .001790585 \ast T \ast\ast 2 - 3.98587\mathrm{E} - 07 \ast T \ast\ast 3 - 12011 \ast T \ast\ast(-1) - 1.033905\mathrm{E} - 20 \ast T \ast\ast 7$
	$1234.93 < T < 3000$	$G_{\mathrm{Ag}}^{\mathrm{Liquid}} = -3587.111 + 180.964656 \ast T - 33.472 \ast T \ast LN(T)$
	$200 < T < 302.91$	$G_{\mathrm{Ga}}^{\mathrm{Liquid}} = -15821.033 + 567.189696 \ast T - 108.228783 \ast T \ast LN(T) + .227155636 \ast T \ast\ast 2 - 1.18575257\mathrm{E} - 04 \ast T \ast\ast 3 + 439954 \ast T \ast\ast(-1) - 7.0171\mathrm{E} - 17 \ast T \ast\ast 7$
	$302.91 < T < 4000$	$G_{\mathrm{Ga}}^{\mathrm{Liquid}} = -1389.188 + 114.049043 \ast T - 26.0692906 \ast T \ast LN(T) + 1.506\mathrm{E} - 04 \ast T \ast\ast 2 - 4.0173\mathrm{E} - 08 \ast T \ast\ast 3 - 118332 \ast T \ast\ast(-1)$
	$298.15 < T < 2000$	${}^{0}L_{\mathrm{Ag,Ga}}^{\mathrm{Liquid}} = -1.96437987\mathrm{E} + 04 + 6.36589658\mathrm{E} + 01 \ast T - 8.62025618\mathrm{E} + 00 \ast T \ast LN(T)$
	$298.15 < T < 2000$	${}^{1}L_{\mathrm{Ag,Ga}}^{\mathrm{Liquid}} = -3.87477601\mathrm{E} + 04 + 1.40716275\mathrm{E} + 02 \ast T - 1.61115178\mathrm{E} + 01 \ast T \ast LN(T)$
	$298.15 < T < 2000$	${}^{2}L_{\mathrm{Ag,Ga}}^{\mathrm{Liquid}} = -2.57456828\mathrm{E} + 04 + 1.40455355\mathrm{E} + 02 \ast T - 1.74166652\mathrm{E} + 01 \ast T \ast LN(T)$
FCC_A1 (Ag)		$G_{\mathrm{Ag}}^{\mathrm{FCC\_A1}} = \mathrm{GHSERAG}$
	$200 < T < 302.91$	$G_{\mathrm{Ga}}^{\mathrm{FCC\_A1}} = -17512.331 + 575.063691 \ast T - 108.228783 \ast T \ast LN(T) + .227155636 \ast T \ast\ast 2 - 1.18575257\mathrm{E} - 04 \ast T \ast\ast 3 + 439954 \ast T \ast\ast(-1)$
	$302.91 < T < 4000$	$G_{\mathrm{Ga}}^{\mathrm{FCC\_A1}} = -3255.643 + 122.53019 \ast T - 26.0692906 \ast T \ast LN(T) + 1.506\mathrm{E} - 04 \ast T \ast\ast 2 - 4.0173\mathrm{E} - 08 \ast T \ast\ast 3 - 118332 \ast T \ast\ast(-1) + 1.64547E + 23 \ast T \ast\ast(-9)$
	$298.15 < T < 2000$	${}^{0}L_{\mathrm{Ag,Ga}}^{\mathrm{FCC\_A1}} = -1.98540439\mathrm{E} + 04 + 2.23059710\mathrm{E} + 01 \ast T$
	$298.15 < T < 2000$	${}^{1}L_{\mathrm{Ag,Ga}}^{\mathrm{FCC\_A1}} = -1.04126067\mathrm{E} + 04 - 2.25102088\mathrm{E} + 01 \ast T$
HCP_A3	$298.15 < T < 3000$	$G_{\mathrm{Ag}}^{\mathrm{FCC\_A1}} = \mathrm{GHCPAG}$
	$298.15 < T < 4000$	$G_{\mathrm{Ga}}^{\mathrm{FCC\_A1}} = \mathrm{GHCPGA}$
	$298.15 < T < 2000$	${}^{0}L_{\mathrm{Ag,Ga}}^{\mathrm{HCP\_A3}} = -1.52032953\mathrm{E} + 04 + 1.78639448\mathrm{E} + 00 \ast T$
	$298.15 < T < 2000$	${}^{1}L_{\mathrm{Ag,Ga}}^{\mathrm{HCP\_A3}} = -2.21349653\mathrm{E} + 04 + 7.17838494\mathrm{E} + 00 \ast T$
ζ' (HCP_ORD)	$298.15 < T < 3000$	$G_{\mathrm{Ag:Ag}}^{\mathrm{HCP\_ORD}} = 3 \ast \mathrm{GHCPAG}$
	$298.15 < T < 2000$	$G_{\mathrm{Ag:Ga}}^{\mathrm{HCP\_ORD}} = 2 \ast \mathrm{GHCPAG} + \mathrm{GHCPGA} - 3.26891668\mathrm{E} + 04 + 1.25713314\mathrm{E} + 01 \ast T$
	$298.15 < T < 2000$	$G_{\mathrm{Ag:Va}}^{\mathrm{HCP\_ORD}} = 2 \ast \mathrm{GHCPAG} + 1.78000000\mathrm{E} + 04$
	$298.15 < T < 2000$	${}^{0}L_{\mathrm{Ag:Ag,Ga}}^{\mathrm{HCP\_ORD}} = 6.36888797\mathrm{E} + 03 - 1.48261554\mathrm{E} + 01 \ast T$
	$298.15 < T < 2000$	${}^{1}L_{\mathrm{Ag:Ag,Ga}}^{\mathrm{HCP\_ORD}} = 3.64122858\mathrm{E} + 03$
$\mathrm{Ag_3Ga_2}$	$298.15 < T < 2000$	$G_{\mathrm{Ag:Ga}}^{\mathrm{Ag_3Ga_2}} = 3 \ast \mathrm{GHSERAG} + 2 \ast \mathrm{GHSERGA} - 4.96638526\mathrm{E} + 041.46044545\mathrm{E} + 01 \ast T$
Orthorhombic_GA (Ga)	$298.15 < T < 4000$	$G_{\mathrm{Ga}}^{\mathrm{Orthorombic\_GA}} = \mathrm{GHSERGA}$
GHSERAG	$298.15 < T < 1234.93$	$-7209.512 + 118.202013^{*}T - 23.8463314^{*}T^{*}LN(T) - .001790585^{*}T^{**}2 - 3.98587\mathrm{E} - 07^{*}T^{**}3 - 12011^{*}T^{**}(-1)$
	$1234.93 < T < 3000.00$	$-15095.252 + 190.266404^{*}T - 33.472^{*}T^{*}LN(T) + 1.411773\mathrm{E} + 29^{*}T^{**}(-9)$
GHSERGA	$200.00 < T < 302.91$	$-21312.331 + 585.263691^{*}T - 108.228783^{*}T^{*}LN(T) + .227155636^{*}T^{**}2 - 1.18575257\mathrm{E} - 04^{*}T^{**}3 + 439954^{*}T^{**}(-1)$
	$302.91 < T < 4000.00$	$-7055.643 + 132.73019^{*}T - 26.0692906^{*}T^{*}LN(T) + 1.506\mathrm{E} - 04^{*}T^{**}2 - 4.0173\mathrm{E} - 08^{*}T^{**}3 - 118332^{*}T^{**}(-1) + 1.64547\mathrm{E} + 23^{*}T^{**}(-9)$
GHCPAG	$298.15 < T < 1234.93$	$-6909.512 + 118.502013^{*}T - 23.8463314^{*}T^{*}LN(T) - .001790585^{*}T^{**}2 - 3.98587\mathrm{E} - 07^{*}T^{**}3 - 12011^{*}T^{**}(-1)$
	$1234.93 < T < 3000.00$	$-14795.252 + 190.566404^{*}T - 33.472^{*}T^{*}LN(T) + 1.411773\mathrm{E} + 29^{*}T^{**}(-9)$
GHCPGA	$200.00 < T < 302.91$	$-16812.331 + 575.763691^{*}T - 108.228783^{*}T^{*}LN(T)$ $+ .227155636^{*}T^{**}2 - 1.18575257\mathrm{E} - 04^{*}T^{**}3 + 439954^{*}T^{**}(-1)$
	$302.91 < T < 4000.00$	$-2555.643 + 123.23019^{*}T - 26.0692906^{*}T^{*}LN(T) + 1.506\mathrm{E} - 04^{*}T^{**}2 - 4.0173\mathrm{E} - 08^{*}T^{**}3 - 118332^{*}T^{**}(-1) + 1.64547\mathrm{E} + 23^{*}T^{**}(-9)$

[*] Multiplications.

[**] Power.

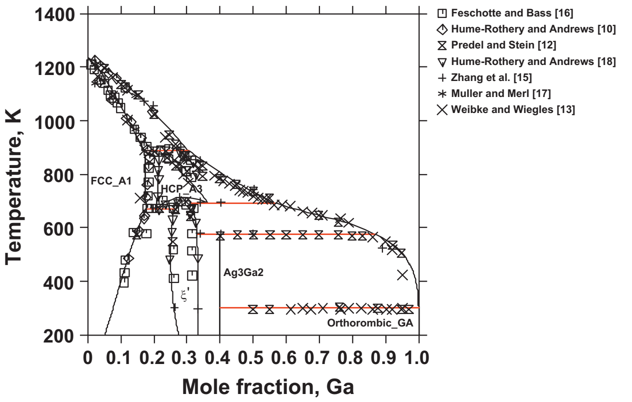

Fig. 1. Calculated phase diagram of the Ag–Ga binary system superimposed with experimental data.

Table 3
Invariant reactions in the Ag–Ga binary system.

Reaction	Calculation		Literature data	
	T [K]	x (Ga)	T [K]	x (Ga)
FCC_A1 + L = HCP_A3	886.8	0.217	888 [17] 888 [19] 885 [16] 884 [12]	0.22 [12]
HCP_A3 = FCC_A1 + HCP_ORD	670	0.208	668 [12]	0.205 [12]
HCP_A3 = ζ' + L	693.6	0.364	693 [16]	. . .
ζ' + L = Ag3Ga2	575	0.4	575 [24] 578 [16] 0.5 [16]	0.4 [24]
L = ζ' + Orthorhombic_GA	302	0.998	299 [12]	. . .

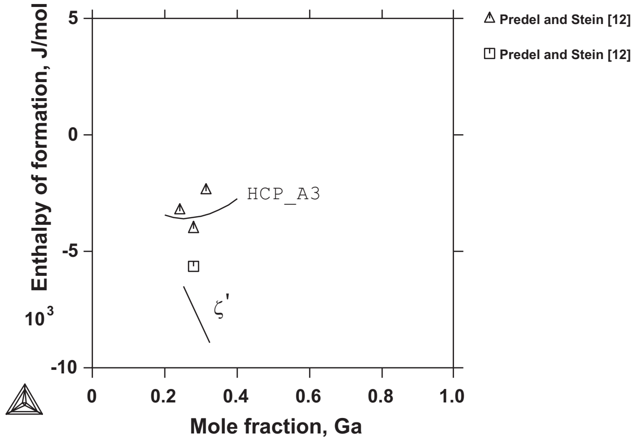

Fig. 3. Enthalpy of formation of HCP_A3 and ζ'(HCP_ORD) at 746 and 864 K, respectively, phases superimposed with experimental data.

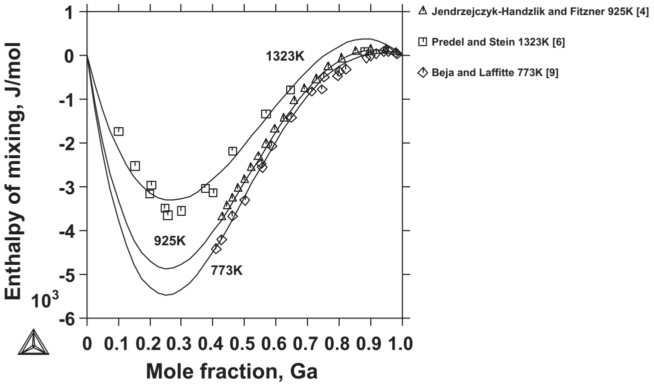

Fig. 4. Calculated enthalpy of mixing at 773, 925 and 1323 K superimposed with experimental data.

the phase boundary between HCP_A3 and liquid agrees more with Zhang et al. [15] than with others. The phase ζ' (ordered HCP) has been described in this work in agreement with Gunneas et al.'s [14] paper what means the homogeneity range of this phase was described by silver atoms and vacancies on the gallium sublattice. Calculated and measured information about invariant reactions are gathered in Table 3. From this table one can see that the calculated values of temperatures of the reactions and compositions of the phases show very good agreement with experimental information. The thermodynamic properties of the solid phase are shown in Figs. 2 and 3. Fig. 2 exhibits chemical potential of gallium in FCC_A1 phase. From this picture it is easy to find that the calculation agrees with Danilin and Yatsenko [2] and lies much higher than values obtained by Predel and Stein [6]. Enthalpies of formation of solid HCP_A3 and ζ' (ordered HCP) are shown in Fig. 3. Taking into account experimental error of the calorimetric method, one can say that the calculated heat of formation of the HCP_A3 and of the ζ phases agrees well with literature data. Thermodynamic properties of the liquid phase are shown in Figs. 4 and 5. Fig. 4 reveals the calculated and measured enthalpy of mixing of the liquid phase at different temperatures. In opposite to Zhang et al. [24] we did not find any evidence for the existence of the liquid associate. The enthalpy of mixing exhibits strong temperature dependency but not sharp extreme. The sharp extreme of the heat of mixing of the

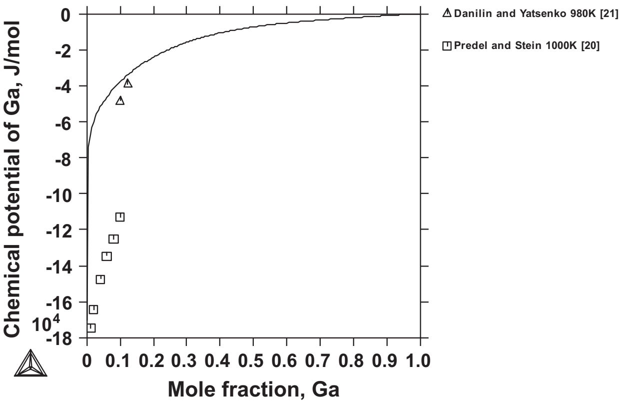

Fig. 2. Calculated chemical potential of Ga in FCC_A1 phase at 1000 K together with experimental data.

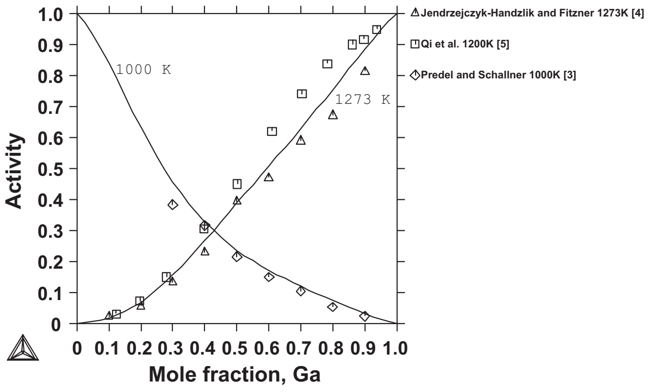

Fig. 5. Calculated activity of gallium and silver at 1273 and 1000 K, respectively, together with an experimental data.

liquid phase in Zhang et al.'s [25] work has been produced by used model, not by experimental data. Moreover, the measured activity of gallium [4] shows only slight negative deviation from the Raoult law, what suggests weak interactions between atoms. Calculated enthalpy of mixing shows very good agreement with the experimental data obtained by Jendrzejczyk-Handzlik and Fitzner [4], Predel and Stein [6] and Beja and Laffite [9]. Fig. 5 shows the calculated activity of gallium at 1273 together with Jendrzejczyk-Handzlik and Fitzner's [4], Qi et al. [5] and Predel and Schallner [3] results. For low concentration of gallium the experimental results obtained by Jendrzejczyk-Handzlik and Fitzner [4] and Qi et al. [5] agree each other and exhibit negative deviation from Raoult's Law. For concentration of gallium higher than 0.4 mole fraction the activity of Ga obtained by Jendrzejczyk-Handzlik and Fitzner [4] shows slightly negative deviation from Raoult's Law when Qi et al. [5] result has positive deviation from the Raoult's Law. The calculated activity of Ga lies between both sets of experimental data. The calculated activity of silver agrees well with the experimental data obtained by Predel and Schallner [3] and exhibits negative deviation from the Raoult's Law for a whole range of concentration of the components. Taking into account comparison of the experimental data and calculated values one can say that the Ag–Ga system is described well using less complicated model for the liquid phase than in previous work [25].

6. Summary

The new thermodynamic description of the binary Ag–Ga system is proposed. Compare to previous optimization available in literature [25] a new available experimental information about the liquid phase [4] and different, more suitable, thermodynamic models were used for describing of the liquid and ζ' (ordered HCP) phases. Good agreement between experimental information and calculation has been found.

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