# Thermodynamic Assessment of the Al-Zr Binary System

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**The thermodynamic parameters of the Al-Zr binary system can be very useful for the development of Zr-Al based amorphous and nanocrystalline materials. Phase diagram and thermochemistry data, especially the enthalpy of mixing of the liquid phase and the standard enthalpy of formation for the intermetallic compounds, are employed to optimize a consistent thermodynamic description for all the phases. The liquid, fcc, bcc, and hcp phases are treated as disordered solutions, while all the intermetallic phases are taken as stoichiometric compounds. The calculated phase diagram and thermochemistry data agree well with most of the experimental values reported in the literature.**

## 1. Introduction

Zr-Al based amorphous and nanocrystalline alloys have recently attracted attention because of their high strength, high ductility, and high glass-forming ability.[1,2] A thermodynamic assessment of the Al-Zr binary system may be used as a base for building a thermodynamic database for higher order systems of glass-forming alloys. In addition, this binary system is part of our effort to perform a thermodynamic assessment of the Ni-Al-Zr ternary system in order to add Zr into the existing Ni database[3] for predicting phase stability in Ni-base superalloys. Although Saunders and Rivlin[4,5] have already performed an assessment of the Al-Zr system, their assessment did not include the $Zr_4Al_3$ phase. In addition, new experimental results on the Zr-rich part of the phase diagram resulted in a revision of some invariant reaction temperatures by as much as 40 °C.[6] Recent data on the enthalpies of formation for some of the intermetallic compounds[7,8] are also significantly different from the thermodynamic assessment of Saunders and Rivlin.[4,5] It is therefore necessary to reassess the thermodynamic parameters of the Al-Zr binary system to be consistent with the new experimental data.

## 2. Review of Experimental Data

### 2.1 Phase Equilibrium Data

The phase equilibria and crystal structure data prior to 1992 were reviewed and summarized by Murray *et al.*[9] and revised by Okamoto[10] to include the new results of Peruzzi.[6] The phase diagram data used in the present assessment were mainly based on them.

The first systematic and comprehensive investigation of the Al-Zr phase diagram was performed by McPherson and Hansen[11] using metallography, x-ray diffraction (XRD), incipient melting, and thermal analysis. The phase diagram proposed by Murray *et al.*[9] was mainly based on this investigation. Peruzzi[6] redetermined the Zr-rich part of the phase diagram in the range 500 to 1300 °C by means of metallography, XRD, electron microprobe analysis, and electrical resistance measurement. In the present thermodynamic assessment, the results from Peruzzi were used for the Zr-rich part of the phase diagram, because the samples used by Peruzzi had higher purity than those used in the previous experimental study.[11] Several investigations[6,11–14] were performed on the solid solubility of Al in Zr, and the results roughly agree. No experimental information could be found concerning the two-phase L + bcc(Zr) field or the hcp(Zr) + bcc(Zr) field.

The Al-rich side of the phase diagram up to 1000 °C was determined by Fink and Willey,[15] Glazov *et al.*,[16] Drits *et al.*,[17] Kuznetsov *et al.*,[18] and Chiotti and Woerner.[19] The results are in good agreement.

The Al-Zr system has a large number of intermetallic compounds. According to the evaluation of Murray *et al.*,[9] there are ten stable intermetallic phases: $Zr_3Al$, $Zr_2Al$, $Zr_5Al_3$, $Zr_3Al_2$, $Zr_4Al_3$, $Zr_5Al_4$, ZrAl, $Zr_2Al_3$, $ZrAl_2$, and $ZrAl_3$. No information is available regarding the composition ranges of these phases.

The selected experiment data of all invariant reactions of the Al-Zr system are summarized in Table 1.

### 2.2 Thermodynamic Data

The partial and integral enthalpies of mixing of liquid Al-Zr alloys were measured using calorimetry by Esin *et al.*[20] at 1970 K, Sudavtsova *et al.*[21] at 1693 K, and Witusiewicz *et al.*[22] at 2010 to 2080 K. The results of Sudavtsova *et al.* were limited to a very narrow composition range from 0 to 10 at.% Al. The results from both Esin *et al.* and Witusiewicz *et al.* covered a much wider composition range up to 60 at.% Al, but Esin *et al.*[20] did not give the experimental details and their results were much more positive than those from Witusiewicz *et al.* Witusiewicz *et al.*[22] conjectured that the data given by Esin *et al.*[20] were referred to solid Zr as the reference state. The most recent results reported by Witusiewicz *et al.* were accepted to optimize the parameters of the

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**Table 1 Comparison between selected and calculated invariant equilibrium data**

| Reaction | Composition of the respective phases (at.% Al) | | | Temperature (K) | Reference |
|---|---|---|---|---|---|
| L ↔ bcc + $Zr_5Al_3$ | 29.5 | 25.9 | 37.5 | 1623 | McPherson[11] |
| | 29.5 | 24.9 | 37.5 | 1621 | This work |
| Bcc + $Zr_5Al_3$ ↔ $Zr_2Al$ | 19.9 | 37.5 | 33.3 | 1488 | Peruzzi[6] |
| | 20.3 | 37.5 | 33.3 | 1487 | This work |
| Bcc + $Zr_2Al$ ↔ $Zr_3Al$ | 12.0 | 33.3 | 25.0 | 1292 | Peruzzi[6] |
| | 12.1 | 33.3 | 25.0 | 1292 | This work |
| Bcc + $Zr_3Al$ ↔ hcp | 6.8 | 25.0 | 8.3 | 1183 | Peruzzi[6] |
| | 6.8 | 25.0 | 8.2 | 1183 | This work |
| L + $Zr_3Al_2$ ↔ $Zr_5Al_3$ | ~35(a) | 40.0 | 37.5 | 1673(a) | McPherson[11] |
| | 32.4 | 40.0 | 37.5 | 1676 | This work |
| $Zr_5Al_3$ ↔ $Zr_2Al$ + $Zr_3Al_2$ | 37.5 | 33.3 | 40.0 | ~1273 | Potzschke[27] |
| | 37.5 | 33.3 | 40.0 | 1273 | This work |
| L + $Zr_5Al_4$ ↔ $Zr_3Al_2$ | ~39 | 44.4 | 40.0 | 1753 | McPherson[11] |
| | 37.8 | 44.4 | 40.0 | 1753 | This work |
| $Zr_3Al_2$ + $Zr_5Al_4$ ↔ $Zr_4Al_3$ | 40.0 | 44.4 | 42.9 | ~1303 | Potzschke[27] |
| | 40.0 | 44.4 | 42.9 | 1304 | This work |
| $Zr_5Al_4$ ↔ $Zr_4Al_3$ + ZrAl | 44.4 | 42.9 | 50.0 | ~1273 | Potzschke[27] |
| | 44.4 | 42.9 | 50.0 | 1272 | This work |
| L ↔ $Zr_5Al_4$ | … | 44.4 | … | 1823(a) | McPherson[11] |
| | … | 44.4 | … | 1831 | This work |
| L ↔ $Zr_5Al_4$ + $Zr_2Al_3$ | ~50 | 44.4 | 60.0 | 1758 | McPherson[11] |
| | 51.0 | 44.4 | 60.0 | 1750 | This work |
| $Zr_5Al_4$ + $Zr_2Al_3$ ↔ ZrAl | 44.4 | 60.0 | 50.0 | 1548(a) | McPherson[11] |
| | 44.4 | 60.0 | 50.0 | 1548 | This work |
| L + $ZrAl_2$ ↔ $Zr_2Al_3$ | ~59 | 66.7 | 60.0 | 1863 | McPherson[11] |
| | 59.7 | 66.7 | 60.0 | 1865 | This work |
| L ↔ $ZrAl_2$ | … | 66.7 | … | 1933(a) | McPherson[11] |
| | … | 66.7 | … | 1931 | This work |
| L ↔ $ZrAl_2$ + $ZrAl_3$ | 73.5 | 66.7 | 75.0 | 1773 | McPherson[11] |
| | 74.7 | 66.7 | 75.0 | 1856 | This work |
| L ↔ $ZrAl_3$ | … | 75.0 | … | 1853 | McPherson[11] |
| | … | 75.0 | … | 1856 | This work |
| $ZrAl_3$ + L ↔ fcc | 75.0 | 99.97 | 99.92 | 933.9 | Fink[15] |
| | 75.0 | 99.97 | 99.92 | 933.8 | This work |

(a) Slightly modified by Murray *et al.*[9]

**Table 2 Standard enthalpy of formation of the Zr-Al intermetallic compounds, kJ/(mole of atoms)**

| | | | | | | |
|---|---|---|---|---|---|---|
| $Zr_3Al$ | … | … | … | … | −27.0 | −36.2 |
| $Zr_2Al$ | … | … | … | … | −33.4 | −48.4 |
| $Zr_5Al_3$ | −48 | … | … | … | −36.2 | −51.5 |
| $Zr_3Al_2$ | −49 | … | … | … | −38.4 | −55.2 |
| $Zr_4Al_3$ | … | … | … | … | … | −58.5 |
| $Zr_5Al_4$ | −52 | … | … | … | −41.0 | −55.4 |
| ZrAl | −53 | … | … | … | −44.5 | −65.0 |
| $Zr_2Al_3$ | −55 | … | … | … | −46.9 | −56.6 |
| $ZrAl_2$ | −54 | −44 | −52.1 | −51.3 | −45.8 | −52.6 |
| $ZrAl_3$ | −49 | −44 | −48.4 | … | −40.5 | −48.5 |
| Ref | Kematick and Franzen[14](a) | Alcock *et al.*[28] | Meschel and Kleppa[7] | Klein *et al.*[8] | Saunders[5] | This work |

(a) Adjusted by Murray et al.[9]

liquid phase, and the partial enthalpies were given a low weight in the optimization process because of the wide scatter.

Batalin *et al.*[23] determined the activity of Al in Al-rich liquid alloys at 1123 K. They reported a significantly higher solubility of Zr in liquid Al than what was reported by other investigations.[15,19] Consequently, the data given by Batalin *et al.* were not used in the present assessment.

Kematick and Franzen[14] measured the equilibrium vapor

**Table 3 Thermodynamic parameters for the phases in the Al-Zr system**

**Liquid**

$^{0}L^{\text{Liquid}}_{\text{Al,Zr}} = -207{,}140 + 42.911T$

$^{1}L^{\text{Liquid}}_{\text{Al,Zr}} = -22{,}643 + 11.442T$

$^{2}L^{\text{Liquid}}_{\text{Al,Zr}} = +56{,}610 - 7.807T$

**Fcc**

$^{0}L^{\text{fcc}}_{\text{Al,Zr}} = -152{,}947 + 21.300T$

**Bcc**

$^{0}L^{\text{bcc}}_{\text{Al,Zr}} = -165{,}348 + 13.235T$

$^{1}L^{\text{bcc}}_{\text{Al,Zr}} = -36{,}570$

$^{2}L^{\text{bcc}}_{\text{Al,Zr}} = +16{,}806$

**Hcp**

$^{0}L^{\text{hcp}}_{\text{Al,Zr}} = -166{,}254 + 13.235T$

$^{1}L^{\text{hcp}}_{\text{Al,Zr}} = -36{,}570$

$^{2}L^{\text{hcp}}_{\text{Al,Zr}} = +16{,}806$

**$Zr_3Al$**

$^{0}G^{Zr_3Al}_{\text{Al:Zr}} = 0.25\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.75\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 36{,}163 + 4.421T$

**$Zr_2Al$**

$^{0}G^{Zr_2Al}_{\text{Al:Zr}} = 0.33333\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.66667\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 48{,}358 + 6.492T$

**$Zr_5Al_3$**

$^{0}G^{Zr_5Al_3}_{\text{Al:Zr}} = 0.375\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.625\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 51{,}484 + 5.749T$

**$Zr_3Al_2$**

$^{0}G^{Zr_3Al_2}_{\text{Al:Zr}} = 0.4\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.6\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 55{,}180 + 6.734T$

**$Zr_4Al_3$**

$^{0}G^{Zr_4Al_3}_{\text{Al:Zr}} = 0.42857\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.57143\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 58{,}480 + 8.236T$

**$Zr_5Al_4$**

$^{0}G^{Zr_5Al_4}_{\text{Al:Zr}} = 0.44444\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.55556\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 55{,}424 + 5.320T$

**ZrAl**

$^{0}G^{ZrAl}_{\text{Al:Zr}} = 0.5\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.5\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 64{,}950 + 11.014T$

**$Zr_2Al_3$**

$^{0}G^{Zr_2Al_3}_{\text{Al:Zr}} = 0.6\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.4\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 55{,}323 - 27.830T + 4.329T \ln T$

**$ZrAl_2$**

$^{0}G^{ZrAl_2}_{\text{Al:Zr}} = 0.66667\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.33333\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 51{,}266 - 29.726T + 4.417T \ln T$

**$ZrAl_3$**

$^{0}G^{ZrAl_3}_{\text{Al:Zr}} = 0.75\ {}^{0}G^{\text{fcc}}_{\text{Al}} + 0.25\ {}^{0}G^{\text{hcp}}_{\text{Zr}} - 47{,}381 - 24.373T + 3.894T \ln T$

All values are in SI units and for one mole of atoms

The thermodynamic descriptions for pure Zr and Al are from Dinsdale[25]

pressure of Al over a number of compounds ($Zr_5Al_3$, $Zr_3Al_2$, $Zr_5Al_4$, ZrAl, $Zr_2Al_3$, $ZrAl_2$, and $ZrAl_3$) by the Knudsen-effusion technique. The enthalpies of formation of the compounds were evaluated by means of the second- and third-law methods. Since they did not take into account the difference between the free energies of the liquid and solid phases of pure Al above its melting point, their results were adjusted by Murray *et al.*[9] It should be mentioned that Kematick and Franzen combined several measurements to obtain the enthalpies of formation, so the cumulative uncertainty could be quite large especially in the Al-rich region. The data were therefore given a low weight in the thermodynamic optimization process.

More recently, Klein *et al.*[8] determined the standard enthalpy of formation for the $ZrAl_2$ phase from calorimetric measurement. Meschel and Kleppa[20] measured the standard enthalpies of $ZrAl_2$ and $ZrAl_3$ again by direct synthesis calorimetry at 1473 K. The results from the two groups agree well.

Esin *et al.*[24] measured the enthalpy of $Zr_2Al_3$, $ZrAl_2$, and $ZrAl_3$ in the temperature range 300 to 2000 K. Those data were used to optimize the parameters of these three compounds.

The enthalpies of formation of the Zr-Al intermetallic phases are listed in Table 2.

## 3. Thermodynamic Models

### 3.1 Solution Phases

The liquid, fcc(Al), bcc(Zr), and hcp(Zr) solution phases are described by a substitution model, and their Gibbs energies are represented by the following equation in terms of one mole of atoms:

$$G^{\alpha}_{m} = x_{\text{Al}}\ {}^{\circ}G^{\alpha}_{\text{Al}} + x_{\text{Zr}}\ {}^{\circ}G^{\alpha}_{\text{Zr}} + \mathrm{R}T\,(x_{\text{Al}} \ln x_{\text{Al}} + x_{\text{Zr}} \ln x_{\text{Zr}}) + {}^{E}G \qquad \text{(Eq 1)}$$

where $x_j$ is the mole fraction of element j (j = Al, Zr). The term $^{\circ}G^{\alpha}_{j}$ denotes the Gibbs energy of pure element j with the structure $\alpha$ ($\alpha$ = Liquid, fcc, bcc, or hcp), and the data for pure elements are taken from the Scientific Group Thermodata Europe (SGTE) database.[25]

The term $^{E}G$ is the excess Gibbs energy with interaction parameters expressed in Redlich-Kister polynomials:

$$^{E}G = x_{\text{Al}}x_{\text{Zr}} \sum_{i=0}^{n} {}^{i}L(x_{\text{Al}} - x_{\text{Zr}})^{i} \qquad \text{(Eq 2)}$$

where $^{i}L$ is the interaction parameter.

### 3.2 Intermetallic Compounds

Since no information is available on the composition ranges of intermetallic phases, all of them are treated as stoichiometric compounds. The Gibbs energy of compound $Zr_aAl_b$ is expressed by the following equation referring to the pure elements' standard state:

$$^{\circ}G^{Zr_aAl_b} = \frac{a}{a+b}\,{}^{\circ}G^{\text{hcp}}_{\text{Zr}} + \frac{b}{a+b}\,{}^{\circ}G^{\text{fcc}}_{\text{Al}} + A + BT + CT \ln T \qquad \text{(Eq 3)}$$

where $A$, $B$, and $C$ are parameters to be evaluated in the course of optimization.

## 4. Results and Discussion

The optimization of parameters was carried out using the PARROT module in the THERMO-CALC™ software.[26] The assessed thermodynamic parameters for the Al-Zr system are listed in Table 3.

Table 1 compares the calculated invariant reaction temperatures with the experimental values in the literature. Agreement is obtained within 10 K except for the L ↔ $ZrAl_2$ + $ZrAl_3$ eutectic reaction. The temperature and composition reported by McPherson and Hansen[11] impose a precipitous slope on the L/(L + $ZrAl_3$) boundary, which implies that the liquid phase has some special thermodynamic properties near

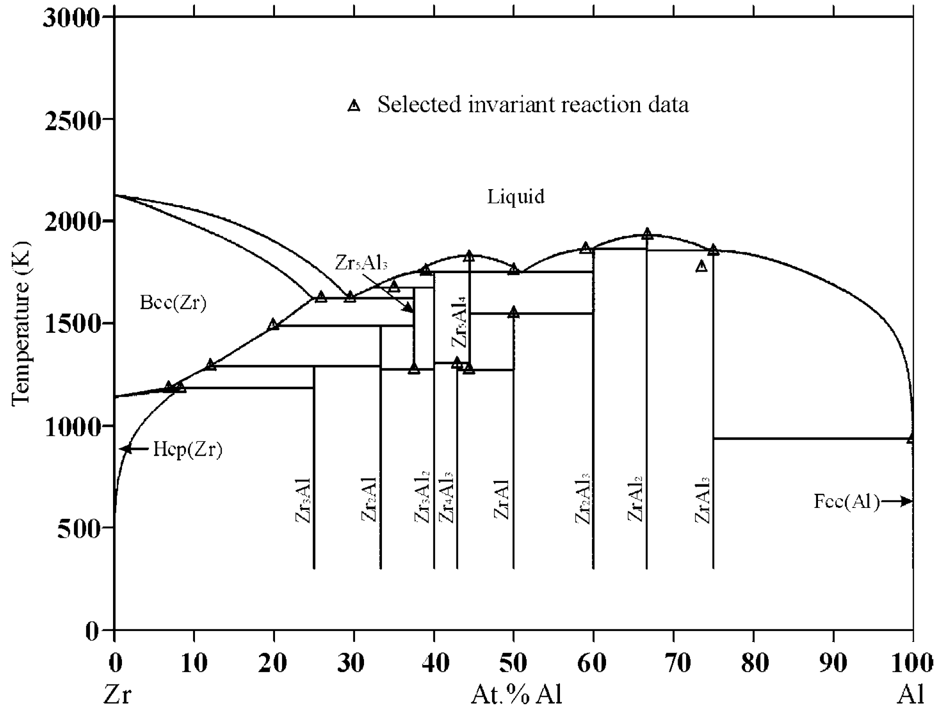

**Fig. 1** Calculated Al-Zr phase diagram compared with selected invariant reaction temperatures

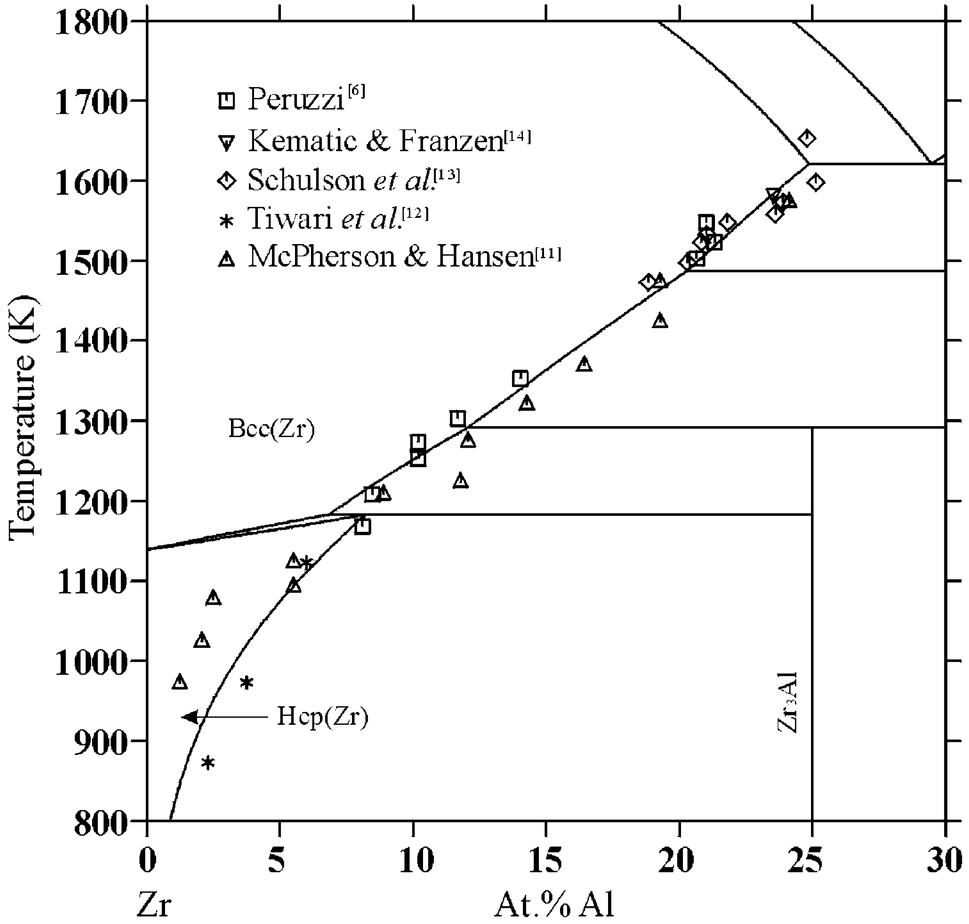

**Fig. 2** Calculated Zr-rich part of the Al-Zr phase diagram together with experimental data

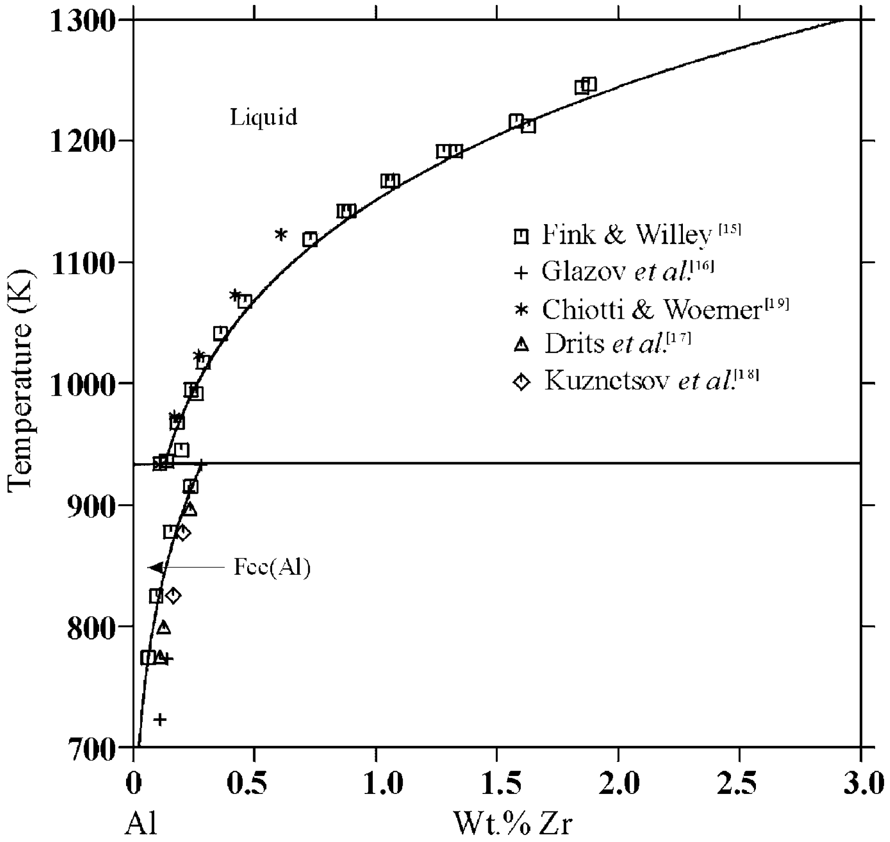

**Fig. 3** Calculated Al-rich part of Al-Zr phase diagram together with the experimental data

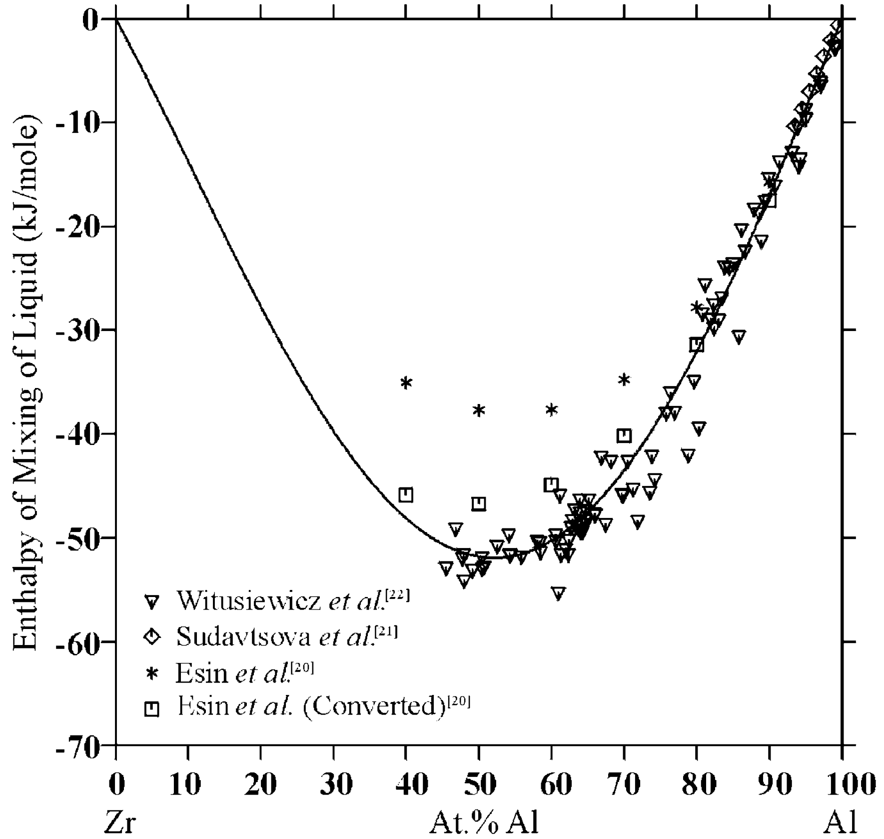

**Fig. 4** Calculated enthalpy of mixing for the liquid phase compared to the experimental values (reference states: liquid-Zr and liquid-Al)

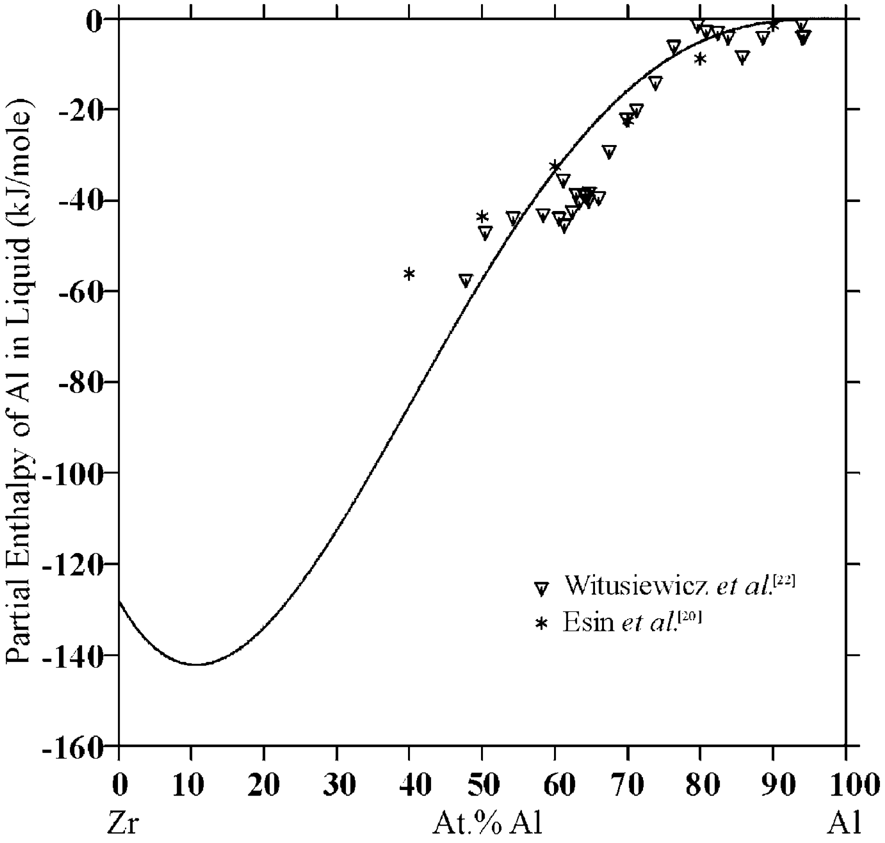

**Fig. 5** Calculated partial enthalpy of Al in liquid phase compared with the experimental data (reference state: liquid-Al)

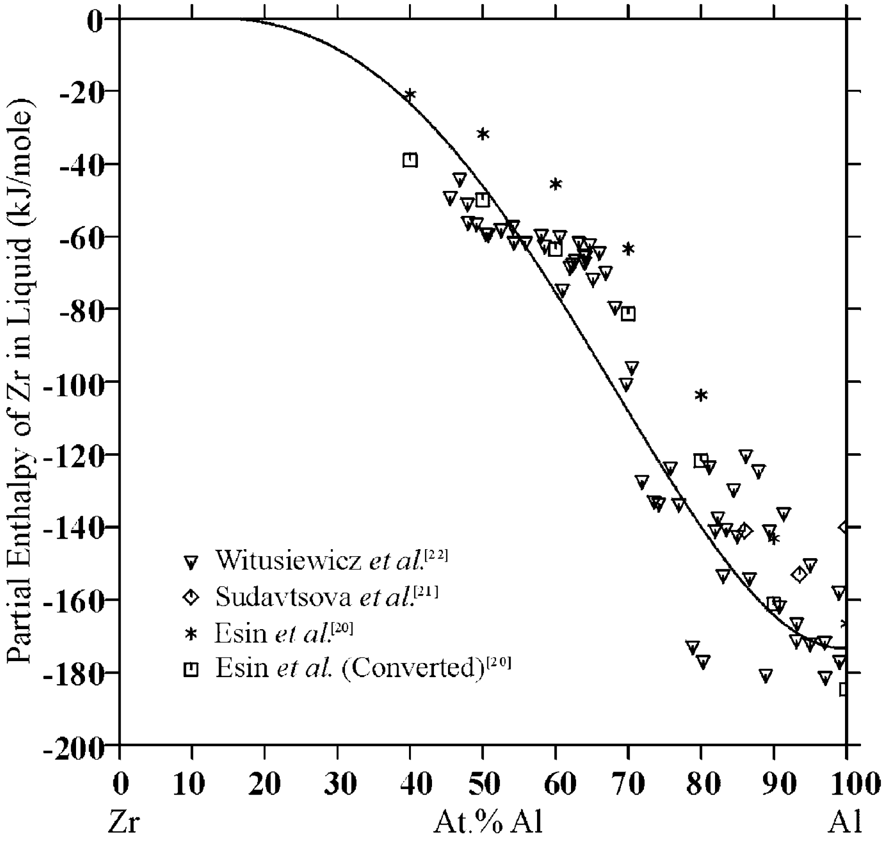

**Fig. 6** Calculated partial enthalpy of Zr in liquid phase compared with the experimental data (reference state: liquid-Zr)

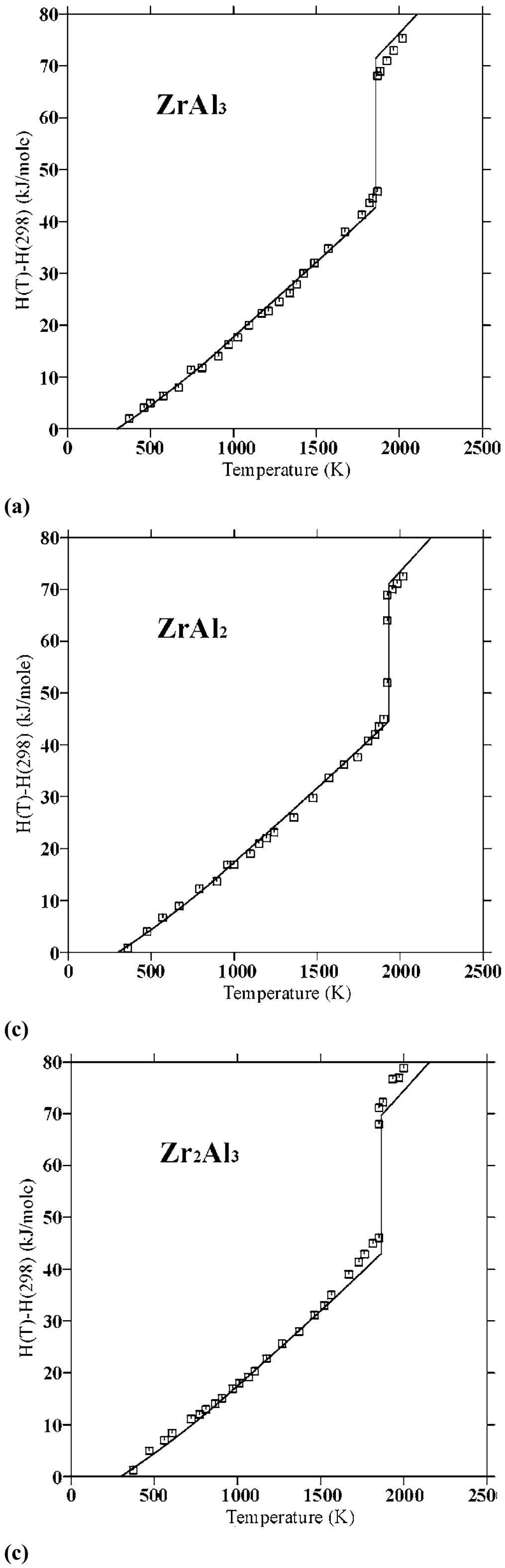

**Fig. 7** Comparison between the calculated and experimental enthalpies for (**a**) $ZrAl_3$, (**b**) $ZrAl_2$, and (**c**) $Zr_2Al_3$. The experimental data were from Esin *et al.*[24]

$ZrAl_3$. Without further experimental information, Saunders and Rivlin[4] suggested that the critical temperature for this reaction should be about 80 K higher than the reported one, thus very close to the melting temperature of $ZrAl_3$. The calculated result is consistent with their conjecture. Further experimental investigation of this part of the phase diagram is necessary.

The calculated Al-Zr phase diagram from the present work is shown in Fig. 1 together with selected invariant reaction temperatures, showing very good agreement. The calculated liquid phase composition of $L + Zr_3Al_2 \leftrightarrow Zr_5Al_3$ peritectic reaction is different from that suggested by McPherson and Hansen,[5] although the calculated temperature is in good agreement with the experimental one. To reproduce the composition suggested by McPherson and Hansen would bring quite a gentle slope on the $L/(L + Zr_5Al_3)$ boundary and then a relatively steep slope on the $L/(L + Zr_3Al_2)$ boundary. Because $Zr_5Al_3$ becomes metastable at low temperatures and decomposes into $Zr_3Al_2$ and $Zr_2Al$,[11,27,28] the difference between the $Zr_3Al_2$ and $Zr_5Al_3$ liquidus slopes implicit in the Hansen-McPherson diagram seems to be thermodynamically implausible.

Figure 2 shows the calculated Zr-rich portion of the phase diagram as compared to experimental data. The agreement is within the experimental uncertainties. The experimental solubilities of Zr in liquid and solid Al are compared to the calculated values in Fig. 3, showing very good agreement.

Figure 4 shows a comparison between the calculated enthalpies of mixing of the liquid phase and experimental data by Esin *et al.*,[20] Sudavtsova *et al.*,[21] and Witusiewicz *et al.*[22] The partial enthalpies of Al and Zr in the liquid phase are shown in Fig. 5 and 6, respectively. The calculated enthalpies reproduced very well the experimental data used in the optimization.

Under the assumption that the data reported by Esin *et al.*[20] were referred to solid Zr as the reference state, those data can be converted to the reference state of the liquid Zr using the following equations:

$$\Delta H^{\mathrm{Mix}}_{(L)} = \Delta H^{\mathrm{Mix}}_{(S)} - x_{\mathrm{Zr}}\, \Delta H^{\mathrm{Fus}}_{\mathrm{Zr}} \qquad \text{(Eq 4)}$$

$$\Delta \overline{H}_{\mathrm{Zr},(L)} = \Delta \overline{H}_{\mathrm{Zr},(S)} - \Delta H^{\mathrm{Fus}}_{\mathrm{Zr}} \qquad \text{(Eq 5)}$$

where the subscripts S and L indicate the enthalpies referred to the solid and liquid Zr, respectively, and $\Delta H^{\mathrm{Fus}}_{\mathrm{Zr}}$ is the molar enthalpy of fusion of Zr. The converted data are quite close to the results of Witusiewicz *et al.*[22] and the calculated curve, as shown in Fig. 4 to 6.

The calculated and experimental standard enthalpies of formation of the intermetallic phases are summarized in Table 2. Good agreement between the calculated values and the data of Meschel and Kleppa[7] and Klein *et al.*[8] was achieved. The calculated enthalpy of formation of ZrAl is quite different from the data reported by Kamatick and Franzen[14] (65 versus 53 kJ/mole). The calculated enthalpies of $ZrAl_3$, $ZrAl_2$, and $Zr_2Al_3$ are presented in Fig. 7, showing good agreement with the experimental data.

## 5. Conclusions

Phase equilibrium and thermodynamic data of the Al-Zr binary system are analyzed using thermodynamic models.

The liquid, fcc, bcc, and hcp phases are described by a substitution model and all intermetallic phases as stoichiometric compounds. A set of self-consistent thermodynamic parameters describing all stable phases in this system is obtained. A comparison between the calculated and experimental results is made. The optimized thermodynamic parameters reproduced most of the available experimental data on both phase diagram and thermochemstry data.

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## References

1. A. Inoue, T. Zhang, M.W. Chen, T. Sakurai, J. Saida, and M. Matsushita: *J. Mater. Res.,* 2000, vol. 15, pp. 2195-2208.
2. A. Inoue, T. Zhang, and M. Matsushita: *Mater. Trans. JIM,* 1990, vol. 31, p. 177.
3. Ni-Data, Version 4.0, Thermo-Tech Ltd., Surrey, United Kingdom, 2000.
4. N. Saunders and V.G. Rivlin: *Mater. Sci. Technol.,* 1986, vol. 2, pp. 521-27.
5. N. Saunders: *Z. Metallkd.,* 1989, vol. 80, pp. 894-903.
6. A. Peruzzi: *J. Nucl. Mater.,* 1992, vol. 186, pp. 89-99.
7. S.V. Meschel and O.J. Kleppa: *J. Alloy Compounds,* 1993, vol. 191, pp. 111-16.
8. R. Klein, I. Jacob, P.A.G. O'Hare, and R.N. Goldberg: *J. Chem. Thermodyn.,* 1994, vol. 26, pp. 599-608.
9. J. Murray, A. Peruzzi, and J.P. Abriata: *J. Phase Equilibria,* 1992, vol. 13, pp. 277-91.
10. H. Okamoto: *J. Phase Equilibria,* 1993, vol. 14, pp. 259-60.
11. D.J. McPherson and M. Hansen: *Trans. ASM,* 1954, vol. 46, pp. 354-74.
12. S.N. Tiwari and K. Tangri: *J. Nucl. Mater.,* 1970, vol. 34, pp. 92-96.
13. E.M. Schulson, D.H. McColl, and V.C. Ling: Report No. AECL-5176, Atomic Energy of Canada Limited, Chalk River Laboratories, Chalk River, Canada, July 1975. Cited in Ref 6.
14. R.J. Kematick and H.F. Franzen: *J. Solid State Chem.,* 1984, vol. 54, pp. 226-34.
15. W.L. Fink and L.A. Willey: *Met. Technol.,* 1939, vol. 1, pp. 69-80.
16. V.M. Glazov, G. Lazarev, and Korolkov: *Metalloved. Term. Obrab. Met.,* 1959, vol. 10, pp. 48-50.
17. M.E. Drits, E.S. Kadaner, and V.I. Kuz'mina: *Izv. Akad. Nauk SSSR,* 1968, vol. 1, pp. 102-05.
18. G.M. Kuznetsov, A.D. Barsukov, and M.I. Abas: *Sov. Non-Ferrous Met. Res.,* 1983, vol. 11 (1), pp. 47-51.
19. P. Chiotti and P.F. Woerner: *J. Less-Common Met.,* 1964, vol. 7, pp. 111-19.
20. Y.O. Esin, N.P. Bobrov, M.S. Petrushevskiii, and P.V. Gel'd: *Izv. Akad. Nauk SSSR, Met.,* 1974, vol. 5, pp. 104-09.
21. V.S. Sudavtsova, G.I. Batalin, and V.S. Tutevich: *Izv. Akad. Nauk SSSR, Met.,* 1985, vol. 5, pp. 185-87.
22. V. Witusiewicz, U.K. Stolz, I. Arpshofen, and F. Sommer: *Z. Metallkd.,* 1998, vol. 89, pp. 704-13.
23. G.I. Batalin, E.A. Beloborodova, V.V. Nerubaschenko, V.D. Galochka, and L.I. Slyuzko: *Izv. Vyssh. Ucheb. Zaved. Tsvetn. Metall.,* 1982, vol. 3, pp. 74-77.
24. Y.O. Esin, N.N. Serebrennikov, E.D. Pletneva, and V.K. Kapustkin: *Izv. Vyssh. Ucheb. Zaved., Chern. Metall.,* 1987, vol. 10, pp. 1-3.
25. A.T. Dinsdale: *CALPHAD,* 1991, vol. 15, pp. 317-425.
26. B. Sundman, B. Jansson, and J.O. Anderson: *CALPHAD,* 1985, vol. 9, pp. 153-90.
27. M. Potzschke and K. Schubert: *Z. Metallkd.,* 1962, vol. 53 (8), pp. 548-61.
28. C.B. Alcock, K.T. Jacob, and S. Zador: in Zirconium: *Physico-Chemical Properties of its Compounds,* Atomic Energy Review No. 6, O. Kubaschewski, ed., IAEA, Vienna, 1976.