Thermochimica Acta 510 (2010) 88–92

Contents lists available at ScienceDirect

Thermochimica Acta

journal homepage: www.elsevier.com/locate/tca

Optimization and calculation of the MCl–$ZnCl_2$ (M = Li, Na, K) phase diagrams

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ARTICLE INFO

Article history:
Received 8 April 2010
Received in revised form 24 June 2010
Accepted 29 June 2010
Available online 4 July 2010

Keywords:
Thermodynamic
Zinc chloride melts
Phase diagram

ABSTRACT

An earlier structural model for binary silicate melts and glasses is extended to zinc chloride–alkali metal chloride systems. The evaluation of the available thermodynamic and phase diagrams data for the MCl–$ZnCl_2$ (M = Li, Na, K) binary systems have been carried out using the structural model for the liquid phase. This thermodynamic model is based on the assumption that each alkali chloride produces the depolymerization of $ZnCl_2$ network with a characteristic free-energy change. A least-squares optimization program permits all available thermodynamic and phase diagram data to be optimized simultaneously. In this manner, data for these binary systems have been analysed and represented with a small number of parameters.

1. Introduction

There is considerable interest in the application of molten salt reactions using zinc chloride. One of these applications is the electrodeposition of refractory metals such as tungsten and molybdenum using molten $ZnCl_2$–NaCl–KCl system at 523 K as electrolyte [1]. Interest in these systems is also related to the recycling of heavy-metal halide waste generated in industrial processes which must consider phase equilibria for the prevention of environmental pollution and the recovery of resources. During the past decades, several investigations of systems with divalent cations have been performed and a large area of molten salt chemistry was discovered. However, the structural and thermodynamic properties and phase diagrams for the zinc chloride–alkali metal chloride systems are not yet accurately known.

The thermodynamics of the binary systems MCl–$ZnCl_2$ (M = Li, Na, K) are of more than usual interest since the component salts are quite dissimilar in character. For example, LiCl is a normal ionic salt while $ZnCl_2$ is evidently associated since it forms a very viscous liquid which is obviously polymeric [2]. Solid $ZnCl_2$ has a structure analogous to SiO_2, in which the Zn^{2+} ions are surrounded tetrahedrally by four chloride ions and each chloride ion is bonded to two zinc ions. Allen et al. [3] used a liquids and amorphous materials diffractometer to show that there exists the tetrahedral coordination of anions around zinc in molten $ZnCl_2$. Hefeng et al. [4] used the EXAFS technique and found that the tetrahedrons consisting of four Cl atoms around Zn are dominant and stable in molten $ZnCl_2$.

The $ZnCl_4{}^{2-}$ tetrahedral shares corners to form a three-dimensional network. The liquid might be expected to have a similar polymeric structure due to the high viscosity and low conductivity of liquid $ZnCl_2$ near its melting point. As LiCl or another alkali chloride is added to molten $ZnCl_2$, the viscosity drops sharply presumably because bridging chloride linkages are broken and the degree of polymerization decreases in a similar way that of SiO_2 is broken up by the addition of alkali or alkaline earth oxides. Seo et al. [5] used a molecular-dynamic simulation for the calculation of some physicochemical properties in $ZnCl_2$-based fluxes, including the enthalpy of solid and liquid $ZnCl_2$, self-diffusion coefficient of each ion in $FeCl_2$, $PbCl_2$ and $ZnCl_2$, and the Gibbs free energies of mixing and phase diagrams of the $PbCl_2$–$ZnCl_2$ binary system.

Lin and Pelton [6] developed a structural model for binary silicate systems MO–SiO_2 (M = Ca, Mn, Mg, Fe, etc.). In this model, one single formalism applies over the entire composition range and accounts for two- and three-dimensional silicate network structures. Later, the model was examined in more depth for binary systems [7] and a more general empirical expression for enthalpy was written, and an empirical nonconfigurational excess entropy was added. Then, the purpose of the present article is to use the structural model, formerly developed for silicate melts, to represent the thermodynamic properties of MCl–$ZnCl_2$ (M = Li, Na, K) melts.

2. Thermodynamic model

The model is based on the depolymerization reaction of $ZnCl_2$:M^+

$$M^+Cl^- + Zn\text{–}Cl\text{–}Zn = Zn\text{–}Cl\text{–}M\text{–}\quad Cl\text{–}Zn \quad M = Li, Na, K \tag{1}$$

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doi:10.1016/j.tca.2010.06.027

or, in shorthand notation:

$$\mathrm{Cl}^- + \mathrm{Cl}^0 = 2\mathrm{Cl}^{-1/2} \tag{2}$$

where Cl^- is a free chloride ion, Cl^0 is a chloride ion bonded to two zinc atoms, and $\mathrm{Cl}^{-1/2}$ is a chloride ion singly bonded to one zinc atom.

The structural model assumes that every zinc atom is bonded to four chlorine atoms. Thus, mass balance considerations require that:

$$N_{\mathrm{Cl}^0} = 2X_{\mathrm{ZnCl_2}} - \frac{N_{\mathrm{Cl}^{-1/2}}}{2} \tag{3}$$

$$N_{\mathrm{Cl}^-} = X_{\mathrm{MCl}} - \frac{N_{\mathrm{Cl}^{-1/2}}}{2} \tag{4}$$

where X_{MCl} and $X_{\mathrm{ZnCl_2}}$ are the mole fractions of the components and N_{Cl^0}, N_{Cl^-} and $N_{\mathrm{Cl}^{-1/2}}$ are the numbers of moles of the various chlorine species per mole of solution. The configurational entropy is calculated by assuming a tetrahedral quasi lattice in which the sites are occupied by Cl^- ions and Zn atoms (each associated with four chlorine atoms bonded to it):

$$\begin{aligned}\Delta S^c = & -R\left[X_{\mathrm{ZnCl_2}} \ln\left(\frac{X_{\mathrm{ZnCl_2}}}{X_{\mathrm{ZnCl_2}} + N_{\mathrm{Cl}^-}}\right) + N_{\mathrm{Cl}^-} \ln\left(\frac{N_{\mathrm{Cl}^-}}{X_{\mathrm{ZnCl_2}} + N_{\mathrm{Cl}^-}}\right)\right] \\ & -R\left[N_{\mathrm{Cl}^0} \ln\left(\frac{N_{\mathrm{Cl}^0}}{N_{\mathrm{Zn-Zn}}}\right) + (N_{\mathrm{Zn-Zn}} - N_{\mathrm{Cl}^0}) \ln\left(\frac{N_{\mathrm{Zn-Zn}} - N_{\mathrm{Cl}^0}}{N_{\mathrm{Zn-Zn}}}\right)\right]\end{aligned} \tag{5}$$

where $N_{\mathrm{Zn-Zn}}$ is the number of moles of neighboring Zn–Zn pairs per mole of solution:

$$N_{\mathrm{Zn-Zn}} = \frac{4X_{\mathrm{ZnCl_2}}}{2}\left(\frac{X_{\mathrm{ZnCl_2}}}{X_{\mathrm{ZnCl_2}} + N_{\mathrm{Cl}^-}}\right) \tag{6}$$

The structural model assumes that reaction (1) is associated with a Gibbs free-energy change containing an enthalpic (ω) and entropic (η) term:

$$\Delta H = \left(\frac{N_{\mathrm{Cl}^{-1/2}}}{2}\right)\omega \tag{7}$$

$$S^{nc} = \left(\frac{N_{\mathrm{Cl}^{-1/2}}}{2}\right)\eta \tag{8}$$

Finally, ω and η are expanded as polynomials:

$$\omega = \omega_0 + \omega_1 X_{\mathrm{ZnCl_2}} + \omega_2 X_{\mathrm{ZnCl_2}}^2 + \ldots \tag{9}$$

$$\eta = \eta_0 + \eta_1 X_{\mathrm{ZnCl_2}} + \eta_2 X_{\mathrm{ZnCl_2}}^2 + \ldots \tag{10}$$

The coefficients ω_i and η_i are the parameters of the model which are obtained by optimization of the data. Given a composition, $X_{\mathrm{ZnCl_2}}$, and values of the parameters ω_i and η_i, the actual value of $N_{\mathrm{Cl}^{-1/2}}$ can be calculated by minimizing the Gibbs free energy at constant $X_{\mathrm{ZnCl_2}}$, ω and η:

$$\Delta G = \Delta H - T(\Delta S^c + S^{nc}) \tag{11}$$

$$\begin{aligned}2\left[\frac{\partial \Delta G}{\partial N_{\mathrm{Cl}^{-1/2}}}\right]_{X_{\mathrm{ZnCl_2}},\omega,\eta} = & (\omega - \eta T) - RT\left[\ln\left(\frac{N_{\mathrm{Cl}^-}}{1 - X_{\mathrm{MCl}} + N_{\mathrm{Cl}^-}}\right) + \ln\left(\frac{N_{\mathrm{Cl}^0}}{N_{\mathrm{Zn-Zn}}}\right)\right. \\ & \left. - \left(1 + \frac{N_{\mathrm{Zn-Zn}}}{1 - X_{\mathrm{MCl}} + N_{\mathrm{Cl}^-}}\right) \ln\left(\frac{N_{\mathrm{Zn-Zn}} - N_{\mathrm{Cl}^0}}{N_{\mathrm{Zn-Zn}}}\right)\right] = 0\end{aligned} \tag{12}$$

Substitution of Eqs. (3), (4) and (6) into (12) gives an equation in terms of X_{MCl} (or $X_{\mathrm{ZnCl_2}}$) and $N_{\mathrm{Cl}^{-1/2}}$, which can be solved numerically at a fixed composition, $X_{\mathrm{ZnCl_2}}$, and for given values of the parameters ω_i and η_i to give $N_{\mathrm{Cl}^{-1/2}}$. This value can then be substituted back into Eqs. (3), (4), (5), (7) and (8) to give ΔS and ΔH.

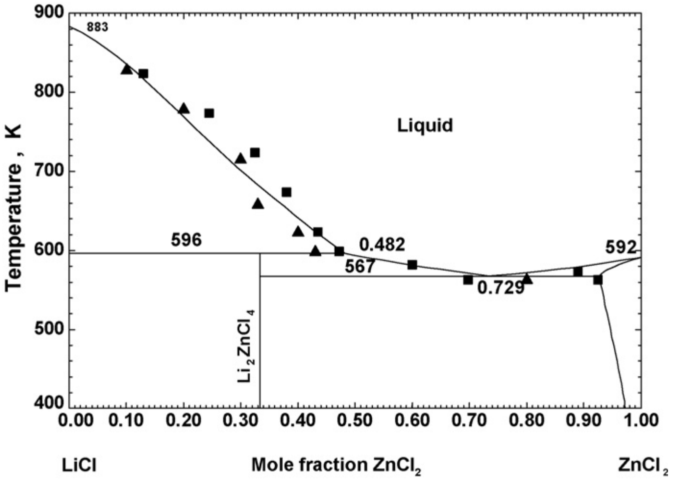

Fig. 1. Calculated optimized LiCl–ZnCl$_2$ phase diagram. Experimental points: (■) Ref. [9]; (▲) Ref. [10].

3. Results and discussion

The coefficients ω_i and η_i are obtained by optimization of experimental data for a given binary system. Since all integral and partial properties are expressed in terms of the same parameters, all available data (phase diagram, activities, enthalpies, etc.) can be considered in one simultaneous least-squares optimization. For the present model, a nonlinear least-squares optimization program was written [8].

3.1. The LiCl–ZnCl$_2$ system

The assessed phase diagram is shown in Fig. 1. The optimization of this system is based on the phase diagram reported by Liu et al. [9] who prepared and examined samples using the visual-polythermal method. They reported that $\mathrm{Li_2ZnCl_4}$ melts incongruently at 598 K and forms one eutectic at 562 K at 69.8 mol% $\mathrm{ZnCl_2}$. They also reported a small solubility of solid LiCl in $\mathrm{ZnCl_2}$. Kanno et al. [10] also determined the phase diagram of LiCl–ZnCl$_2$ but they did not report solid solubility in the $\mathrm{ZnCl_2}$ rich region. Fig. 1 shows that the calculated LiCl–ZnCl$_2$ phase diagram is in good agreement with the experimental values.

The integral enthalpies of mixing of the liquid LiCl–ZnCl$_2$ system were determined calorimetrically at 938 K by Papatheodorou and Kleppa [11]. They found that this system has an *S*-shaped enthalpy curve with positive values in the high $\mathrm{ZnCl_2}$ range. Calculated enthalpies of mixing are plotted in Fig. 2, where they may be compared with the results of Papatheodorou and Kl eppa [11].

$\Delta H_{298}{}^\circ$ and $S_{298}{}^\circ$ as well as C_p for LiCl and $\mathrm{ZnCl_2}$ were taken from Barin [12], and they are shown in Table 1. For $\mathrm{Li_2ZnCl_4}$ ($\mathrm{2LiCl{\cdot}ZnCl_2}$) no thermodynamic data are available. The values of C_p were calculated from Berman and Brown formula [13]:

$$C_p\,\mathrm{2LiCl{\cdot}ZnCl_2} = 2C_p\,\mathrm{LiCl} + C_p\,\mathrm{ZnCl_2} \tag{13}$$

$\Delta H_{298}{}^\circ$ and $S_{298}{}^\circ$ were then chosen to reproduce the experimental invariant temperatures. The optimized properties of this intermediate compound are given in Table 1.

The solid solution in the rich $\mathrm{ZnCl_2}$ region reported by Liu et al. [9] can be treated as a Henrian solution; that is, the activity of the solvent is ideal ($a_{\mathrm{ZnCl_2}} = X_{\mathrm{ZnCl_2}}$), while for the solute, $a_{\mathrm{LiCl}} = \gamma_{\mathrm{LiCl}}{}^\circ X_{\mathrm{LiCl}}$, where the Henrian activity coefficient ($\gamma_{\mathrm{LiCl}}{}^\circ$) is independent of composition. At the eutectic temperature in Fig. 1, LiCl in the $\mathrm{ZnCl_2}$ rich solid solution at about $X_{\mathrm{ZnCl_2}} = 0.92$ exists in equilibrium with virtually pure solid LiCl. Thus, in this solution $a_{\mathrm{LiCl}} \approx 1$ with

Table 1
Thermodynamic properties of the compounds in the MCl–$ZnCl_2$ (M = Li, Na, K) systems relative to elements at 298.15 K.

	A	*B*	*a*	*b*	*c*	*d*	*e*
LiCl(s)	−408266.35	59.299832	41.417416	23.396928	–	–	–
LiCl(l)	−395776.31	66.277403	73.383176	−9.472576	–	–	–
NaCl(s)	−411119.84	72.13216	45.94032	16.31760	–	–	–
NaCl(l)	−394956.03	76.076101	77.763824	−7.53120	–	–	–
KCl(s)	−436684.08	82.55032	40.015776	25.46801	3.64845	–	–
KCl(l)	−421824.91	86.52225	73.596560	–	–	–	–
$ZnCl_2$(s)	−416308.00	108.3656	60.66800	23.0120	–	–	–
$ZnCl_2$(l)	−414823.91	104.9669	100.83440	–	–	–	–
Li_2ZnCl_4(s)	−1232726.57	230.29116	349.2560	–	150.887	−4656.9	−21.714
Na_2ZnCl_4(s)	−1241069.22	276.951864	154.82164	6.1300	–	–	–
K_2ZnCl_4(s)	−1302071.39	317.232224	159.91357	50.9360	7.29689	–	–
$K_5Zn_4Cl_{13}$(s)	−3945410.82	846.99094	451–84288	242.00	18.2422	–	–
KZn_2Cl_5(s)	−1265792.27	348.851632	165.89778	82.798	3.64845	–	–

$H(\mathrm{J\ mol^{-1}}) = A + \int_{298.15}^{T} C_p dT$; $S(\mathrm{J\ mol^{-1}\ K^{-1}}) = B + \int_{298.15}^{T} (C_p/T) dT$; $C_p\ (\mathrm{J\,mol^{-1}\,K^{-1}}) = a + b\,(10^{-3})\,T + c\,(10^{5})\,T^{-2} + d\,T^{-1/2} + e\,(10^{8})\,T^{-3}$.

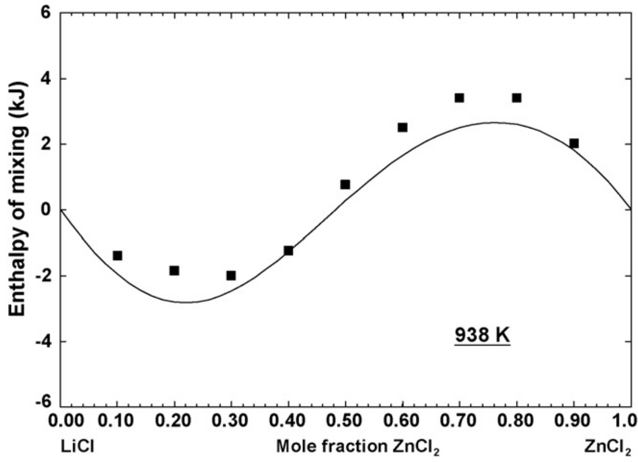

Fig. 2. Calculated optimized integral enthalpy of mixing of the liquid LiCl–$ZnCl_2$ system at 938 K. Experimental points: (■) Ref. [11].

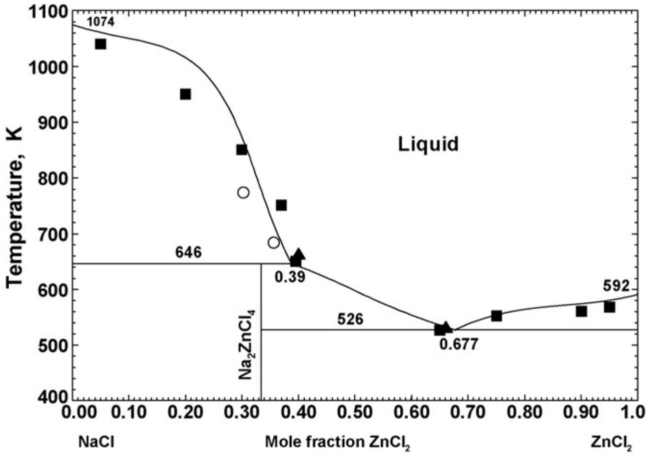

Fig. 3. Calculated optimized NaCl–$ZnCl_2$ phase diagram. Experimental points: (▲) Ref. [14]; (■) Ref. [15]; (○) Ref. [16].

respect to pure solid LiCl as standard state. Then,

$$\gamma_{\mathrm{LiCl}}^{\circ} = \frac{a_{\mathrm{LiCl}}}{X_{\mathrm{LiCl}}} = \frac{1.0}{1 - 0.92} = 12.5$$

and the partial excess Gibbs free energy of LiCl is given by:

$$g_{\mathrm{LiCl}}^{E} = RT\ \ln(g_{\mathrm{LiCl}}^{\circ}) = 11906\,\mathrm{J} \tag{14}$$

All the above experimental data were used as input to a least-squares optimization program in order to find the coefficients of Eqs. (9) and (10) which best reproduce all the data. The following parameters were found for the liquid:

$$\omega = -12005.68 + 15123.89X_{\mathrm{ZnCl_2}} + 20236.80X_{\mathrm{ZnCl_2}}^{2}\ \mathrm{J\ mol^{-1}} \tag{15}$$

$$\eta = -6.9521 + 36.1927X_{\mathrm{ZnCl_2}}^{2}\ \mathrm{J\ mol^{-1}\ K^{-1}} \tag{16}$$

3.2. The NaCl–$ZnCl_2$ system

The NaCl–$ZnCl_2$ binary phase diagram was determined in 1944 by Johnstone and Winsche [14]. They found an eutectic point at 66 mol% $ZnCl_2$ (530 K) and a peritectic at 40 mol% $ZnCl_2$ (662 K) but they did not determine the composition of the corresponding compound. Shaw and Perry [15] reported the eutectic at 65 mol% $ZnCl_2$ (526 K) and a peritectic at 40 mol% $ZnCl_2$ (650 K) and an incongruently melting compound Na_2ZnCl_4. Evseeva and Bergman [16] reported that Na_2ZnCl_4 melts incongruently at 683 K. The assessed phase diagram is shown in Fig. 3 together with the experimental points.

$\Delta H_{298}{}^{\circ}$, $S_{298}{}^{\circ}$ and C_p for NaCl were taken from Barin [12]. The thermodynamic data for Na_2ZnCl_4 were taken from the FACTSage database [17], and they are shown in Table 1. Fig. 4 shows the Gibbs free energy of mixing for the binary NaCl–$ZnCl_2$ system at 873 K calculated by the thermodynamic model and the results obtained by Lesourd et al. [18] using the electrochemical cells technique. This figure shows that the minimum Gibbs free energy of mixing

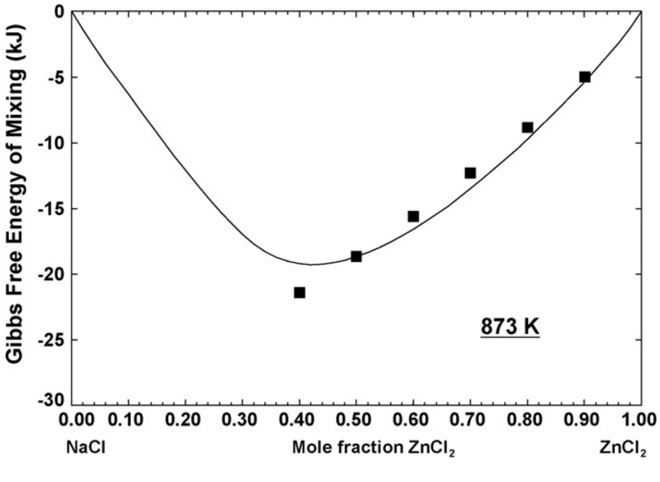

Fig. 4. Calculated Gibbs free energy of mixing of the NaCl–$ZnCl_2$ binary melt at 873 K. Experimental points: (■) Ref. [18].

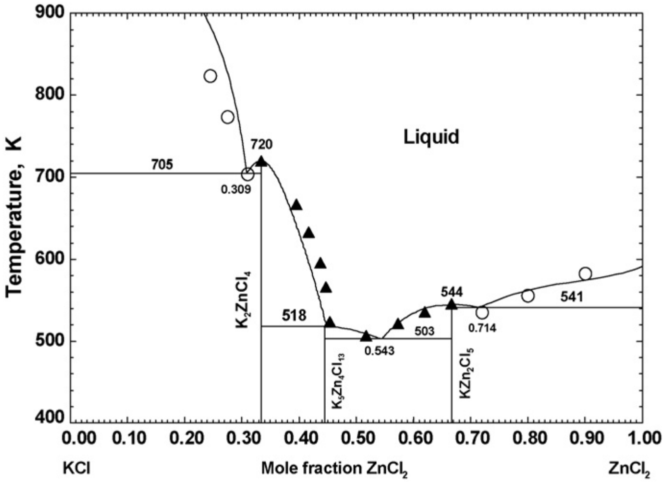

Fig. 5. Calculated optimized KCl–$ZnCl_2$ phase diagram. Experimental points: (○) Ref. [19]; (▲) Ref. [20].

is obtained in the concentration range of $X_{ZnCl_2} = 0.30–0.40$, corresponding to the Na_2ZnCl_4 compound. The following parameters were found for the liquid NaCl–$ZnCl_2$ system:

$$\omega = 12084.25 - 31327.20X_{ZnCl_2} + 43967.69X^2_{ZnCl_2}\ \text{J mol}^{-1} \tag{17}$$

$$\eta = 34.3975 + 21.2217X^2_{ZnCl_2}\ \text{J mol}^{-1}\ \text{K}^{-1} \tag{18}$$

3.3. The KCl–$ZnCl_2$ system

The assessed phase diagram is shown in Fig. 5. The optimization of this system is based on the phase diagram proposed by Duke and Fleming [19] and on the pseudo-binary 2KCl·$ZnCl_2$–KCl·2$ZnCl_2$ system which was investigated by Jiang et al. [20] using visual-polythermal, DTA and XRD methods. Duke and Fleming [19] showed that K_2ZnCl_4 and KZn_2Cl_5 melted congruently at 719 K and 547 K, respectively. They also reported that the compound $K_3Zn_2Cl_7$ melted incongruently at 523 K. Jiang et al. [20] did not report the presence of the compound $K_3Zn_2Cl_7$, instead of it they found the compound $K_5Zn_4Cl_{13}$ which melted incongruently at 522 K. In the present assessment, most weight was accorded to the results of Jiang et al. [20] since they have been obtained recently.

There is a significant uncertainty in the thermodynamic data of the intermediate compounds of the KCl–$ZnCl_2$ system. We decided to take the values reported in the FACTSage database [17].

$\Delta H_{298}{}^\circ$, $S_{298}{}^\circ$ and C_p for K_2ZnCl_4, KZn_2Cl_5 and $K_5Zn_4Cl_{13}$ are shown in Table 1.

Robertson and Kucharski measured the activities of $ZnCl_2$ in the liquid solutions by galvanic cell techniques [21] between 723 K and 1073 K. Data points are shown in Fig. 6 which shows that the model predictions agree well with the experimental results. The phase diagram and activity data were optimized simultaneously. The following parameters were found for the liquid:

$$\omega = -30059.4 + 8610.9X_{ZnCl_2} + 25269.9X^3_{ZnCl_2}\ \text{J mol}^{-1} \tag{19}$$

$$\eta = -2.3446 + 42.4086X^2_{ZnCl_2}\ \text{J mol}^{-1}\ \text{K}^{-1} \tag{20}$$

Fig. 7 shows the mixing free energy of the LiCl–$ZnCl_2$, NaCl–$ZnCl_2$ and KCl–$ZnCl_2$ systems at 800 K. This figure also shows that the energy of the KCl–$ZnCl_2$ is much lower than that of the LiCl–$ZnCl_2$ system. This means that K^+ and Li^+ must play a different role in the network. We can explain this behavior according to the following reaction:

$$\text{Zn–Cl}\overset{\text{Li}^+}{\quad}\text{Cl–Zn} + \text{K}^+\text{Cl}^- = \text{Zn–Cl}\overset{\text{K}^+}{\quad}\text{Cl–Zn} + \text{Li}^+\text{Cl}^- \quad \Delta\omega \tag{21}$$

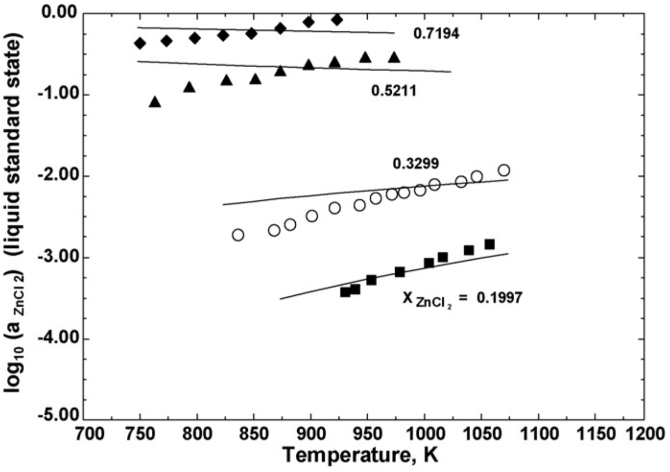

Fig. 6. Calculated and experimental [21] activities of $ZnCl_2$ in the KCl–$ZnCl_2$ liquid system.

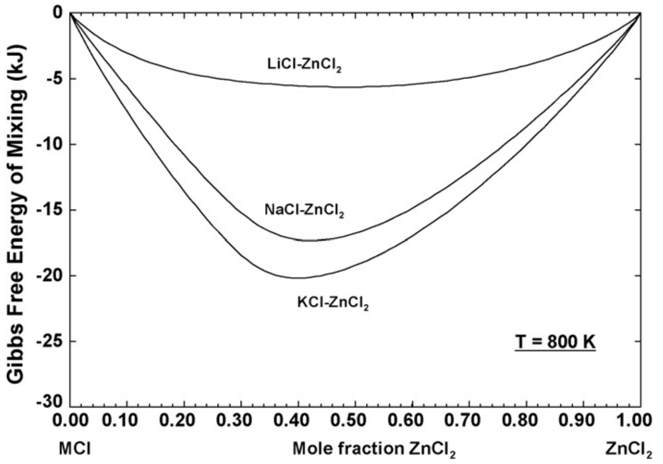

Fig. 7. Calculated Gibbs free energy of mixing of the MCl–$ZnCl_2$ (M = Li, Na, K) binary systems at 800 K.

where $\Delta\omega = (\omega - \eta T)_{KCl-ZnCl_2} - (\omega - \eta T)_{LiCl-ZnCl_2}$. At 800 K and $X_{ZnCl_2} = 1/3$ the value of $\Delta\omega$ for the $ZnCl_2$–LiCl–KCl system is around −25.8 kJ/mol and reaction (21) moves to the right, then the cations K^+ will be found associated to the Zn–Cl network and the cations Li^+ will be close to the free chloride ion Cl^-.

4. Conclusions

The structural model provides a simple method for representing the thermodynamic properties of structurally ordered liquid solutions. This model is based on the assumption that each alkali chloride produces the depolymerization of the $ZnCl_2$ polymeric network with a characteristic free-energy change.

Evaluations of all available thermodynamic and phase diagram data for the LiCl–$ZnCl_2$, NaCl–$ZnCl_2$ and KCl–$ZnCl_2$ systems have been carried out. Through the technique of least-squares optimization, all data were evaluated simultaneously to obtain one set of self-consistent model coefficients for the Gibbs free energies of mixing of liquid solutions as function of temperature and composition. The evaluations are valid from room temperature to above the liquidus temperatures.

Acknowledgment

The authors wish to thank the Institutions CONACyT, SNI, COFAA and IPN for their permanent assistance to the Process Metallurgy Group at ESIQIE- Metallurgy and Materials Department.

References

[1] H. Nakajima, T. Nohira, R. Hagiwara, K. Nitta, S. Inazawa, K. Okada, Electrochem. Acta 53 (2007) 24–27.
[2] A.K. Soper, Pramana J. Phys. 63 (2004) 41–50.
[3] D.A. Allen, R.A. Howe, N.D. Wood, W.S. Howells, J. Phys.: Condens. Matter 4 (1992) 1407–1418.
[4] L. Hefeng, L. Kunquan, W. Zhonghua, D. Jun, J. Phys.: Condens. Matter 6 (1994) 3629–3640.
[5] W.-G. Seo, H. Matsuura, F. Tsukihashi, Metall. Mater. Trans. B 37B (2006) 239–251.
[6] P.L. Lin, A.D. Pelton, Metall. Trans. B 10B (1979) 667–676.
[7] A. Romero-Serrano, A.D. Pelton, Metall. Mater. Trans. B 26B (1995) 305–315.
[8] A. Romero-Serrano, Un modèle Structural de Silicates Fondus, Ph.D. Thesis, EcolePolytechnique, Montréal, 1992.
[9] S.Q. Liu, Y. Liu, Q.Y. Zhang, Gaodeng Xuexiao Huaxue Xuebao 5 (1984) 765–768.
[10] R. Kanno, Y. Takeda, M. Mori, O. Yamamoto, Chem. Lett. 18 (1989) 223–226.
[11] G.N. Papatheodorou, O.J. Kleppa, Z. Anorg. Allg. Chem. 401 (1973) 132–144.
[12] I. Barin, Thermochemical Data of Pure Substances, ed. VCH Verlagsgesellschaft, Germany, 1989.
[13] R.G. Berman, T.H. Brown, Contrib. Mineral Petrol 89 (1985) 168–183.
[14] H.F. Johnstone, W.E. Winsche, Ind. Eng. Chem. 36 (1944) 435–439.
[15] S.J. Shaw, G. Perry, Thermochim. Acta 157 (1990) 329–333.
[16] N.N. Evseeva, A.G. Bergman, Izv. Sekt. Fiz.-Khim. Anal., Inst. Obshch. Neorg. Khim., Akad. Nauk SSSR 21 (1952) 208–227.
[17] C.W. Bale, A.D. Pelton, W.T. Thompson, FACTSage, v. 6.1., User's manual, 2009.
[18] J.-B. Lesourd, Y.Y. Rocca-Serra, Y. Doucet, J. Chem. Thermodyn. 9 (1977) 333–343.
[19] F.R. Duke, R.A.J. Fleming, J. Electrochem. Soc. 104 (1957) 251–254.
[20] L. Jiang, A. Meng, Q. Zhang, Acta Phys. Chim. Sin. 22 (2006) 131–134.
[21] R.J. Robertson, A.S. Kucharski, Can. J. Chem. 51 (1973) 3114–3122.