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Theoretical Assessment of the Thermodynamics of Molten Mg-In-Cd Alloys and Concerned Binary Systems

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Abstract

The concentration dependent thermodynamic behaviour of Mg-In-Cd melts at 850 K has been analysed in terms of the excess free energy of mixing, free energy of mixing, activity coefficient and activity of first element *i.e.* Mg on applying MIVM known as molecular interaction volume model. The computations of the mentioned thermodynamic functions require the input parameters, which are ascertained from the parameters needed for the concerned binary system at 850 K. The theoretical values for the excess free energy of mixing, free energy of mixing and activity for In-Mg at 923 K, In-Cd at 800 K and Cd-Mg at 923 K are in well agreement with the corresponding experimental results. The concentration dependence of the excess free energy of mixing, free energy of mixing, activity coefficient and activity of first element *i.e.* Mg for Mg-In-Cd system at 850 K for three cross-sections namely $x_{Cd} : x_{In}$ = 3:2, 2:3 and 1:4 indicate that Mg-In-Cd melts at 850 K is more stable for cross-section 3:2 followed by 2:3 and 1:4 respectively.

Keywords

MIVM Model, Excess Free Energy of Mixing, Activity Coefficient, Activity, Free Energy of Mixing, Mg-In-Cd melts

1. Introduction

Mg-In-Cd liquid alloys are composed of Mg, In and Cd. The presence of In and

Cd significantly decreases the melting point of Mg. The interactions between Mg, In, and Cd in the liquid state become crucial for explaining the behavior of Mg-In-Cd melts. The specific properties of Mg-In-Cd melts depend upon the characteristics of each constituent elements. Mg-In-Cd melts have wide range of applications in soldering due to the specific thermal characteristics having low melting point. It is clear that Mg-In-Cd consist of three binaries, namely In-Mg, Cd-Mg and In-Cd, in which In-Mg and Cd-Mg are ordered alloys while In-Cd is a segregating alloy [1]. Further, Cd-Mg at 923 K and Cd-In at 800 K are complex forming alloy [1] which influence the thermodynamic behavior of Mg-In-cd alloys. It is interesting to mention that Cd-In melt at 800 K is an exceptional alloy having both the complex formation tendency as well as segregating character. The researchers have employed theoretical model such as CALPHAD technique [2] as well as experimental studies [3] to assess the phase diagram as well as thermodynamic properties of Mg-In-Cd melts. The Mg-In-Cd melts are a matter of ongoing research to promote the understanding of their characteristics and potential applications. It is factual that Mg-In-Cd melt is not directly applicable to local industries but critical for material scientists interested in growing new materials.

In-Mg melt at 923 K is an ordered alloy [1] in which there is the existence of $InMg_2$, $InMg_3$ and In_2Mg_5 chemical complexes (or chemical compounds). The concentration dependence of G_M^E, S_M^E, and H_M are asymmetric while G_M and S_M are symmetric about equiatomic composition, x = 0.5 for In-Mg melts at 923 K. The activities a_{In} and a_{Mg} exhibit negative deviation from Raoult's law. The negative values of G_M^E and H_M, and negative deviations of a_{In} and a_{Mg} from ideal mixing behaviour indicate the ordering character of In-Mg melts at 923 K. The unique properties of In like ability of wetting as well as bonding to non-metallics such as glass, mica, quartz, glazes, ceramics and different metallic oxides make In and In- based alloys suitable for wide range of applications as solders and contact alloys. It is to be noted that in In-Mg liquid alloys, there exists primary bonding known as metallic bonding, where delocalized electrons from Mg form a shared "sea" of electrons that hold the positive ions together [4]. Therefore, it becomes necessary to have a good knowledge of the properties of mixing like thermodynamic, microscopic, transport and surface properties of In-Mg liquid alloys. The interesting behavior and potential applications of In-Mg melts have drawn the attentiveness of several researchers [5]-[7]. The mixing properties of In-Mg liquid alloys at 900 K have been theoretically explored [8] on employing the complex formation model [9] [10]. Thus, In-Mg melts is a suitable candidate for theoretical investigation.

The phase diagram [1] indicates the existence of CdMg and $CdMg_3$ chemical complexes in Cd-Mg system. The properties of mixing of Cd-Mg melts at 923 K illustrate symmetries for G_M^E, G_M, S_M^E, S_M and H_M about x = 0.5. The activities of Cd and Mg *i.e.* a_{Cd} and a_{Mg} illustrate the negative deviations from linearity. The negative values of G_M^E and H_M, and negative deviations of

a_{Cd} and a_{Mg} from linear law advocate the ordering nature of Cd-Mg melts at 923 K. In periodic table Cd lies in group 12 (IIB). The pure Cd is highly reactive due to which it has limited applications but the Cd- based alloys have a wide range of industrial applications [11] [12]. Cd-Mg system possesses low melting point, excellent corrosion resistance, low electrical resistance, low friction coefficient, good galvanic compatibility, excellent damping property, solderability. Therefore, Cd-Mg system has potential applications in aerospace, mining, nuclear, electrical etc. [3] [13]. The mixing properties of Cd-Mg liquid system have drawn the attention of many researchers [3] [13]-[18]. Therefore, Cd-Mg liquid alloys are an appropriate prospective material for theoretical investigation.

The phase diagram [1] indicates that there exists $InCd_3$ chemical complexes in In-Cd system. The properties of mixing like G_M^E exhibit asymmetric nature while G_M, S_M^E, S_M and H_M show symmetric character of In-Cd melts at 800 K relative to the concentration. It is interesting to note that concentration dependent values of G_M^E and H_M are positive in the whole concentration region, x_{In} = 0.1 to 0.9 while the activities a_{In} and a_{Cd} exhibit positive deviations from ideal behavior. Thus, In-Cd melt at 800 K is a segregating system with the existence of chemical complexes, which is an exceptional case. This shows the anomalous behavior of In-Cd melts at 800 K with regards to the mixing properties. In-Cd melts have potential applications including casting, soldering, bearing assembly, radiation shielding and ballast. Again, In-Cd-based ternary alloy like Ag-In-Cd are very important and utilized in nuclear power plants [19]. Earlier, phase diagram of Cd-In system has been investigated [20]. It is required to point out that there is scanty of theoretical and experimental data of the thermodynamic behavior of In-Cd melt in the literature. Thus, In-Cd melt is a proper binary melt for theoretical exploration.

Therefore, the interesting thermodynamic behaviour and potential applications of the Mg-In-Cd as well as the concerned binaries alloys become indispensable for the theoretical understanding of the Mg-In-Cd molten alloys.

In present research work, MIVM approach [21] is employed for the analysis of the thermodynamic properties namely excess free energy of mixing, G_M^E, free energy of mixing, G_M, activity coefficient and activity of Mg-In-Cd melts at 850 K. Earlier, the thermodynamics of several binary liquid alloys such as Zn-Bi, Bi-Sn, Pb-Bi, Fe-Mn, Cd-Tl, Ti-Al, Ni-Pd etc. [22]-[28] and several ternary liquid alloys namely In-Bi-Sn, Al-Sn-Zn, Mn-Fe-C, Sn-Ag-Cu etc. [29]-[33] have been investigated by MIVM model.

2. Formalism

The fluid-based model, MIVM (*i.e.* molecular interaction volume model) has been described by Tao [21] and deduced from statistical thermodynamics, fluid-phase equilibria and the fundamental concept of the non-random exchange of liquid molecules. The molecular excess free energy of mixing of the ternary molten alloys (1-2-3) is expressed as [21].

$$\frac{G_M^E}{RT} = x_1\left(\frac{V_{m1}}{x_1V_{m1}+x_2V_{m2}A_{21}+x_3V_{m3}A_{31}}\right)+x_2\ln\left(\frac{V_{m2}}{x_2V_{m2}+x_1V_{m1}A_{12}+x_3V_{m3}A_{32}}\right)$$
$$+x_3\ln\left(\frac{V_{m3}}{x_3V_{m3}+x_1V_{m1}A_{13}+x_2V_{m2}A_{23}}\right)-\frac{1}{2}\left[Z_1x_1\left(\frac{x_2A_{21}\ln A_{21}+x_3A_{31}\ln A_{31}}{x_1+x_2A_{21}+x_3A_{31}}\right)\right. \quad (1)$$
$$\left.+Z_2x_2\left(\frac{x_1A_{12}\ln A_{12}+x_3A_{32}\ln A_{32}}{x_1A_{12}+x_2+x_3A_{32}}\right)+Z_3x_3\left(\frac{x_1A_{13}\ln A_{13}+x_3A_{23}\ln A_{23}}{x_1A_{13}+x_2A_{23}+x_3}\right)\right]$$

where, Z_i ($i=1,2,3$) stands for the first coordination numbers for the constituent molecules 1,2 and 3 respectively, x_i ($i=1,2,3$) represents the concentration (or mole fraction) of the constituents 1,2 and 3 respectively A_{12}, A_{21}; A_{23}, A_{32}; and A_{31}, A_{31} denote the pair-potential energy interaction parameters between the constituent elements 1-2, 2-3 and 1-3 for the concerned binary systems (1-2), (2-3) and (1-3) respectively, V_{m1}, V_{m2} and V_{m3} represent the molar volume of elements 1, 2 and 3 respectively. Since, the ternary system (1-2-3) is composed of three binary systems (1-2), (2-3) and (1-3). It is remarkable to note that in MIVM, the computations for the ternary system require only binary interaction parameters. The ternary interaction term used in general solution model (GSM) [34], is not taken into account [21]. Despite this, the MIVM is successfully employed to predict the thermodynamic properties of several ternary alloys. Therefore, the potential energy interaction parameters are determined for each binary system.

Let us consider a binary system ($i-j$) for which the expression for the molar excess free energy of mixing may be represented by [21].

$$\frac{G_M^E}{RT} = x_i\ln\left(\frac{V_{mi}}{x_iV_{mi}+x_jV_{mj}A_{ji}}\right)+x_j\ln\left(\frac{V_{mj}}{x_jV_{mj}+x_iV_{mi}A_{ij}}\right)$$
$$-\frac{x_ix_j}{2}\left(\frac{Z_iA_{ji}\ln A_{ji}}{x_i+x_jA_{ji}}+\frac{Z_jA_{ij}\ln A_{ij}}{x_j+x_iA_{ij}}\right) \quad (2)$$

where, x_i and x_j are the compositions (or mole fractions) of i and j components respectively, Z_i and Z_j stands for the first coordination numbers for the constituent molecules i and j respectively. A_{ij} and A_{ji} denote the pair-potential energy interaction parameters and V_{mi} and V_{mj} are the molar volumes of elements i and j respectively. Now, A_{ij} and A_{ji} may be expressed as [21].

$$A_{ji}=\exp\left[-\frac{\varepsilon_{ji}-\varepsilon_{ii}}{kT}\right] \text{ and } A_{ij}=\exp\left[-\frac{\varepsilon_{ij}-\varepsilon_{jj}}{kT}\right] \quad (3)$$

with, ε_{ii}, ε_{jj} and ε_{ji} refer to pair potential energies for $i-i$, $j-j$ and $i-j$ pairs respectively, so that $\varepsilon_{ji}=\varepsilon_{ij}$, k and T represent Boltzmann constant and absolute temperature of the binary liquid alloy respectively.

Again, the value of co-ordination number of an element of the binary system can be determined from the relation given below [21].

$$Z_i=\frac{4\sqrt{2\pi}}{3}\left(\frac{r_{mi}^3-r_{oi}^3}{r_{mi}-r_{oi}}\right)\rho_i r_{mi}\exp\left(\frac{\Delta H_{mi}\left(T_{mi}-T\right)}{Z_cRTT_{mi}}\right) \quad (4)$$

with ΔH_{mi} and T_{mi} are enthalpy at melting temperature and melting temperature

respectively; Z_C is taken to be 12 for closed packed structure; $\rho_i = N_i V_i = \dfrac{0.6022}{V_{mi}}$ = molecular number density; r_{mi} and r_{oi} = initial and fist peak values of radial distribution function of the molten metal i near melting temperature respectively, and R is the molar gas constant. The radial distances are expressed as

$$r_{oi} = 0.918 d_{\mathrm{cov}\,i} \quad \text{and} \quad r_{mi} = \sigma_i \tag{5}$$

where, σ_i and $d_{\mathrm{cov}\,i}$ = atomic diameter and atomic covalent diameter respectively.

The activity coefficients of the component $\mu(=i,j)$ of a binary melt in terms of G_M^E can be expressed as [21].

$$RT \ln \gamma_\mu = G_M^E + (1 - x_\mu) \frac{\partial G_M^E}{\partial x_\mu}$$

Therefore,

$$\ln \gamma_\mu = \frac{G_M^E}{RT} + \frac{(1 - x_\mu)}{RT} \frac{\partial G_M^E}{\partial x_\mu} \tag{6}$$

From equation (6), the activity coefficients for constituents i and j of the binary melt $i-j$ can be represented respectively as

$$\ln \gamma_i = \frac{G_M^E}{RT} + \frac{x_j}{RT} \frac{\partial G_M^E}{\partial x_i} \tag{7}$$

$$\ln \gamma_j = \frac{G_M^E}{RT} + \frac{x_i}{RT} \frac{\partial G_M^E}{\partial x_j} \tag{8}$$

where, $x_j = (1 - x_i)$ and $x_i = (1 - x_j)$

Employing equation (2) in (7) and (8), we can obtain respectively

$$\begin{aligned} \ln \gamma_i = {} & \ln\left(\frac{V_{mi}}{x_i V_{mi} + x_j V_{mj} A_{ji}}\right) + x_j \left(\frac{V_{mj} A_{ji}}{x_i V_{mi} + x_j V_{mj} A_{ji}} - \frac{V_{mi} A_{ji}}{x_j V_{mj} + x_i V_{mi} A_{ij}}\right) \\ & - \frac{x_j^2}{2} \left(\frac{Z_i A_{ji}^2 \ln A_{ji}}{(x_i + x_j A_{ji})^2} + \frac{Z_j A_{ij} \ln A_{ji}}{(x_j + x_i A_{ij})^2}\right) \end{aligned} \tag{9}$$

$$\begin{aligned} \ln \gamma_j = {} & \ln\left(\frac{V_{mj}}{x_j V_{mj} + x_i V_{mi} A_{ij}}\right) - x_i \left(\frac{V_{mj} A_{ji}}{x_i V_{mi} + x_j V_{mj} A_{ji}} - \frac{V_{mi} A_{ij}}{x_j V_{mj} + x_i V_{mi} A_{ij}}\right) \\ & - \frac{x_i^2}{2} \left(\frac{Z_j A_{ij}^2 \ln A_{ij}}{(x_j + x_i A_{ij})^2} + \frac{Z_i A_{ji} \ln A_{ji}}{(x_i + x_j A_{ji})^2}\right) \end{aligned} \tag{10}$$

The equations (9) and (10) are the analytical expressions from which γ_i and γ_j of the binary melt $i-j$ can be calculated.

From definition, the activity coefficient and activity of the component μ of a binary melt are related as

$$a_\mu = \gamma_\mu x_\mu \quad (\text{where}, \ \mu = i, j) \tag{11}$$

From equation (11), the activities of the components i and j of the binary

melt $i-j$ can be expressed as [30].

$$a_i = \gamma_i x_i \tag{12}$$

$$a_j = \gamma_j x_j \tag{13}$$

The equations (12) and (13) can be utilized to determine the activities a_i and a_j respectively of the binary melt $i-j$.

The expressions for activity coefficients of the components of the alloy in infinite dilute solution range *i.e.* x_i or $x_i \to 0$, are, respectively, given by

$$\ln \gamma_i^{\infty} = 1 - \ln\left(\frac{V_{mj}A_{ji}}{V_{mi}}\right) - \frac{V_{mi}A_{ji}}{V_{mj}} - \frac{1}{2}\left(Z_i \ln A_{ji} + Z_j A_{ij} \ln A_{ij}\right) \tag{14}$$

and

$$\ln \gamma_j^{\infty} = 1 - \ln\left(\frac{V_{mi}A_{ij}}{V_{mj}}\right) - \frac{V_{mj}A_{ji}}{V_{mi}} - \frac{1}{2}\left(Z_j \ln A_{ij} + Z_i A_{ji} \ln A_{ji}\right) \tag{15}$$

The pair-potential energy interaction parameters, A_{ij} and A_{ji} can be determined by solving equation (14) and (15) on applying Newton-Rapson method.

Now, for a ternary melt (1-2-3), the activity coefficient of the component i ($i \equiv 1$) is expressed as [15].

$$RT \ln \gamma_1 = G_M^E + x_2\left(\frac{\partial G_M^E}{\partial x_1}\right) - x_3\left(\frac{\partial G_M^E}{\partial x_3}\right) \tag{16}$$

Using equations (1) in (16), we can obtain

$$\begin{aligned}\ln \gamma_i = {} & 1 + \ln\left(\frac{V_{m1}}{x_1V_{m1} + x_2V_{m2}A_{21} + x_3V_{m3}A_{31}}\right) - \frac{x_1V_{m1}}{x_1V_{m1} + x_2V_{m2}A_{21} + x_3V_{m3}A_{31}} \\ & - \frac{x_2V_{m1}A_{12}}{x_1V_{m1}A_{12} + x_2V_{m2} + x_3V_{m3}A_{32}} - \frac{x_3V_{m1}A_{13}}{x_1V_{m1}A_{13} + x_2V_{m2}A_{23} + x_3V_{m3}} \\ & - \frac{1}{2}\left(\frac{Z_1\left(x_2A_{21} + x_3A_{31}\right)\left(x_2A_{21} \ln A_{21} + x_3A_{31} \ln A_{31}\right)}{\left(x_1 + x_2A_{21} + x_3A_{31}\right)^2}\right. \\ & + \frac{Z_2x_2A_{21}\left[\left(x_2 + x_3A_{32}\right)\ln A_{12} - x_3A_{32} \ln A_{32}\right]}{\left(x_1A_{12} + x_2 + x_3A_{32}\right)^2} \\ & \left. + \frac{Z_3x_3A_{13}\left[\left(x_2A_{23} + x_3\right)\ln A_{13} - x_2A_{23} \ln A_{23}\right]}{\left(x_1A_{13} + x_2A_{23} + x_3\right)^2}\right)\end{aligned} \tag{17}$$

which is the analytical expression for the activity coefficient of the component i ($i \equiv 1$) of a ternary system (1-2-3).

Now, the activity coefficient and activity of the component 1 may be related as

$$a_1 = \gamma_1 x_1 \tag{18}$$

The equations (17) and (18) are utilized to determine the theoretical values of the activity of component i of a ternary system (1-2-3).

Now, the free energy of mixing, G_M for a ternary system may be represented as

$$\frac{G_M}{RT} = \frac{G_M^E}{RT} + \frac{G_M^{id}}{RT}$$

Again, for a ternary system, the ideal free energy of mixing, G_M^{id} at a given temperature T may be represented by

$$G_M^{id} = RT\left[x_1 \ln x_1 + x_2 \ln x_2 + x_3 \ln x_3\right] \tag{20}$$

Using equation (1) and (20), we get

$$\begin{aligned}\frac{G_M}{RT} = {} & x_1 \ln\left(\frac{V_{m1}}{x_1 V_{m1} + x_2 V_{m2} A_{21} + x_3 V_{m3} A_{31}}\right) + x_2 \ln\left(\frac{V_{m2}}{x_2 V_{m2} + x_1 V_{m1} A_{12} + x_3 V_{m3} A_{32}}\right) \\ & + x_3 \ln\left(\frac{V_{m3}}{x_3 V_{m3} + x_1 V_{m1} A_{13} + x_2 V_{m2} A_{23}}\right) - \frac{1}{2}\left[Z_1 x_1 \left(\frac{x_2 A_{21} \ln A_{21} + x_3 A_{31} \ln A_{31}}{x_1 + x_2 A_{21} + x_3 A_{31}}\right)\right. \\ & \left. + Z_2 x_2 \left(\frac{x_1 A_{12} \ln A_{12} + x_3 A_{32} \ln A_{32}}{x_1 A_{12} + x_2 + x_3 A_{32}}\right) + Z_3 x_3 \left(\frac{x_1 A_{13} \ln A_{13} + x_3 A_{23} \ln A_{23}}{x_1 A_{13} + x_2 A_{23} + x_3}\right)\right] \\ & + \left[x_1 \ln x_1 + x_2 \ln x_2 + x_3 \ln x_3\right]\end{aligned} \tag{21}$$

which is the required analytical expression for G_M of a ternary liquid alloy.

3. Result and Discussion

The analytical expressions (1), (21), (17) and (18) are employed to compute G_M^E/RT, G_M/RT, γ_i and a_i respectively of Mg-In-Cd melts at 850 K. For calculations, the input parameters required are evaluated from the concerned binary systems *i.e.* In-Mg melts at 923 K, In-Cd melts at 800 K and Cd-Mg melts at 923 K.

The necessary parameters of pure In, Cd and Mg are presented in **Table 1** [35]. For a binary system i-j, the coordination number Z_i and Z_j of the constituents are determined from equation (4) which are presented in **Table 2**. The values of A_{ji} and A_{ij} are determined on solving equations (14) and (15) by Newton-Raphson method using the experimental values of the infinite dilute activity coefficients *i.e.* γ_i^∞ and γ_j^∞ [1]. The values of A_{ji} and A_{ij} slightly changed in order to achieve a good agreement between the theory and experiment [1] for the excess free energy of mixing, G_M^E/RT of the concerned binary alloys [25] [26]. The best fit values A_{ji} and A_{ij} at required temperature are also depicted in **Table 2**.

Table 1. Input parameters for the pure metals [35].

Metal,i	ΔH_{mi} (KJ/mole)	σ_i ($\times 10^{-8}$ cm)	r_{oi} ($\times 10^{-8}$ cm)	V_{mi} (cm^3/mole) at m.p.
Mg	8.8	3.10	2.52	$15.3\left[1+1.6\times10^{-4}\left(T-923\right)\right]$
In	3.26	3.14	2.70	$16.3\left[1+0.97\times10^{-4}\left(T-429.5\right)\right]$
Cd	6.4	3.0	2.54	$14.0\left[1+1.6\times10^{-4}\left(T-594\right)\right]$

Table 2. Estimated values of A_{ij}, A_{ji}, Z_i, Z_j as well as γ_i^∞ and γ_j^∞ of the binary liquid alloys.

$i-j$	T(K)	A_{ij}	A_{ji}	Z_i	Z_j	γ_i^∞ [1]	γ_j^∞ [1]
In-Mg	923	1.6886	0.9315	9.48	9.69	0.010	0.068
In-Cd	800	1.1871	0.6983	9.59	9.63	2.386	1.571
Cd-Mg	923	1.1047	1.2997	9.45	9.69	0.118	0.082

3.1. Results for G_M^E, G_M and $a_\mu(\mu = i, j)$ of In-Mg and Cd-Mg at 923 K, and In-Cd at 800 K

The equation (2) is used to ascertain the values of G_M^E/RT for In-Mg and Cd-Mg at 923 K, and In-Cd at 800 K as a function of concentration, x_p (p = In, In, Cd). The theoretical results and correlated experimental results [1] depicted in **Figure 1**, demonstrate well concord in the complete range of composition, x = 0.1 to 0.9.

For In-Mg system at 923 K, G_M^E/RT vs x_{In} isotherm denotes the negative values of G_M^E/RT in the complete composition range of In *i.e.* x_{In} = 0.1 to 0.9 with minima at x_{In} = 0.4 *i.e.* −0.8684 (Theory) and −0.8581 (Experiment) having an error of 1.2%. Thus, the asymmetry in G_M^E/RT as well as ordering nature [36] of In-Mg melts at 923 K are successfully explained.

Again, Cd-Mg melts at 923 K, it is found that G_M^E/RT are negative in the whole concentration range of Cd *i.e.* x_{Cd} = 0.1 to 0.9 having minima at x_{Cd} = 0.5 *i.e.* −0.6005 (Theory) and −0.6055 (Experiment) with an error of 0.83%. Thus, the symmetry in G_M^E/RT as well as ordering nature [36] of Cd-Mg melts at 923 K are successfully discussed.

Further, for In-Cd liquid alloys at 800 K, G_M^E/RT exhibit positive values in the entire composition range of In *i.e.* x_{In} = 0.1 to 0.9 with maxima at x_{In} = 0.4 *i.e.* 0.1577 (Theory) and 0.1517 (Experiment) having an error of 3.96%. Thus, the asymmetry in G_M^E/RT as well as segregating nature [36] of In-Cd melts at 800 K are well reproduced.

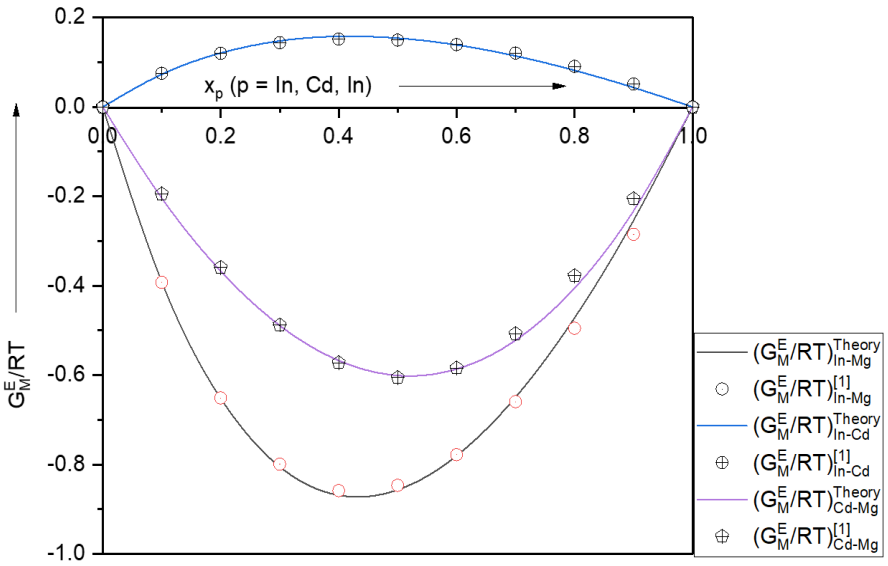


Figure 1. G_M^E/RT vs X_p (p = In, Cd, In) for In-Mg melts at 923 K, In-Cd melts at 923 K and Cd-Mg melts at 800 K.

Equation (19) is used to determine the values of G_M/RT for In-Mg and Cd-Mg both at 923 K, and In-Cd at 800 K as a function of concentration, x_p (p = In, In, Cd). The theoretical results and correlated experimental results [1] presented in **Figure 2**, exhibit well agreement in the complete range of composition, x = 0.1

to 0.9.

For In-Mg system at 923 K, G_M/RT - x_{In} isotherm represents the symmetry in G_M/RT for In-Mg melts at 923 K and the minima are observed at x_{In} = 0.5 *i.e.* –1.5495 (Theory) and –1.5405 (Experiment) with an error of 0.6%.

For Cd-Mg melts at 923 K, G_M/RT - x_{Cd} isotherm explains the symmetry in G_M/RT for Cd-Mg melts at 923 K because the lowest values of G_M/RT are observed at x_{Cd} = 0.5 *i.e.* –1.2937 (Theory) and –1.2994 (Experiment) having an error of 0.4%.

For In-Cd melts at 800 K, the symmetric nature of G_M/RT for In-Cd melts at 800 K is displayed by G_M/RT - x_{In} isotherm because the minimum values of G_M/RT are found at x_{In} = 0.5 *i.e.* –0.5393 (Theory) and –0.5444 (Experiment) with an error of 0.9%.

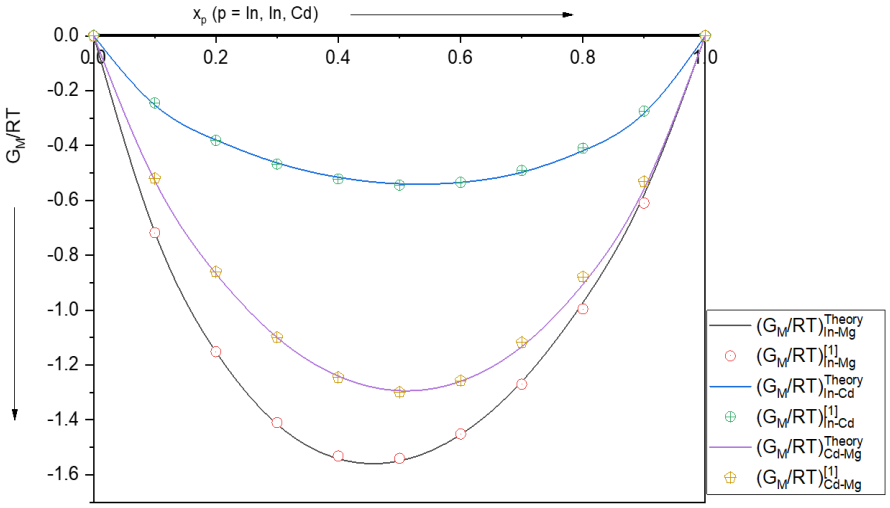


Figure 2. G_M/RT vs X_p (p = In, Cd, In) for In-Mg melts at 923 K, In-Cd melts at 923 K and Cd-Mg melts at 800 K.

For the computations of activity of both the components of each alloy namely In-Mg at 923 K, Cd-Mg at 923 K and In-Cd at 800 K from the equations (12) and (13), the theoretical values of activity coefficients of both the components of the concerned binary alloys are required. For this, the equations (9) and (10) are utilized to determine the theoretical values of both the components of the alloys such as In-Mg at 923 K, Cd-Mg at 923 K and In-Cd at 800 K. The theoretical results and corresponding experimental results [6] for both the components of the alloys under consideration are depicted in **Figure 3** with respect to the concentration.

For In-Mg liquid alloys at 923 K, the theoretical results for a_{In} and a_{Mg} are compared with the correlated experimental results [1] which are in well harmony as illustrated in **Figure 3**. The negative departures of a_{In} and a_{Mg} from ideal mixing value refer to the ordering character [36] for In-Mg melts at 923 K. It is remarkable to mention that the well harmony between theory and experiment for a_{In} and a_{Mg} validates the reasonable values of A_{ji} and A_{ij}.

For comparison of a_{Cd} and a_{Mg} of Cd-Mg melts at 923 K, the theoretical

results and corresponding experimental results [1] are illustrated in **Figure 3**. A well concord is noticed between theory and experiment. The negative deviations of a_{Cd} and a_{Mg} from ideal behavior stand for the ordering nature [36] of Cd-Mg melts at 923 K. Again, the harmony between theory and experiment provides the validity to the approximated values of A_{ji} and A_{ij}.

For In-Cd melts at 800 K, the theoretical results as well as correlated experimental results of a_{In} and a_{Cd} [1] are mentioned in **Figure 3**. A well harmony is observed between theory and experiment. The positive deviations of a_{In} and a_{Cd} from ideal mixing behavior advocate the segregating character [36] of In-Cd melts at 800 K. Again, the harmony between theory and experiment justifies the evaluated values of A_{ji} and A_{ij}.

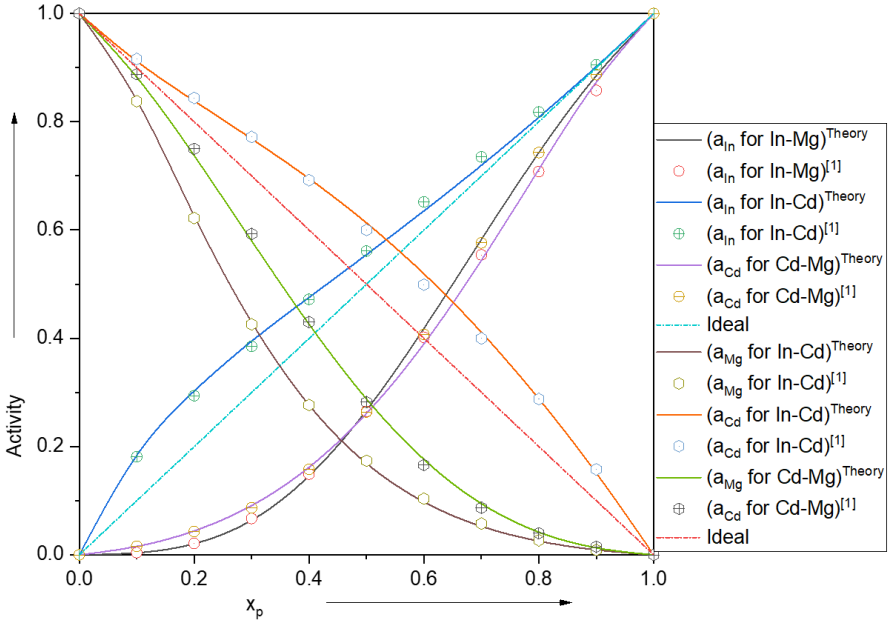


Figure 3. Activity vs X_p (p = In, Cd, In) for In-Mg melts at 923 K, In-Cd melts at 923 K and Cd-Mg melts at 800 K.

3.2. Results for G_M^E, G_M and $a_\mu(\mu = i, j)$ of Mg-In-Cd Melts at 850 K

The MIVM model has further been employed to investigate the thermodynamic behaviour of Mg-In-Cd melts at 850 K in terms of G_M^E/RT, G_M/RT, γ_{Mg} and a_{Mg} as a function of concentration of Mg. For the computations of the thermodynamic properties of Mg-In-Cd melts, the required input parameters for the concerned binaries are evaluated at 850 K.

At a desired temperature *i.e.* TK, the values of A_{ji} and A_{ij} are estimated using equations [21] as mentioned below

$$-\frac{\varepsilon_{ji}-\varepsilon_{ii}}{kT} = T\ln A_{ji}(T) = T_0 \ln A_{ji}(T_0)$$

$$A_{ji}(T) = \exp\left(\frac{T_0 \ln A_{ji}(T_0)}{T}\right) \tag{22}$$

and

$$-\frac{\varepsilon_{ij}-\varepsilon_{jj}}{kT}=T\ln A_{ij}\left(T\right)=T_0\ln A_{ij}\left(T_0\right)$$

$$A_{ij}=\exp\left(\frac{T_0\ln A_{ij}\left(T_0\right)}{T}\right) \tag{23}$$

where, T_0 = 923 K (for In-Mg and Cd-Mg); and 800 K (for In-Cd)

The evaluated input parameters are mentioned in **Table 3**.

Table 3. Input parameters for binary systems.

$i-j$	T(K)	V_{mi} (cm³/mole)	V_{mj} (cm³/mole)	A_{ij}	A_{ji}	Z_i	Z_j
Cd-Mg	850	14.57	15.12	1.1142	1.3293	9.56	9.81
In-Cd	850	16.96	14.57	1.1752	0.7132	9.55	9.56
In-Mg	850	16.96	15.12	1.7663	0.9258	9.55	9.81

Now, expression (1) is utilized to determine the theoretical values of G_M^E/RT relative to the concentration of Mg for Mg-In-Cd liquid alloys at 850 K for the cross-sections namely, $x_{Cd}:x_{In}$ = 3:2, 2:3 and 1:4. The choice of these cross sections is due to the fact that the activities of the component, Mg for Mg-In-Cd melts at 850 K are available in the literature [3]. The theoretical results of G_M^E/RT for Mg-In-Cd melts at 850 K relative to the composition of Mg are reported in **Table 4** and displayed in **Figure 4**. It is obvious that, for each cross-section, G_M^E/RT exhibit negative value at each composition of Mg in the region, x_{Mg} = 0.1 to 0.9 for Mg-In-Cd melts at 850 K. The negative values of G_M^E/RT for each cross-section in the entire concentration range indicate that Mg-Cd and Mg-In are the dominating systems in Mg-In-Cd melts at 850 K as a result of which Mg-In-Cd melt at 850 K is an ordered system. Again, the magnitude and position of minima are changed on changing the cross-section *i.e.* the minimum values of G_M^E/RT are – 0.8265 at x_{Mg} = 0.6 for cross-section $x_{Cd}:x_{In}$ = 3:2; which is followed by – 0.7958 at x_{Mg} = 0.4 for cross-section 1:4; and – 0.7896 at x_{Mg} = 0.5 for cross-section 2:3 respectively. In the region $0.0\le x_{Mg}\le 0.4$, the values of G_M^E/RT are minimum for cross-section 1: 4 which is followed by those for the cross-sections 2:3 and 3:2 respectively and in the region $0.5\le x_{Mg}\le 1.0$, the values of G_M^E/RT are minimum for cross-section 3:2 which is followed by those for the cross-sections 2:3 and 1:4 respectively. It is necessary to mention that the experimental results for Mg-In-Cd melts at 850 K are not found in the literature for comparison.

Expression (21) is used to ascertain the theoretical values of G_M/RT for Mg-In-Cd liquid alloys at 850 K for the aforesaid cross-sections. The theoretical results of G_M/RT are mentioned in **Table 5** and shown in **Figure 5**. Obviously, G_M/RT indicates negative value at each concentration of Mg in the region, x_{Mg} = 0.1 to 0.9 for Mg-In-Cd melts at 850 K for each cross-section. The negative value

of G_M/RT is minimum for the cross-section $x_{Cd}:x_{In}$ = 3:2 followed by that for the cross-section 2:3 and 1:4 respectively in the composition region $0.0 \le x_{Mg} \le 0.3$ and in the region, $0.4 \le x_{Mg} \le 0.1$, the negative value of

Table 4. G_M^E/RT for Mg-In-Cd Liquid Alloys at 850 K.

For $x_{Cd}:x_{In}=3:2$			
x_{Mg}	x_{Cd}	x_{In}	G_M^E/RT
0.1000	0.5400	0.3600	−0.1158
0.2000	0.4800	0.3200	−0.3802
0.3000	0.4200	0.2800	−0.5878
0.4000	0.3600	0.2400	−0.7347
0.5000	0.3000	0.2000	−0.8161
0.6000	0.2400	0.1600	−0.8265
0.7000	0.1800	0.1200	−0.7591
0.8000	0.1200	0.0800	−0.6057
0.9000	0.0600	0.0400	−0.3566
For $x_{Cd}:x_{In}=2:3$			
x_{Mg}	x_{Cd}	x_{In}	G_M^E/RT
0.1000	0.3600	0.5400	−0.2308
0.2000	0.3200	0.4800	−0.4580
0.3000	0.2800	0.4200	−0.6282
0.4000	0.2400	0.3600	−0.7395
0.5000	0.2000	0.3000	−0.7896
0.6000	0.1600	0.2400	−0.7756
0.7000	0.1200	0.1800	−0.6941
0.8000	0.0800	0.1200	−0.5411
0.9000	0.0400	0.0600	−0.3116
For $x_{Cd}:x_{In}=1:4$			
x_{Mg}	x_{Cd}	x_{In}	G_M^E/RT
0.1000	0.1800	0.7200	−0.5027
0.2000	0.1600	0.6400	−0.6506
0.3000	0.1400	0.5600	−0.7483
0.4000	0.1200	0.4800	−0.7958
0.5000	0.1000	0.4000	−0.7932
0.6000	0.0800	0.3200	−0.7398
0.7000	0.0600	0.2400	−0.6349
0.8000	0.0400	0.1600	−0.4775
0.9000	0.0200	0.0800	−0.2664

G_M/RT becomes minimum for cross-sections 1 :4 followed 2 :3 and 3:2 respectively. Overall, the magnitude of G_M/RT is minimum *i.e.* – 1.8458 at x_{Mg} = 0.5 for cross-section 3:2; – 1.8192 for cross-section 2:3 at x_{Mg} = 0.5 and – 1.7691 for cross-section 1:4 at x_{Mg} = 0.4. Thus, the theoretical results predict that Mg-In-Cd melts at 850 K have lowest values of G_M/RT for cross-section $x_{Cd}:x_{In}$ = 3:2 followed by $x_{Cd}:x_{In}$ = 2:3 and $x_{Cd}:x_{In}$ = 1:4 respectively.

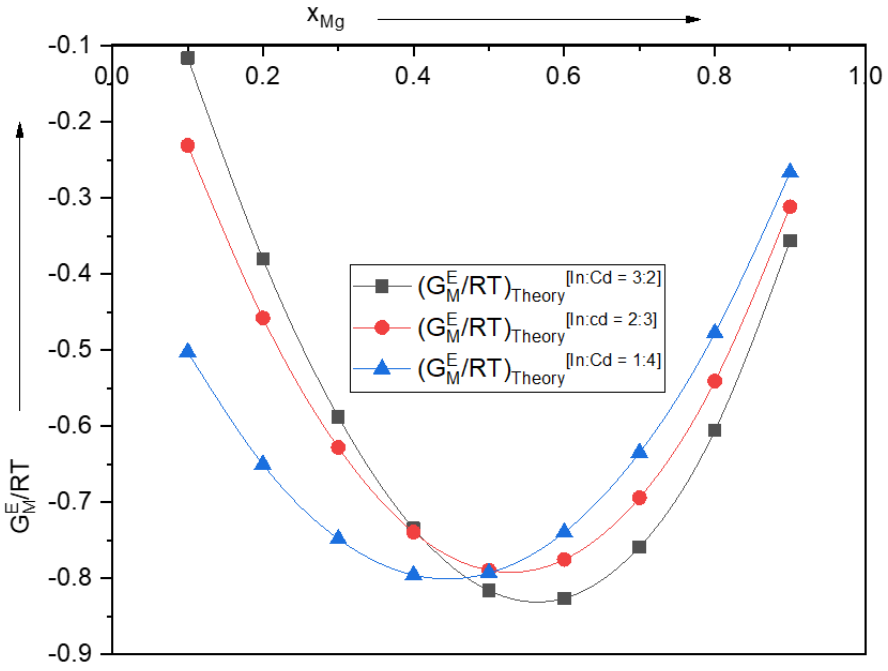


Figure 4. G_M^E/RT vs x_{Mg} for Mg-In-Cd system at 850 K for cross-sections, $x_{Cd}:x_{In}$ = 3:2, 2:3 and 1:4.

Table 5. G_M/RT for Mg-In-Cd Liquid Alloy at 850 K.

For $x_{Cd}:x_{In}=3:2$			
x_{Mg}	G_M^E/RT	G_M^{id}/RT	G_M/RT
0.1000	−0.1158	−0.9308	−1.0466
0.2000	−0.3802	−1.0388	−1.4190
0.3000	−0.5878	−1.0820	−1.6697
0.4000	−0.7347	−1.0768	−1.8115
0.5000	−0.8161	−1.0297	−1.8458
0.6000	−0.8265	−0.9422	−1.7687
0.7000	−0.7591	−0.8128	−1.5718
0.8000	−0.6057	−0.6350	−1.2407
0.9000	−0.3566	−0.3924	−0.7490
For $x_{Cd}:x_{In}=2:3$			
x_{Mg}	G_M^E/RT	G_M^{id}/RT	G_M/RT
0.1000	−0.2308	−0.9308	−1.1616

Continued

0.2000	**−0.4580**	**−1.0388**	**−1.4968**
0.3000	−0.6282	−1.0820	−1.7101
0.4000	−0.7395	−1.0768	−1.8163
0.5000	−0.7896	−1.0297	−1.8192
0.6000	−0.7756	−0.9422	−1.7178
0.7000	−0.6941	−0.8128	−1.5069
0.8000	−0.5411	−0.6350	−1.1761
0.9000	−0.3116	−0.3924	−0.7040
For $x_{Cd} : x_{In} = 1:4$			
x_{Mg}	G_M^E/RT	G_M^{id}/RT	G_M/RT
0.1000	−0.5027	−0.7754	−1.2782
0.2000	−0.6506	−0.9007	−1.5513
0.3000	−0.7483	−0.9611	−1.7094
0.4000	−0.7958	−0.9733	−1.7691
0.5000	−0.7932	−0.9433	−1.7365
0.6000	−0.7398	−0.8732	−1.6129
0.7000	−0.6349	−0.7610	−1.3959
0.8000	−0.4775	−0.6005	−1.0780
0.9000	−0.2664	−0.3751	−0.6416

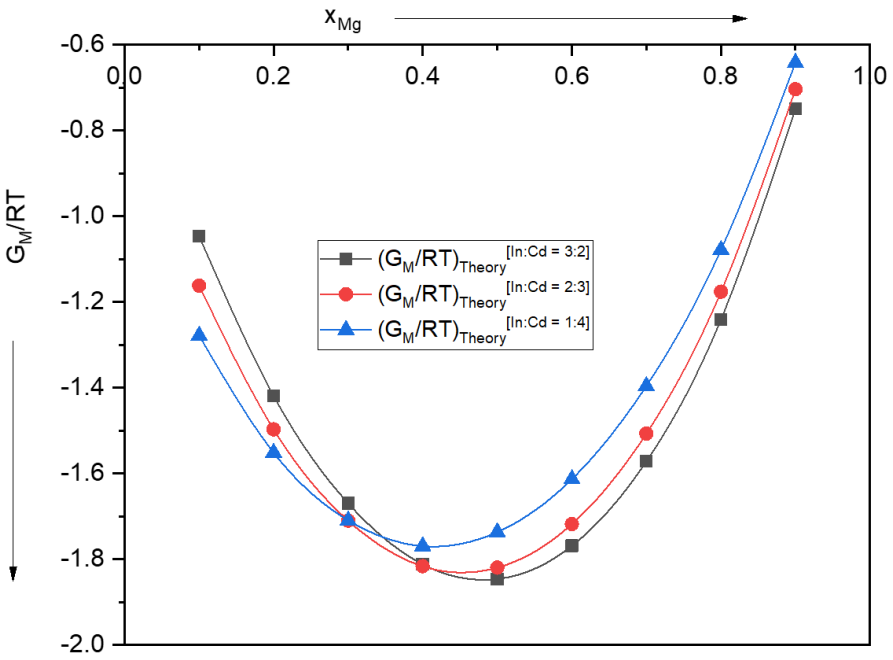


Figure 5. G_M/RT vs x_{Mg} for Mg-In-Cd system at 850 K for cross-sections, $x_{Cd} : x_{In}$ = 3:2, 2:3 and 1:4.

Equation (17) is used to determine the concentration dependence of γ_{Mg} for Mg-In-Cd liquid alloys at 850 K on using the same values of input parameters in

order to maintain the consistency for the cross-sections $x_{Cd} : x_{In}$ = 3:2, 2:3 and 1:4. The theoretical results are reported in Table 6 and displayed in Figure 6. It is obvious that the value of γ_{Mg} increases on increasing the composition of Mg for each cross-section. Overall, the values of γ_{Mg} are maximum for the cross-section 1:4 followed by that for cross-sections 2:3 and 3:2 respectively.

Table 6. Activity Coefficient of Mg in Mg-In-Cd Ternary Liquid Alloys at 850 K.

For $x_{Cd} : x_{In} = 3:2$			
x_{Mg}	x_{Cd}	x_{In}	γ_{Mg}
0.1000	0.5400	0.3600	0.0687
0.2000	0.4800	0.3200	0.1080
0.3000	0.4200	0.2800	0.1654
0.4000	0.3600	0.2400	0.2464
0.5000	0.3000	0.2000	0.3553
0.6000	0.2400	0.1600	0.4930
0.7000	0.1800	0.1200	0.6526
0.8000	0.1200	0.0800	0.8151
0.9000	0.0600	0.0400	0.9861
For $x_{Cd} : x_{In} = 2:3$			
x_{Mg}	x_{Cd}	x_{In}	γ_{Mg}
0.1000	0.3600	0.5400	0.0624
0.2000	0.3200	0.4800	0.1066
0.3000	0.2800	0.4200	0.1727
0.4000	0.2400	0.3600	0.2655
0.5000	0.2000	0.3000	0.3868
0.6000	0.1600	0.2400	0.5331
0.7000	0.1200	0.1800	0.6926
0.8000	0.0800	0.1200	0.8435
0.9000	0.0400	0.0600	1.0194
For $x_{Cd} : x_{In} = 1:4$			
x_{Mg}	x_{Cd}	x_{In}	γ_{Mg}
0.1000	0.1800	0.7200	0.0733
0.2000	0.1600	0.6400	0.1289
0.3000	0.1400	0.5600	0.2101
0.4000	0.1200	0.4800	0.3188
0.5000	0.1000	0.4000	0.4520
0.6000	0.0800	0.3200	0.6006
0.7000	0.0600	0.2400	0.7494
0.8000	0.0400	0.1600	0.8787
0.9000	0.0200	0.0800	1.0563

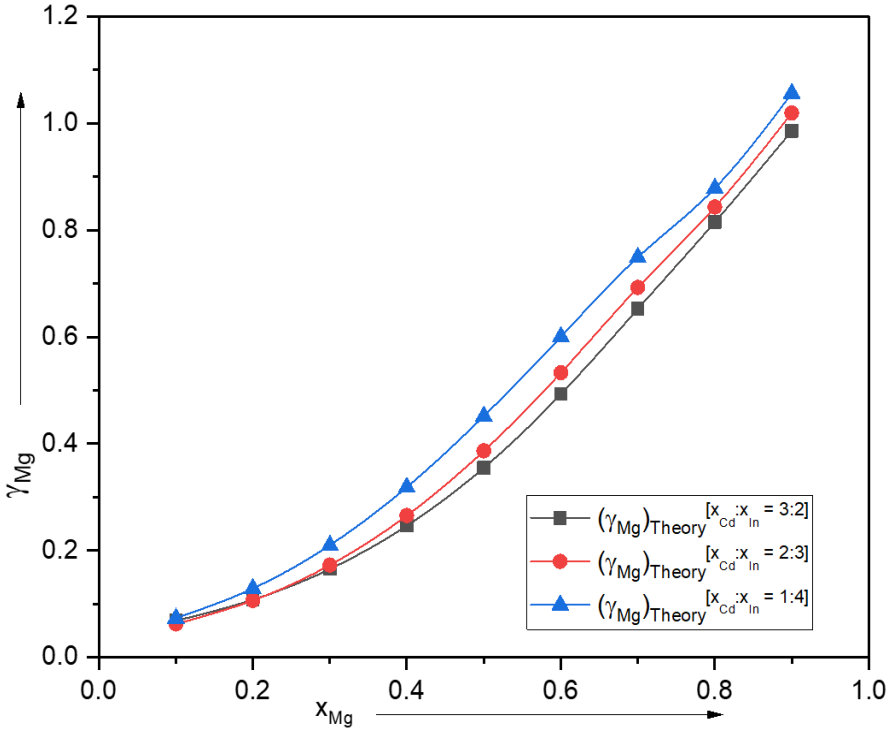


Figure 6. γ_{Mg} vs x_{Mg} for Mg-In-Cd system at 850 K for cross-sections, $x_{Cd} : x_{In}$ = 3:2, 2:3 and 1:4.

The activity, a_{Mg} for Mg-In-Cd at 850 K has been calculated from equation (18) on using the theoretical results of γ_{Mg} for the aforementioned cross-sections. The theoretical data for a_{Mg} of Mg-In-Cd at 850 K are presented in **Table 7** and illustrated in **Figure 7**. The experimental data for the concentrations, x_{Mg} = 0.1 to 0.6 of a_{Mg}, available in the literature [3] are also included in **Table 7** and **Figure 7**. The a_{Mg} - x_{Mg} isotherms [**Figure 7(a)~(c)**] indicate reasonable agreement between the theoretical results and experimental results of a_{Mg} for each cross-section in the region, $0.0 \le x_{Mg} \le 0.6$. The theoretical results for a_{Mg} of Mg-In-Cd at 850 K exhibit negative deviation from ideal mixing behavior for each cross-section under consideration in the concentration region, $0.0 \le x_{Mg} \le 0.85$, which refers to the ordering nature of Mg-In-Cd melts at 850 K. However, the Mg-In-Cd melt at 850 K demonstrate weak segregating nature beyond x_{Mg} = 0.85 as mentioned in **Figure 7(d)**.

Table 7. Activity of Mg in Mg-In-Cd Liquid Alloys at 850 K.

For $x_{Cd} : x_{In} = 3 : 2$					
x_{Mg}	x_{Cd}	x_{In}	a_{Mg} (Theory)	a_{Mg} [3]	$\lvert a_{Mg,\text{Expt.}} - a_{Mg,\text{Theory}} \rvert$
0.1000	0.5400	0.3600	0.007	0.010	0.003
0.2000	0.4800	0.3200	0.022	0.026	0.005
0.3000	0.4200	0.2800	0.050	0.052	0.002
0.4000	0.3600	0.2400	0.099	0.109	0.011

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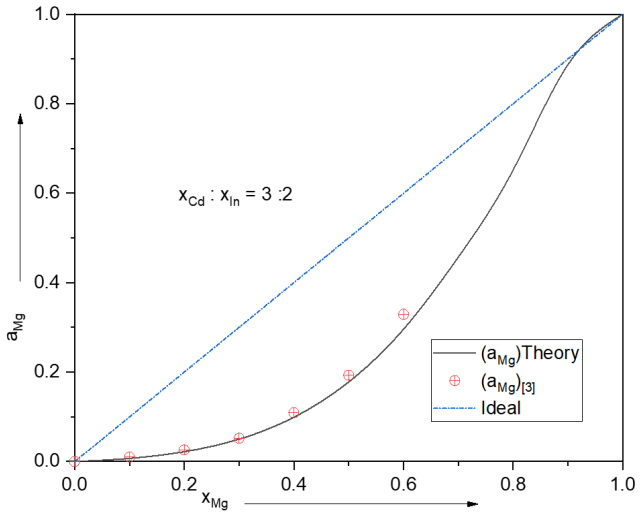
0.5000	**0.3000**	**0.2000**	**0.178**	**0.193**	**0.016**
0.6000	0.2400	0.1600	0.296	0.329	0.014
0.7000	0.1800	0.1200	0.457	-	
0.8000	0.1200	0.0800	0.652	-	
0.9000	0.0600	0.0400	0.887	-	

For $x_{Cd} : x_{In} = 2:3$

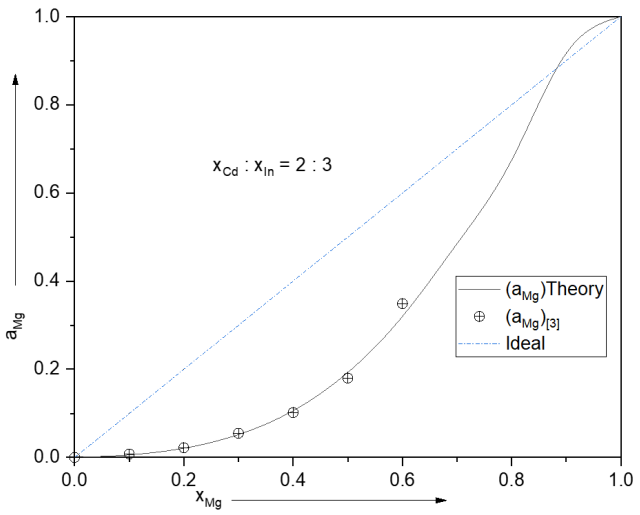
x_{Mg}	x_{Cd}	x_{In}	a_{Mg} (Theory)	a_{Mg} [3]	$\lvert a_{Mg,\text{Expt.}} - a_{Mg,\text{Theory}} \rvert$
0.1000	0.3600	0.5400	0.006	0.008	0.002
0.2000	0.3200	0.4800	0.021	0.022	0.001
0.3000	0.2800	0.4200	0.052	0.055	0.003
0.4000	0.2400	0.3600	0.106	0.102	0.004
0.5000	0.2000	0.3000	0.193	0.180	0.013
0.6000	0.1600	0.2400	0.320	0.349	0.061
0.7000	0.1200	0.1800	0.485	-	
0.8000	0.0800	0.1200	0.675	-	
0.9000	0.0400	0.0600	0.917	-	

For $x_{Cd} : x_{In} = 1:4$

x_{Mg}	x_{Cd}	x_{In}	a_{Mg} (Theory)	a_{Mg} [3]	$\lvert a_{Mg,\text{Expt.}} - a_{Mg,\text{Theory}} \rvert$
0.1000	0.1800	0.7200	0.007	0.009	0.001
0.2000	0.1600	0.6400	0.026	0.022	0.004
0.3000	0.1400	0.5600	0.063	0.048	0.015
0.4000	0.1200	0.4800	0.128	0.091	0.036
0.5000	0.1000	0.4000	0.226	0.178	0.048
0.6000	0.0800	0.3200	0.360	0.293	0.231
0.7000	0.0600	0.2400	0.525	-	
0.8000	0.0400	0.1600	0.703	-	
0.9000	0.0200	0.0800	0.951	-	



(a)



(b)

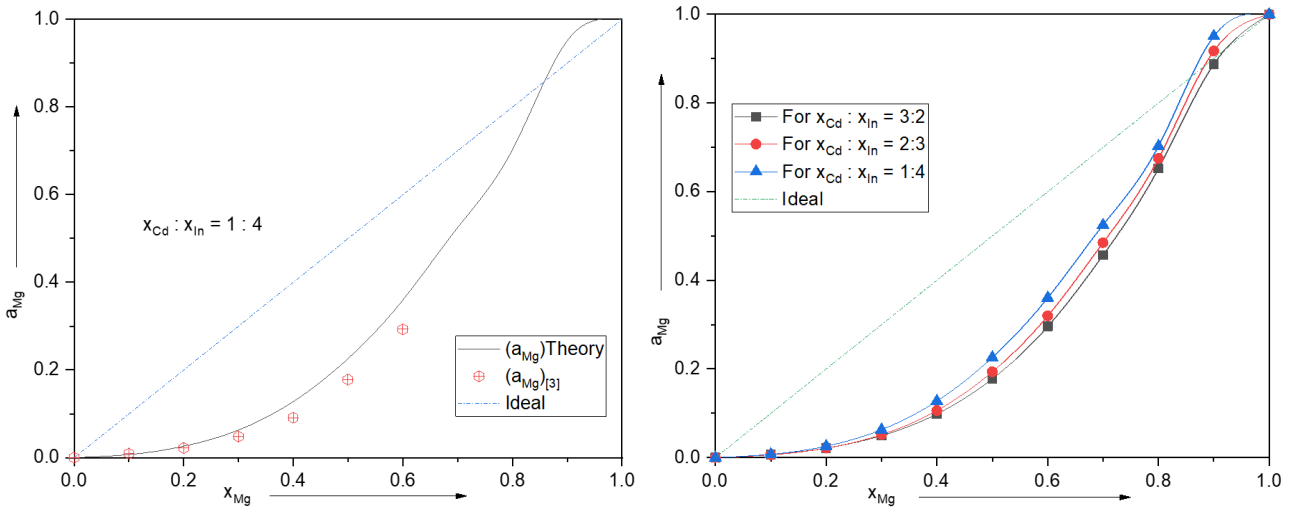


Figure 7. (a) a_{Mg} vs x_{Mg} for Mg-In-Cd system at 850 K for cross-sections, $x_{Cd} : x_{In}$ = 3:2; (b) a_{Mg} vs x_{Mg} for Mg-In-Cd system at 850 K for cross-sections, $x_{Cd} : x_{In}$ = 2:3; (c) a_{Mg} vs x_{Mg} for Mg-In-Cd system at 850 K for cross-sections, $x_{Cd} : x_{In}$ = 1:4; (d) a_{Mg} vs x_{Mg} for Mg-In-Cd system at 850 K for cross-sections, $x_{Cd} : x_{In}$ = 3:2, 2:3 and 1:4.

The standard errors for a_{Mg} have been computed from the equation given below:

$$\text{Standard error}\left(S_i^*\right) = \pm\left[\frac{1}{n}\sum_{i=1}^{n}\left(a_{i,\text{Expt}} - a_{i,\text{Pre}}\right)^2\right]^{1/2} \tag{24}$$

The computed values of the standard errors for a_{Mg} are found to be 0.0099%, 0.0255% and 0.0977% respectively for cross-sections $x_{Cd} : x_{In}$ = 3:2, 2:3 and 1:4.

4. Conclusions

From present theoretical study, it may be concluded that

- The theoretical results of G_M^E and G_M agree well with the correlated experimental results available in the literature for the systems like In-Mg at 923 K, Cd-Mg at 923 K and In-Cd at 800 K.
- The observed asymmetries in G_M^E/RT for In-Mg at 923 K and In-Cd at 800 K, as well as symmetries in G_M^E/RT for Cd-Mg at 923 K are successfully explained.
- The sign and magnitude of the values of G_M^E/RT indicate that In-Mg and Cd-Mg at 923 K are weakly ordering in nature while In-Cd at 800 K is feebly segregating in nature.
- The negative departures of a_{In} and a_{Mg} for In-Mg at 923 K; a_{Cd} and a_{Mg} for Cd-Mg at 923 K from ideal mixing behavior indicate the weakly ordering character of the alloy *i.e.* In-Mg and Cd-Mg at 923 K, while the positive departures of a_{In} and a_{Cd} for In-Cd at 800 K from ideal mixing behavior exhibit the weakly segregating nature of the In-Cd at 800 K.
- The theoretical results for G_M^E/RT indicate that Mg-In-Cd melt at 850 K is an ordered system for each cross-section under consideration because the

values of G_M^E/RT are negative in the complete concentration region, x_{Mg} = 0.1 to 0.9.

- The concentration dependence of G_M/RT for Mg-In-Cd melts at 850 K shows that the values of G_M/RT are negative in the whole range of concentration for each cross-section having minima –1.8458 at x_{Mg} = 0.5 for cross-section $x_{Cd}:x_{In}$ = 3:2 followed by –1.8192 at x_{Mg} = 0.5 for cross-section $x_{Cd}:x_{In}$ = 2:3 and –1.7691 at x_{Mg} = 0.4 for cross-section $x_{Cd}:x_{In}$ = 1:4 respectively. This explores that Mg-In-Cd system at 850 K may be more stable for cross-section $x_{Cd}:x_{In}$ = 3:2 followed for the cross-section $x_{Cd}:x_{In}$ = 2:3 and $x_{Cd}:x_{In}$ = 1:4 respectively about x_{Mg} = 0.5.
- The theoretical results for a_{Mg} of Mg-In-Cd at 850 K calculated from the theoretical data of activity coefficient γ_{Mg}, exhibit good agreement with the corresponding experimental results for above mentioned cross sections in the concentration region x_{Mg} = 0.1 to 0.6. It is pointed out that the experimental results a_{Mg} of Mg-In-Cd at 850 K are available only for the concentrations x_{Mg} = 0.1 to 0.6 with negligible standard error. The present results of a_{Mg} indicate that Mg-In-Cd system at 850 K is an ordered system. However, in higher concentration region of Mg, Mg-In-Cd system at 850 K exhibits slightly segregating nature for the cross-section $x_{Cd}:x_{In}$ = 2:3 and $x_{Cd}:x_{In}$ = 1:4.

Thus, MIVM model is a reliable and suitable model to explain the thermodynamic behaviour of binary as well as ternary alloys.

Author Contributions

Conceptualization, I. S. Jha and J. Mandal; methodology, N. K. Roy; validation, I.S. Jha & J. Mandal; formal analysis, N. K. Roy, N. Kumari & S. K. Bhagat; investigation, N. K. Roy & S. K. Bhagat; writing original draft preparation, N. K. Roy; writing-review and editing, R. Prabhu; visualization, I. S. Jha; supervision, J. Mandal. All authors have read and agreed to published version of the manuscript.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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