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Research Article

MIXING PROPERTIES OF Cu-Mg LIQUID ALLOY USING EXPONENTIAL MODEL

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ABSTRACT

The Redlich-Kister (R-K) polynomial has been generally used to model the mixing properties of binary and higher order alloys. The interaction energy parameters of the R-K polynomial are assumed to be either linear or exponentially temperature-dependent. When these parameters are assumed to be linear temperature-dependent, the computed thermodynamic functions sometimes show unusual trends. But when they are assumed to be exponential temperature-dependent, such trends do not appear in the theoretical calculations. Therefore, the mixing properties of Cu-Mg liquid alloy have been studied using the exponential temperature-dependent parameters of the above-mentioned model. These parameters for excess Gibb's free energy of mixing have been optimised using the experimental values of enthalpy of mixing and excess entropy of mixing. The study of thermodynamic properties involves the measurement of excess Gibb's free energy of mixing, enthalpy of mixing and activities of monomers at different temperatures. Likewise, the assessment of surface property includes surface tension and surface concentration. Similarly, the structural properties have been studied by computing concentration fluctuation in long wave-length limit and short-range order parameter at different temperatures. The investigation revealed that the exponential model can explain mixing behavior of Cu-Mg liquid alloy and the system is found to have strong compound forming tendency at its melting temperature. This mixing tendency has been observed to decrease with the increase in temperature above its melting temperature.

Keywords: Cu-Mg alloy, R-K polynomial, surface concentration, surface tension, structural properties

INTRODUCTION

Today's world places a great deal of importance on alloys. The modern era has seen a revolution in the growth of technology, and one way of doing so is through the study of alloys and their formation, which is mainly done in the molten state of respective elements (Koirala *et al.*, 2013; Yadav *et al.*, 2016a; Yadav *et al.*, 2018a). The alloying phenomenon is becoming a very useful tool in the field of material science for the production of different types of materials with specific properties (Yadav *et al.*, 2018a). It has a wide range of applications in many fields like industries, medicine, automobiles, the military, nuclear reactors, piping systems, aeronautics (Yadav *et al.*, 2016b), etc. The study of the thermodynamic properties of liquid alloys is very important in alloying phenomena (Redlich & Kister, 1948; Desai, 1987; Zhou & Napolitano, 2007; Yadav *et al.*, 2015a) because the alloying process involves the mixing of elements to obtain desired materials at near-melting and elevated temperatures.

The enhancement of properties like corrosion resistance, high metallic strength, high conductivity, and resistance to oxidation (Yadav *et al.*, 2016a) has drawn the considerable consent of researchers working in this field. An intriguing Cu-based alloy with significant industrial use is the Cu-Mg alloy. Its employment in technological domains is advantageous due to its metallic glass composition (Godbole *et al.*, 2004). The wire of this alloy is utilized in the railway electrification system (Nairn, 2013). Some ternary alloys, such as Al-Cu-Mg, are important industrially as they have a variety of uses, like casting, step soldering, and radiation shielding. Additionally, the Pb-Sn alloy, which has a low melting point, is used for soldering. However, because lead is toxic, an excellent replacement is an alloy based on copper (Peng *et al.*, 1998). The Cu-Mg alloy with a glass-forming tendency is more important industrially and is used extensively (Zhou & Napolitano, 2007). Hence, the study of this system has great importance in the fields of material science and industry, and it has been the subject of several research studies (Hultgren *et al.*, 1973; Nayeb-Hashemi & Clark, 1984; Juneja *et al*, 1986; Feufel & Sommer, 1995; Godbole *et al.*, 2004; Kumar *et al.*, 2005; Zhou & Napolitano, 2007; Zhou *et al.*, 2007; Mezbahul-Islam *et al.*,2014; Yadav *et al.*, 2020). Recently, Yadav *et al.* (2020) have studied the mixing behaviours of the system using quasi-lattice model assuming the existence of the Cu_2Mg complex. They have assumed the linear temperature-dependence of the model fit parameters in order to assess the thermo-physical properties of the system at elevated temperatures.

To date, a number of theoretical models (Bhatia & Hargrove, 1974; Bhatia & Singh, 1980; Desai, 1987; Peng *et al.*, 1998; Godbole *et al.*, 2004; Awe *et al.*, 2008; Awe *et al.*, 2011; Nairn, 2013; Yadav *et al.*, 2015a; Kaptay, 2016;

Yadav *et al.*, 2016a; Fima & Novakovic, 2018; Yadav *et al.*, 2018a) have been suggested or revised in order to explain how various binary and ternary alloys are formed at varying temperatures. In this context, the Redlich-Kister polynomial has also been profoundly used to model the mixing properties of alloys. This polynomial is based on interaction energy parameters which can be assumed either linear or exponential temperature-dependent (Yuan *et al.*, 2009; Kaptay, 2016). It has been observed that when the interaction energy parameters are assumed to be linear temperature dependent, the mixing behaviours predicted by them sometimes, but not in all cases, do not show natural trends of variations. The main cause of such trends may be either due to poor optimisation of modeling parameters or due to their low temperature range acceptability. But when the interaction energy parameters of the R-K polynomial are assumed to be exponentially temperature-dependent, the above-mentioned properties are correctly predicted at elevated temperatures. Moreover, these parameters have a wide temperature range of acceptability. Therefore, exponential temperature dependent parameters have been optimised and used for the prediction of mixing behaviours of Cu-Mg liquid alloy at different temperatures in the present work.

In thermodynamic properties, excess Gibbs free energy of mixing (ΔG_M^{XS}), heat of mixing (ΔH_M), and activity (a_i =A,B) of the constituent atoms of the alloy have been computed. For the purpose, the exponential temperature-dependent interaction energy parameters of R-K polynomial for ΔG_M^{XS} have been optimised using the experimental data of ΔH_M and excess entropy of mixing (ΔS_M^{XS}) (Hultgren *et al.*, 1973). The validity of the model parameters has been tested by comparing the theoretically computed values with the experimental results. The same parameters have been then used to compute the structural functions, such as concentration fluctuation in long wavelength limit ($S_{CC}(0)$) and Warren-Cowley short range order parameter (α_1). The surface tension (σ) and surface concentration (C_i^s) of the system have been determined with the help of Renovated Butler model (Yuan *et al.*, 2009; Kaptay, 2017).

THEORETICAL FORMALISM

Thermodynamic Property

The determination and analysis of thermodynamic functions, such as excess Gibb's free energy of mixing, enthalpy of mixing, entropy of mixing, and activity of the constituent atoms, are required to understand the behaviour of binary system. The well-known formula that connects enthalpy of mixing, excess entropy of mixing, and excess Gibbs free energy of mixing (Bhatia & Hargrove, 1974; Singh *et al.*, 1990; Yuan *et al.*, 2009; Yadav *et al.*, 2015a; Yadav *et al.*, 2015b; Yadav *et al.*, 2016b; Cui & Jung, 2017; Yadav *et al.*, 2018a; Yadav *et al.*, 2018b; Gohivar *et al.*, 2021a; Gohivar *et al.*, 2021b; Mehta *et al.*, 2022) can be expressed as

$$\Delta G_M^{XS} = \Delta H_M - T\Delta S_M^{XS} \tag{1}$$

According to R-K polynomial (Redlich & Kister, 1948), the thermodynamic quantity (ΔY) for any binary liquid alloy system of type A-B can be expressed as

$$\Delta Y = C_A C_B \sum_{i=0}^{n} M_i\,(C_A - C_B)^i \tag{2}$$

where, ΔY is thermodynamic quantity that may be ΔG_M^{XS} or ΔH_M or ΔS_M^{XS} depending upon the value of M_i and C_A (i=A,B) is the concentration of element. The temperature dependent interaction parameter M_i in Equation (2) can be expressed by considering linear temperature dependence (Chen *et al.*, 2001; Kaptay, 2016) as

$$M_i = a_i + b_i T \tag{3}$$

where a_i is related to the enthalpy of mixing and b_i is related to the entropy of mixing for alloy. The values of a_i and b_i are determined by optimisation and Equation (3) is used to estimate M_i which is finally utilized for estimation of exponential temperature dependent interaction parameters from the following expression (Kaptay, 2004; Gohivar *et al.*, 2021b)

$$M_i = h_i exp\left(\frac{-T}{\tau_i}\right) \tag{4}$$

where h_i is the parameter associated with the enthalpy at temperature of zero Kelvin (T=0 K) and τ_i is temperature at which extraplotation of M_i linearly above temperature of zero Kelvin would cause sign change in parameter M_i. Here, the value of ΔG_M^{XS} can be calculated by

$$\Delta G_M^{XS} = C_A C_B \sum_{i=0}^{n} h_i exp\left(\frac{-T}{\tau_i}\right)(C_A - C_B)^i \tag{5}$$

Equation (5) gives the required values for excess Gibb's free energy of Cu-Mg liquid alloy at selected temperatures. Similarly, the excess entropy of mixing and enthalpy of mixing can be calculated from the expressions

$$\Delta S_M^{XS} = C_A C_B \sum_{i=0}^{n} \left(\frac{1}{\tau_i}\right) h_i exp\left(\frac{-T}{\tau_i}\right)(C_A - C_B)^i \tag{6}$$

and

$$\Delta H_M = C_A C_B \sum_{i=0}^{n} \left(1 + \frac{T}{\tau_i}\right) h_i exp\left(\frac{-T}{\tau_i}\right)(C_A - C_B)^i \tag{7}$$

To forecast the likelihood of compound formation from a liquid mixture, the activity of the monomers (a_{Cu} and a_{Mg}) is of utmost significance. To analyze the mixing behaviour of the binary liquid alloys, it is therefore required to calculate the activity of each component of the liquid mixture. This calculation can be done using expressions

$$a_A = C_A exp\left(\frac{\Delta G_A^{XS}}{RT}\right) \quad (8)$$

and

$$a_B = C_B exp\left(\frac{\Delta G_B^{XS}}{RT}\right) \quad (9)$$

where R is the universal gas constant whose value is 8.314 J/(molK) and T is the absolute temperature at which activity of the constituent element is to be calculated. Also, ΔG_A^{XS} and ΔG_B^{XS} represent partial excess Gibb's free energy of mixing for individual elements that are being mixed together.

SURFACE PROPERTIES

The study of the surface properties of the binary liquid alloy system involves the computation of surface tension (σ) of the system and surface concentration (C_i^s) of constituents. We can make the conclusion about which element among two in liquid mixture comes to the surface or segregates on the surface and which one will segregate to the bulk, from the calculation of surface tension and surface concentration of individual components (Koirala *et al.*, 2013; Yadav *et al.*, 2015b; Fima & Novakovic, 2018; Yadav *et al.*, 2018a).

The Renovated Butler model (Cui & Jung, 2017; Yadav *et al.*, 2018b) is used for investigation of surface properties using equation

$$\sigma = \sigma_A^0 \frac{\lambda_A^0}{\lambda_A} + \frac{RT}{\lambda_A}\ln\left(\frac{C_A^S}{C_A}\right) + \frac{\Delta G_{S,A}^{XS} - \Delta G_A^{XS}}{\lambda_A} = \sigma_B^0 \frac{\lambda_B^0}{\lambda_B} + \frac{RT}{\lambda_B}\ln\left(\frac{C_B^S}{C_B}\right) + \frac{\Delta G_{S,B}^{XS} - \Delta G_B^{XS}}{\lambda_B} \quad (10)$$

where σ = surface tension of the liquid mixture at its melting temperature, $\sigma_i^0 =$ surface tension for pure ith component of liquid mixture, λ_i = molar surface area of ith component in liquid mixture and λ_i^0 = molar surface area of ith component of pure liquid. Here, the molar surface area of component in pure liquid is equal to molar surface area of component in liquid solution i.e. $\lambda_i^0 = \lambda_i$(Yadav *et al.*, 2017; Yadav *et al.*, 2018b). Moreover, $\Delta G_{S,i}^{XS}$and $\Delta G_i^{XS}$are respectively the surface partial excess free energy and bulk partial excess free energy for the ith component of binary liquid alloy.

STRUCTURAL PROPERTIES

The concentration fluctuation in long wavelength limit and short-range order parameter can be utilized for the study of structural property for binary liquid alloy. These two parameters can be calculated by using the expressions (Akinlade, 1996; Singh & Sommer, 1997)

$$S_{cc}(0) = \frac{RT}{\frac{RT}{C_A C_B} - 2M_0 - (12C_A - 6)M_1 - (48{C_A}^2 - 48C_A + 10)M_2 - (160{C_A}^3 - 240{C_A}^2 + 108C_A - 14)M_3} \quad (11)$$

$$\text{and, } \alpha_1 = \frac{\Phi - 1}{1 + \Phi(Z-1)} \quad (12)$$

where Φ is the parameter that is related with $S_{cc}(0)$ and $S_{cc}^{ideal}(0)$ by the expression

$$\Phi = \frac{S_{cc}(0)}{S_{cc}^{ideal}(0)} \quad (13)$$

And the parameter Z is called co-ordination number whose value is taken to be 10 in this work. Here, the ideal value of $S_{cc}(0)$ is calculated by

$$S_{cc}^{ideal}(0) = C_A C_B \quad (14)$$

RESULTS AND DISCUSSION

Thermodynamic Properties

For the theoretical investigation of thermodynamic properties of alloy at molten state, optimization technique for R-K polynomial has been carried out. Here, the interaction energy parameters for excess Gibbs free energy of mixing (ΔG_M^{XS}) have been first assumed to be linearly temperature dependent and with this assumption, the parameter a_i and b_i are determined with the help of Eq. (1-3) and the experimental values of the enthalpy of mixing (ΔH_M) and excess entropy of mixing (ΔS_M^{XS}) of Cu-Mg liquid alloy (Hultgren *et al.*, 1973). These values have been then used to determine the exponential temperature dependent parameters using Eqs. (4-7). The optimised values of this work and linear parameters from the work of Yadav *et al.* (2020) are presented in Table 1.

Table 1. The optimised energy interaction parameters for ΔG_M^{XS} for Cu-Mg system

Interaction energy parameters		
This work [Exponential]		Yadav *et al.* (2020) [Linear] [J/mol]
h_i [J/mol]	τ_i [J/mol]	
$h_0 = -45145$	$\tau_0 = 2143$	$\omega = -18058.6 + 10.1431 * dT$
$h_1 = -9743$	$\tau_1 = 17015$	$\omega_{AB} = -16131.1 + 6.48492 * dT$
$h_2 = -23$	$\tau_2 = -270$	$\omega_{AA} = -16465.3 + 0.08314 * dT$
$h_3 = 857217$	$\tau_3 = 82$	

These parameters have been then used to calculate values of ΔG_M^{XS} for the system at the temperature 1100 K. The values computed using the exponential parameters of this work and experimental data (Hultgren *et al.*, 1973) are plotted as a function of concentration of Cu in Figure 1. It can be observed that the values computed using the parameters of this work are consistent with the experimental data and the results from the work of Yadav *et al.* (2020). This establishes the validity of the present optimisation procedure.

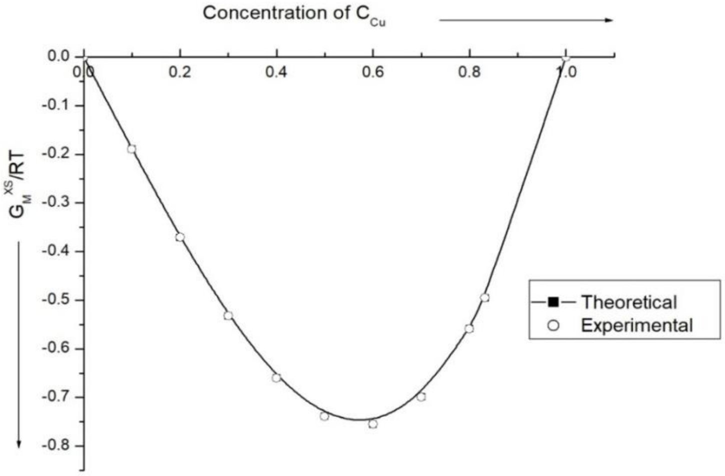

Figure 1: $\Delta G_M^{XS}/\mathrm{RT}$ vs concentration of Cu at 1100 K

Further, the values of ΔG_M^{XS} for this system are found negative throughout the entire concentration range which signify that the system is completely ordering in nature at 1100 K. The maximum negative value of ΔG_M^{XS} as calculated theoretically is -0.7555 RT and experimentally is -0.7551 RT at the concentration of copper C_{Cu} = 0.6. This result concludes that there is tendency of hetero-atomic bonding of the system at 1100 K. The same optimised interaction parameters (Table 1) have been used to investigate ΔG_M^{XS} of the system at elevated temperatures using Equation (5) and they are plotted in Figure 2.

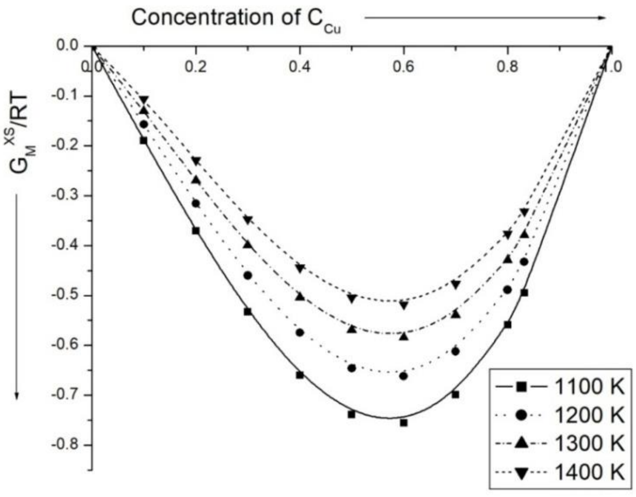

Figure 2. ΔG_M^{XS}**/RT vs** C_{Cu}**for Cu-Mg liquid alloy at different temperatures**

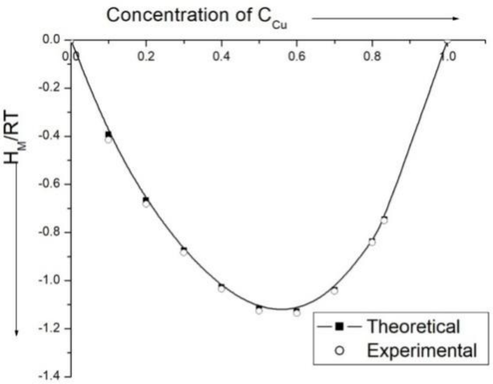

Figure 3. Theoretical and experimental values of $\Delta H_M/RT$ **vs concentration of Cu at 1100 K temperature**

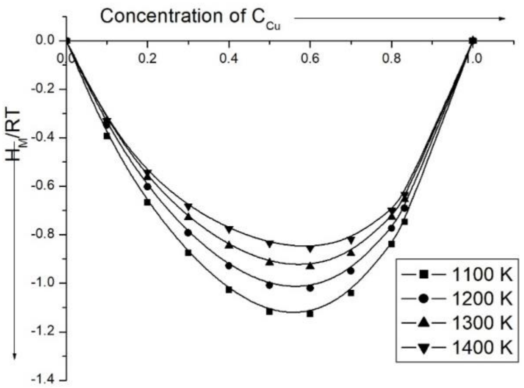

Figure 4. Δ**H**$_M$**/RT vs**C_{Cu}**for Cu-Mg liquid alloy at different temperatures**

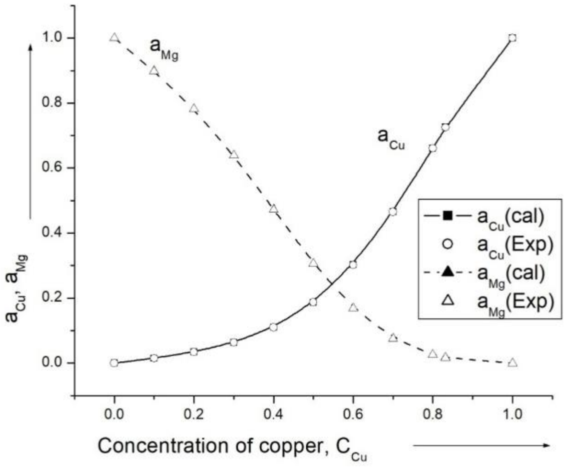

Figure 5. Plots of activities of Cu (a_{Cu}**) and Mg (**a_{Mg}**) vs concentration of Cu for Cu-Mg liquid alloy at 1100 K**

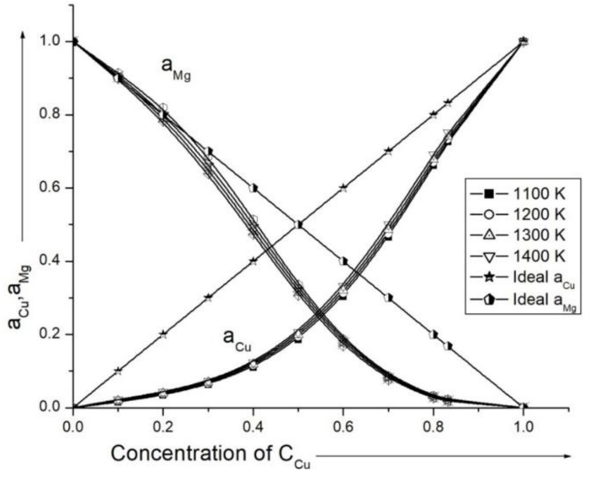

Figure 6. Activity vs C_{Cu} **for Cu-Mg liquid alloy at different temperatures**

It can be observed that the plot of ΔG_M^{XS} vs C_{Cu} gradually shallows up with rise in temperature indicating the gradual decrement of its negative values with increased temperature above 1100 K (Figure 2). The maximum negative value of ΔG_M^{XS} at 1100 K, 1200K, 1300 K and 1400 K are computed to be -0.7555 RT, -0.6621 RT, -0.5841 RT and -0.5179 RT respectively at the concentration of Cu, $C_{Cu} = 0.6$. These results conclude that the compound forming tendency of liquid mixture continuously decreases with the rise in temperature above its melting temperature and it is pronounced at its melting temperature. This finding is in accordance with the results of Yadav *et al.* (2020).

The total quantity of heat contained in the system is represented by its enthalpy (ΔH_M), which is linked to its internal energy. The positive and the negative values of ΔH_M of the metallic solution depend on the types of components being mixed. When two or more elements are mixed, the low negative or positive value of ΔH_M indicates the demixing or segregating tendency of system whereas its high negative value represents ordering or complex formation tendency (Singh *et al.*, 1990; Yadav *et al.*, 2018a). However, when ΔH_M=0, mixing is assumed to be ideal in nature.

The values of ΔH_M have been computed at 1100 K using Equation (7) and the parameters of Table 1. The computed values are plotted as a function of concentration of Cu in Figure 3. It can be observed that the values computed using optimised parameters of this work are found to be consistent with the experimental data (Hultgren *et al.*, 1973) and the results from the work of Yadav *et al.* (2020). Moreover, the values of ΔH_M are found to be negative indicating the compound forming tendency at its melting temperature. Following the similar method, ΔH_M has been computed at different temperatures and plotted in Figure 4. The computed values of ΔH_M gradually decrease with increase in temperature of the system indicating gradual decrease in compound forming tendency of the system beyond its melting temperature. These results confirm the findings obtained from the study of ΔG_M^{XS}.

The activities of monomers of Cu-Mg liquid alloy at 1100 K and different temperatures have been theoretically calculated using Equations (5), (8) and (9) and parameters from Table 1. The computed values of this work and experimental values (Hultgren *et al.*, 1973) as a function of concentration of Cu are plotted in Figures 5 and 6. This comparison reveals that theoretically computed values of activities of monomers and experimental data are in well agreement (Figure 5). Thus, the optimised exponential parameters of this work have well explained the thermodynamic properties of the system. Moreover, the computed values of activities of the components Cu and Mg gradually increase with increase in the temperature of the system corresponding to the decrease in its compound forming tendency (Figure 6). These findings are in accordance with the results predicted by ΔG_M^{XS} and ΔH_M as computed above.

SURFACE PROPERTIES

The surface tension (σ) and the surface concentration (C_i^S) of each constituent of Cu-Mg liquid alloy at the melting temperature have been calculated using Equation (10),parameters from Table 2 and partial excess Gibbs free energy (ΔG_i^{XS}; $i = Cu, Mg$). ΔG_i^{XS} have been estimated with the help of parameters in Table 1 and the relation $\Delta G_i^{XS} = RT \ln\left(\frac{a_i}{C_i}\right)$, where the terms have meanings as stated above. Herein, the required values of surface tension (σ_i^0) and density (ρ_i^0) of pure component i at the temperature of interest (T_k) have been calculated using the following relations (Brandes & Brook, 1992)

$$\sigma_i^0 = \sigma^0 + \frac{d\sigma}{dT}(T_k - T_0) \text{ and } \rho_i^0 = \rho^0 + \frac{d\rho}{dT}(T_k - T_0) \tag{15}$$

where T_0 is the melting temperature of component i and $d\sigma/dT$ and $d\rho/dT$ are the temperature derivative terms of surface tension and density respectively.

Table 2. Input parameters for surface tension (Brandes & Brook, 1992)

Element	T_0 (K)	ρ^0 ($\mathrm{kgm^{-3}}$)	$d\rho/dT$ ($\mathrm{kgm^{-3}K^{-1}}$)	σ^0 ($\mathrm{Nm^{-1}}$)	$d\sigma/dT$ ($\mathrm{mNm^{-1}K^{-1}}$)
Cu	1356	8000	-0.80	1.285	-0.13
Mg	924	1590	-0.2647	0.559	-0.35

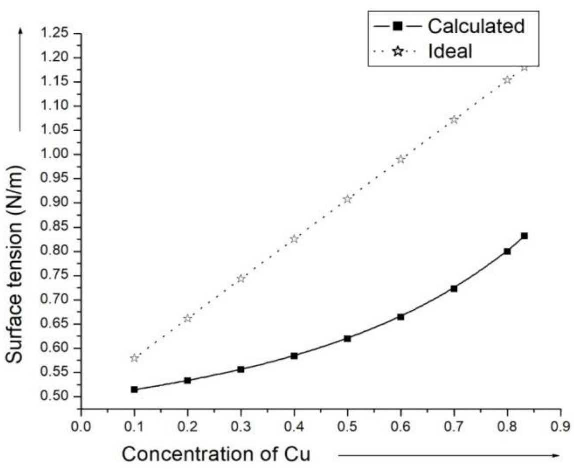

Figure 7. σ vs C_{Cu} for Cu-Mg liquid alloy at 1100 K

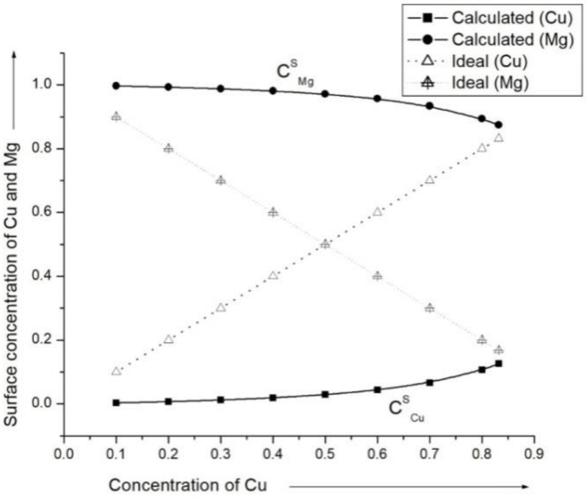

Figure 8. C_i^S vs $C_{Cu}$for Cu-Mg liquid alloy at 1100 K

The computed values of σ and $C_i^S$for the binary liquid alloy at 1100 K are plotted in Figures 7 and 8 respectively. The surface tension of the system gradually increases with increase in the bulk concentration of Cu, and it is found to be less than ideal value at all bulk concentrations (Figure 7). The surface concentration of Mg is found to be greater than its ideal value whereas that of Cu is found to be less than its ideal value (Figure 8). These results indicate that among the two components, Mg atoms segregate on the surface phase whereas Cu remains in the bulk phase of the initial melt at 1100 K (Yadav *et al.*, 2020).

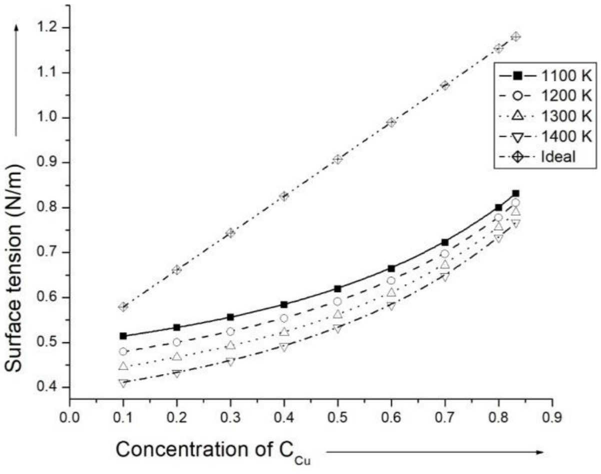

Figure 9. σ vs C_{Cu} for Cu-Mg liquid alloy at different temperatures

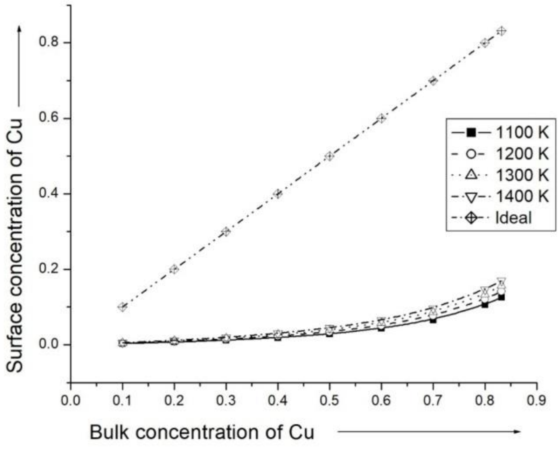

Figure 10. C_{Mg}^S vs C_{Cu} for Cu-Mg liquid alloy at different temperatures

The surface tension and surface concentrations of Cu and Mg have also been computed at above mentioned temperatures following a similar procedure. It can be observed that the surface tension of the system gradually decreases with increase in temperature (Figure 9). This may be due to the decrease in the cohesive energy of the system with an increase in its temperature and the results are as expected. Moreover, at higher temperature, the values of C_{Mg}^{S} gradually decreases indicating the movement of respective atoms from surface to the bulk phase (Figure 10). Moreover, the values of C_{Cu}^{S} gradually increases indicating the movement of respective atoms from bulk phase to the surface phase (Figure 11). The movements of atoms take place in order to regain the stability of the liquid mixture which has been disturbed by the rise in temperature. These results are similar to those predicted from the study of thermodynamic functions and are also in accordance with the results from the works of other researchers (Yadav *et al.*, 2020; Mehta *et al.*, 2022).

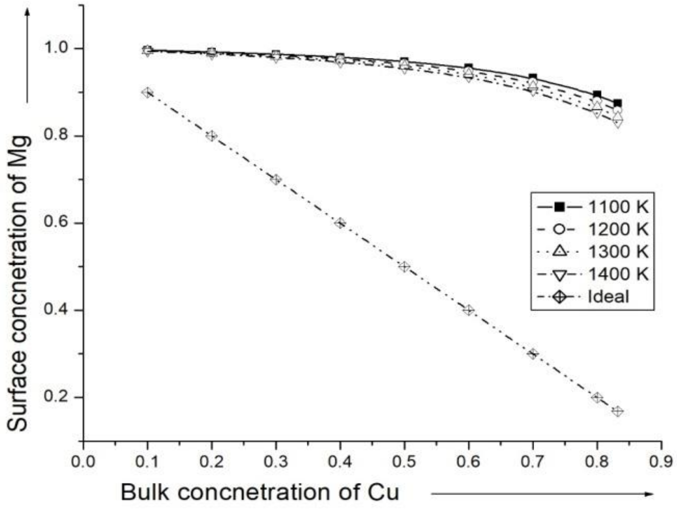

Figure 11: C_{Cu}^{S} vs $C_{Cu}$for Cu-Mg liquid alloy at differenttemperatures

STRUCTURAL PROPERTIES

The knowledge of structural functions gives an idea about the local pairing of atoms of the liquid alloy. In structural functions, concentration fluctuation in long wavelength limit ($S_{CC}(0)$) and Warren-Cowley short range order parameter (α_1) have been computed in this work. At a temperature and concentration, if $S_{cc}(0) > S_{cc}^{ideal}(0)$, then $S_{cc}(0)$ is said to have positive deviation from its ideal value $S_{cc}^{ideal}(0)$ and at this condition, the alloy shows segregating behaviour or demixing nature (Singh & Sommer, 1997). On the other side, if $S_{cc}(0) < S_{cc}^{ideal}(0)$, then it is said to have negative deviation from its ideal value and at this condition, the alloy shows ordering behaviour or mixing nature (Singh & Sommer, 1997).

The theoretical and ideal values of $S_{cc}(0)$ at 1100 K and different temperatures have been calculated using Equations (11) and (14) respectively with the aid of required parameters from Table 1. These values are plotted as a function of concentration in Figures 12 and 13. The values of $S_{cc}(0)$ calculated in this work are found to be less than $S_{cc}^{ideal}(0)$ at all concentrations corresponding the ordering nature of the system. As the temperature of the system is gradually increased beyond 1100 K, the values of $S_{cc}(0)$ gradually increases and get closure to ideal values. These results convey that the ordering or complex forming tendency of the system gradually decreases with rise in its temperature and it shows ideal mixing tendency. Thus, it can be concluded that the exponential temperature-dependent parameters for Cu-Mg liquid alloy optimised in this work fruitfully explain its thermodynamic, surface and structural properties.

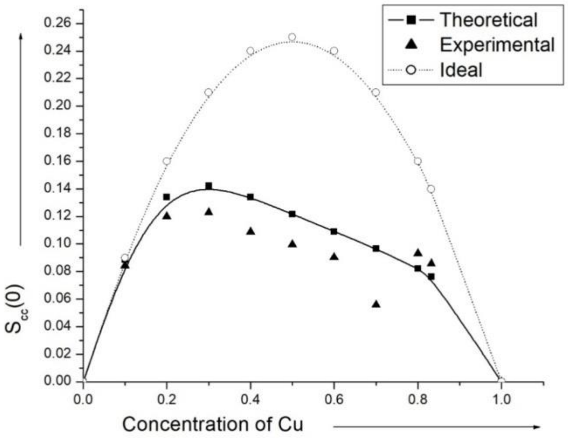

Figure 12. $S_{cc}(0)$ vs concentration of Cu for Cu-Mg liquid alloy at 1100 K

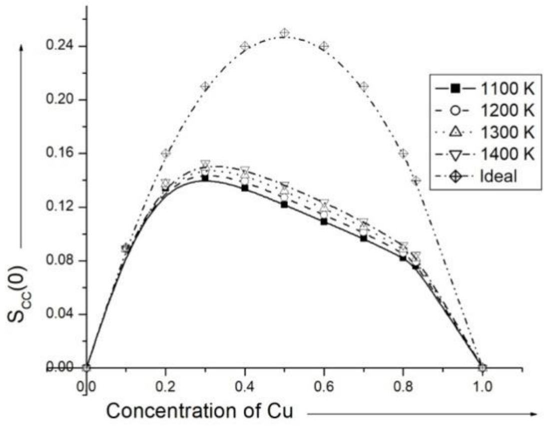

Figure 13. $S_{cc}(0)$ vs concentration of Cu at different temperatures

The values of (α_1) have been calculate using Equations (12) and (13) and above determined values of $S_{cc}(0)$. The temperature and composition dependence of these values are displayed in Figures 14 and 15. The value for this parameter can be positive as well as negative and both of them incorporate valuable information regarding the mixing behaviour of the liquid alloy (Butler, 1932; Bhatia & Thorntorn, 1970; Zhou & Napolitano, 2007; Yadav *et al.*, 2015c; Yadav *et al.* 2016b; Gohivar *et al.*, 2020). When $\alpha_1 > 0$ i.e., positive then, the liquid mixture shows segregating nature, when $\alpha_1 < 0$ i.e., negative, then the liquid mixture shows ordering nature and when $\alpha_1 = 0$, it shows ideal mixing tendency.

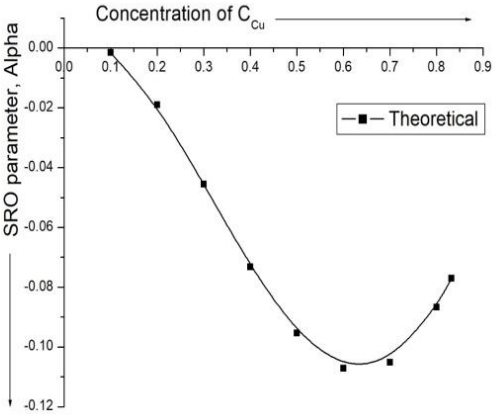

Figure 14. Compositional dependence of α_1 for Cu-Mg liquid alloy at 1100 K

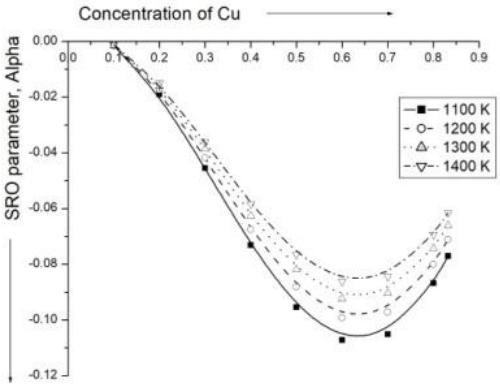

Figure 15. α_1 vs concentration of Cu at different temperatures

The observation of curve reveals that α_1 has negative value at all concentrations of copper which agrees to the fact that Cu-Mg liquid alloy has strong compound forming tendency at its melting temperature (Figure 14). This result further puts on strong evidence for acceptance of the exponential model for investigation of mixing behaviour for binary liquid alloy. Further, the negative value of α_1 at higher temperatures gradually decreases indicating the gradual decrease in the compound forming tendency of the system. These findings are similar to the results obtained from the investigations of other thermodynamic, surface and structural functions.

CONCLUSIONS

The optimised values of self-consistent exponential temperature-dependent interaction energy parameters for excess Gibb's free energy of mixing for Cu-Mg liquid alloy successfully explains the mixing behaviours at different temperatures. Present investigations correspond that the system shows complete ordering nature at its melting temperature. However, this tendency gradually decreases at elevated temperatures.

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AUTHOR CONTRIBUTIONS

All authors have equal contributions.

CONFLICT OF INTEREST

The author declares no conflict of interest.

DATA AVAILABILITY STATEMENT

The corresponding author will provide the dataset created during the research process and/or analyzed during the current study upon reasonable request.

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