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The role of thermophysical properties of liquid mercury-lead alloy

Malti*, Deapartment of Physics, H.No. 532, Housing Board Colony, Jind, Haryana (India)
Email id- mudgilmalti@gmail.com

Abstract

The HgPb2 complex has been taken into consideration when reporting the thermophysical parameters of the compound that forms binary liquid mercury-lead alloy at a temperature of 600 K as a function of concentration. By using a quasi-chemical approximation, it is possible to study the alloy's micro- and macro-scopical properties, including the Gibbs free energy, enthalpy of mixing, chemical activity of each component, and concentration fluctuation in the long-wavelength limit. The interaction energy characteristics between the alloy's atoms are stressed more in this research report. The validity of the model is assessed by contrasting the theoretical and experimental results. Surface tension has been studied using the compound formation model, statistical mechanical technique, and improved Butler equation derivation.

Keyword: liquid mercury-lead alloy, macroscopic properties, temperature, and pressure, Viscosity, Transportable Quality, HgPb2

Introduction

It is thought that understanding alloy thermophysical properties is a prerequisite for creating innovative materials. Changes in a system's structural organisation and atom-to-atom bonds are related to the formation of an alloy. Studying how constituent atoms interact and rearrange structurally during alloy formation helps us understand the topic in greater detail. Atoms of specific elements align in either a self-coordinated or strong ordering pattern according to the alloy's mixing capabilities, which are influenced by the electrochemical effect, atom size, and constituent element concentration. According to composition, temperature, and pressure, which are all crucial for the materials' strength, stability, and electrical resistivity, liquid alloys have different alloying properties. As a result, metallurgists and physicists have been curious to learn more about how metals mix to form alloys. The research of the characteristics of different alloys is still not complete, nevertheless, due to experimental challenges and time constraints.

To address these issues, facilitate study, and expedite the inquiry process, different concentration-dependent theoretical models have been developed by various theoreticians to understand the alloying behaviour of compound producing binary alloys (e,f,g), Mercury and lead are the most extensively researched metals due to their direct effects on human health. Assuming the presence of the HgxPby (x = 1, y = 2) complex in the melt, our work focuses on one of the lead alloys, Hg-Pb, to theoretically determine various properties at 600 K [6]. Due to its extreme ductility and softness, lead is frequently employed in commercial lead alloys [8]. By altering the atomic weight % of Hg, Zabdyr [9] investigated phase diagram, crystal structure, and lattice parameters, however the full thermophysical examination is incomplete. The most desirable in metallurgical research for describing the surface and transport properties of liquid mixtures are concentration-dependent surface tension and viscosity of binary liquid alloys. As a result, scientists are attempting to investigate these aspects by proposing various models [10-16]. Furthermore, one of the most crucial aspects to be investigated in metallurgical research is surface segregation, which basically relates to the concentration disparity between the alloys' surface and bulk materials. The difference in surface energy between the alloy's constituent ele- ments is the fundamental source of this disparity, the element with lower surface energy tending to segregate on the surface [17]. A theoretical analysis indicates that bigger atoms have a tendency to cluster on surfaces.

The current research also seeks to investigate the alloy's surface tension using a compound formation model [13]. The computed result is contrasted with two additional models due to the absence of experimental data: a statistical mechanical approach [12] and an updated Butler equation derivation [16]. Three models are used in this work to analyse viscosity: the Budai-Benko-Kaptay model [10], the Kaptay equation, and the Kozlov-Ronanov-Petrov equation [11].

Conceptualization of the theory

Processes Thermodynamic

Let's say an alloy of A and B atoms has NA and NB number of each. The model presupposes that complexes AxBy exist in such a way that

xA + yB = AxBy (1)

where x and y are small integers.

With this presumption, the grand partition function is solved in terms of configurational energy [6] and excess free energy of mixing, which is given in Eq. (2) and used to derive various features.

$$G_M^{XS} = RT \int_0^C \gamma dC \qquad (2)$$

where γ is the activity coefficient ratio of atom A to B, C is the concentration of A atom and R is universal gas constant. After simple mathematical calculation, the solution of Eq. (2) is given as

$$G_M^{XS} = N[\theta\omega + \theta_{AB}\Delta\omega_{AB} + \theta_{AA}\Delta\omega_{AA} + \theta_{BB}\Delta\omega_{BB}] \qquad (3)$$

where θ = C(1 − C) and θj,k’s are the simple polynomials in C that depend on the values of integers x and y, ω is interchange energy, and Δωjk are the interaction energy parameters. For A =Hg, B =Pb, x = 1, y = 2, the values of θj,k’s are found to be [6, 19]

$$\theta_{AA}(C) = 0 \qquad (4)$$

$$\theta_{AB}(C) = \frac{1}{6}C + C^2 - \frac{5}{3}C^3 + \frac{1}{2}C^4 \qquad (5)$$

$$\theta_{BB}(C) = -\frac{1}{4}C + \frac{1}{2}C^2 - \frac{1}{4}C^4 \qquad (6)$$

The Gibbs free energy of mixing for complex formation is given by

$$\begin{aligned} G_M &= G_M^{XS} + G_M^{ideal} \\ &= G_M^{XS} + RT(C\ln C + (1-C)\ln(1-C)) \\ &= RT\left[\theta\frac{\omega}{k_BT} + \theta_{AB}\frac{\Delta\omega_{AB}}{k_BT} + \theta_{AA}\frac{\Delta\omega_{AA}}{k_BT}\right. \\ &\qquad \left. + \theta_{BB}\frac{\Delta\omega_{BB}}{k_BT} + C\ln C + (1-C)\ln(1-C)\right] \end{aligned}$$

Because x is valued at 1 in the model being employed, AA is taken to be zero in this instance. The coefficient of AA kBT in Eq. (6) likewise tends to zero in this situation since there is no chance that the pair A and A will be a member of the complex. If the alloy contains no complexes, then jk is zero. In this situation, the aforementioned equation has the form shown below:

$$G_M = RT\left[\theta\frac{\omega}{k_BT} + C\ln C + (1-C)\ln(1-C)\right] \tag{8}$$

The enthalpy of mixing is calculated with the standard thermodynamic relation:

$$\begin{aligned}\frac{H_M}{RT} &= \frac{G_M}{RT} - \left[\frac{dG_M}{RdT}\right]_{C,N,P}\\ &= \theta\left[\frac{\omega}{k_BT} - \frac{1}{k_B}\frac{d\omega}{dT}\right]\\ &\quad + \theta_{AB}\left[\frac{\Delta\omega_{AB}}{K_BT} - \frac{1}{k_B}\frac{d\Delta\omega_{AB}}{dT}\right]\\ &\quad + \theta_{BB}\left[\frac{\Delta\omega_{BB}}{K_BT} - \frac{1}{k_B}\frac{d\Delta\omega_{BB}}{dT}\right] \end{aligned} \tag{9}$$

The theoretical value of activity for each constituent component is now given by solving Eqs. (7) and (10), as follows:

$$\begin{aligned}\ln a_A = \frac{G_M}{RT} + \frac{1-C}{k_BT}&\bigg[(1-2C)\omega + \theta'_{AB}\Delta\omega_{AB}\\ &+ \theta'_{BB}\Delta\omega_{BB} + \ln\frac{C}{1-C}\bigg]\end{aligned} \tag{11}$$

$$\begin{aligned}\ln a_B = \frac{G_M}{RT} - \frac{C}{k_BT}&\bigg[(1-2C)\omega + \theta'_{AB}\Delta\omega_{AB}\\ &+ \theta'_{BB}\Delta\omega_{BB} + \ln\frac{C}{1-C}\bigg]\end{aligned} \tag{12}$$

where, θ ′ AB, θ ′ AA and θ ′ BB, respectively, are derivatives of θAB, θAA and θBB with respect to concentrations.

Microscale Operations

According to the connection, the alloy's concentration variation in the long-wavelength limit SCC (0) is given as [20],

$$S_{CC}(0) = RT\left[\frac{\partial^2 G_M}{\partial C^2}\right]_{T,P,N} \tag{13}$$

With the aid of the subsequent Eq, the value of SCC (0) can be determined using experimentally recorded activities (14). Therefore, the SCC (0) values produced from this equation are referred to as experimental values.

$$\begin{aligned}S_{CC}(0) &= a_A(1-C)\left[\frac{\partial a_A}{\partial C_A}\right]^{-1}_{T,P,N}\\ &= a_BC\left[\frac{\partial a_B}{\partial C_B}\right]^{-1}_{T,P,N}\end{aligned} \tag{14}$$

where aA and aB represent, respectively, the observed activity of elements A and B. We can write C and 1-C instead of CA and CB, respectively, to keep things simple. Equations (7) and (14) are solved, and the result for SCC (0) is,

$$S_{CC}(0) = C(1-C)\left[1 + C(1-C)\left(-2\frac{\omega}{K_BT} + \theta''_{AB}\frac{\Delta\omega_{AB}}{K_BT} + \theta''_{BB}\frac{\Delta\omega_{BB}}{K_BT}\right)\right]^{-1} \quad (15)$$

Where θ”jk are second concentration derivatives of θjk.
The concentration fluctuation in the long-wavelength limit is related to the Warren-Cowley short-range order parameter (1) as follows:

$$\alpha_1 = (S-1)[S(Z-1)+1]^{-1} \quad (16)$$

where Z is coordination number and

$$S = \frac{S_{CC}(0)}{S^{id}_{CC}(0)} \quad (17)$$

Viscosity, a Transportable Quality

The mixing characteristics of a molten alloy can be evaluated at the microscopic level in terms of viscosity, which forms the basis for some of the most fundamental theories about atomic transport properties. In metallurgical study, which largely deals with industrial processes and a range of natural occurrences, it is recognised as one of the most significant thermophysical properties. Molar volume, cohesion energy, and the composition of the liquid all have an impact on it [23, 24]. The atomic transport characteristics of the Hg-Pb alloy are examined by computing the composition dependency of viscosity at 600 K. But because there aren't any experimental data, three distinct models—the Kozlov-Ronanov-Petrov equation, the Kaptay equation, and the BBK (Budai-BenkoKaptay) model—are used to compare viscosity.
Cohesive interaction, which is a product of geometric and electrical shell effects, is what causes viscous flow in liquids [25]. In order to take into account the viscous flow in a liquid alloy, the cohesion interaction in terms of the enthalpic effect has been incorporated into the KRP equation. The equation is presented as follows for T:

$$\ln\eta = C\ln C\ln\eta_A + (1-C)\ln\eta_B - \frac{H_M}{3RT} \quad (18)$$

where the viscosity of the alloy and the individual elements A and B are denoted by and j, respectively. The variation in viscosity with temperature for metals is given as [26].

$$\eta_j = \eta_0 \exp\frac{\epsilon}{RT} \quad (19)$$

where η0 and ϵ are constants of each metal’s units of viscosity and energy per mole.
Equation of Kaptay
By taking into account the theoretical connection between the cohesive energy and activation energy of the viscous flow, Kaptay created an equation. The equation is as follows at temperature T:

$$\eta = \frac{hN_{Av}}{CV_A + (1-C)V_B + V^E} \times exp\left(\frac{CG_A + (1-C)G_B - \Phi H_M}{RT}\right) \quad (20)$$

where h is Plank's constant, NAv is Avogadro's number, Vj (j = A, B) is the molar volume of pure metal, V E is excess molar volume upon alloy formation, Gj is Gibb's energy of activation of the viscous flow in pure metals, and φ is a constant whose value is (0.155±0.015) [27]. The Gibb's energy of activation of pure metal is calculated by the following equation:

$$G_j = RT \ln\left(\frac{\eta_j V_j}{hN_{Av}}\right) \tag{21}$$

BBK (Budai-Benko-Kaptay) model

The BBK model is used for the viscosity of multicomponent alloys. At temperature, it is given as:

$$\begin{aligned}\eta = {} & LT^{1/2}(CM_A+(1-C)M_B)^{1/2} \\ & \times (CV_A+(1-C)V_B+V^E)^{-2/3} \\ & \times exp\left[(CT_{m,A}+(1-C)T_{m,B}-\frac{H_M}{\chi R})\frac{I}{T}\right]\end{aligned} \tag{22}$$

where L and I are constants whose values are (1.80±0.39)×10−8 j/Kmol1/3) 1/2 and (2.34±0.02), respectively, and χ is a semi-empirical parameter having a value equal to 25.4. Similarly Mj and TmJ are, respectively, molar mass and the effective melting temperature of constituent elements of the alloy.

Dimensional quality

Due to their relationship with both surface and interface in the liquid metal process, the surface properties (surface tension and surface concentration) of liquid alloy or liquid metal are regarded in metallurgy and industry as key factors for processing as well as for the production of new materials [28, 29]. The importance placed on the surface and interfacial behaviours of liquid metals in the metallurgical process for solidification, controlling the processes of welding and casting, is due to the fact that the interfacial motion caused by the surface tension of liquid plays a significant role in many industrial phenomena [30].

Model for Compound Formation

The model implies that because the intermetallic compound AxBy forms in the melt, there is a tendency for compounds to develop in the binary liquid alloy that is comparable to the tendency for compounds to form in the solid state, in the form of short-ranged volume elements. The grand partition function, which is akin to the quasi-chemical approximation, is used to develop the equation in this model. The following is the equation at temperature T:

$$\begin{aligned}\sigma = \sigma_A & + \frac{k_BT}{\rho}\ln\frac{C^s}{C} + \frac{\omega}{\rho}[p(f^S-f)-qf] \\ & + \frac{\Delta\omega_{AB}}{\rho}[p(f^S_{AB}-f_{AB})-qf_{AB}] \\ & + \frac{\Delta\omega_{BB}}{\rho}[p(f^S_{BB}-f_{BB})-qf_{BB}] \qquad (23) \\ = \sigma_B & + \frac{k_BT}{\rho}\ln\frac{1-C^s}{1-C} + \frac{\omega}{\rho}[p(\varphi^S-\varphi)-q\varphi] \\ & + \frac{\Delta\omega_{AB}}{\rho}[p(\varphi^S_{AB}-\varphi_{AB})-q\varphi_{AB}] \\ & + \frac{\Delta\omega_{BB}}{\rho}[p(\varphi^S_{BB}-\varphi_{BB})-q\varphi_{BB}] \qquad (24)\end{aligned}$$

where ϕ, f, ϕjk and fjk are bulk concentration functions. Similarly, ϕ S, f S, ϕ S jk and f S jk are surface concentration functions, and ρ is the mean area of the surface per atom. For x = 1 and y = 2, the bulk concentration functions are [13, 31]:

$$\varphi = C^2 \tag{25}$$

$$\varphi_{AB} = \frac{1}{6} + 2(1-C) - 6(1-c)^2 + \frac{16}{3}(1-C)^3 - \frac{3}{2}(1-C)^4 \tag{26}$$

$$\varphi_{BB} = -\frac{1}{4} + (1-C) - \frac{1}{2}(1-C)^2 + (1-C)^3 - \frac{3}{4}(1-C)^4 \tag{27}$$

$$f = (1-C)^2 \tag{28}$$

$$f_{AB} = (1-C)^2 + \frac{10}{3}(1-C)^3 - \frac{3}{2}(1-C)^4 \tag{29}$$

$$f_{BB} = -(1-C)^2 + \frac{3}{4}(1-C)^4 \tag{30}$$

The functions ϕ s , ϕ S jk, f s and f s jk can be obtained from Eqs. (26) to (30) by replacing bulk concentration C with surface concentration C S, while p and q are surface coordination fractions that indicate the fraction of the number of nearest neighbors of an atom within its own layer and in the adjoining layers, respectively, and and are related as p + 2q = 1. In a simple cubic crystal, p = 2/3 and q = 1/6. In a bcc crystal, p = 3/5 and q = 1/5, and in close packed crystal, p = 1/2 and q = 1/4. The mean atomic surface area is given by following relation [13]:

$$\rho = \sum_j C_j \rho_j \tag{31}$$

The atomic surface area of each component is given as

$$\rho_j = 1.012 \left(\frac{V_j}{N_{Av}}\right)^{2/3} \tag{32}$$

Mechanical statistical approach

The idea of layered structure close to the interface serves as the basic foundation for this approach. Through the activity coefficient (j) and the energy exchange between an alloy's constituent parts, the model links surface tension to thermodynamic parameters. The following is the equation at temperature T:

$$\sigma = \sigma_j + \frac{K_B T}{\rho} \ln \frac{C_j^S}{C_j \gamma_j} + \left[p(1-C_j^S)^2 - q(1-C_j)^2\right] \frac{\omega}{\rho} \tag{33}$$

Improved Derivation of the Butler equation

In accordance with this theory, a liquid's surface has a monoatomic layer known as a surface monolayer that functions as a separate phase and is in thermodynamic equilibrium with the bulk phase. The modified Butler equation yields the surface tension () of a binary alloy at temperature T as:

$$\sigma = \frac{S_j^0}{S_j}\sigma_j^0 + \frac{RT}{S_j}\ln\frac{C_j^S}{C_j^b} + \frac{G_j^{S,XS} - G_j^{b,XS}}{S_j} \qquad (34)$$

where, σ 0 j , S 0 j , Sj are surface tension of pure liquid metal, molar surface area of pure liquid metal, and partial molar surface area of j th component, respectively. G S,Xs j and G b,Xs j are partial excess free energy of mixing in the surface and bulk of constituent elements of the alloy, respectively. The molar surface area of pure component is given as:

$$S_j^0 = \delta\left(\frac{M_j^0}{\lambda_j^0}\right)^{2/3} N_{Av}^{1/3} \qquad (35)$$

where δ, M0 j , λ 0 j , δ and NAv are geometrical constant, molar mass, density of each constituent element at its melting temperature, and Avogadro's number, respectively. The value of geometrical constant is expressed as,

$$\delta = \left(\frac{3f_v}{4}\right)^{2/3}\frac{\pi}{f_s} \qquad (36)$$

where fv is volume packing fraction and fs is surface packing fraction. For liquid metal, the values of fv and fs are 0.66 and 0.906 respectively [33].

Results and analysis

Microstructure and thermodynamics

Binary liquid alloys' characteristics are often influenced by temperature, composition, and pressure.

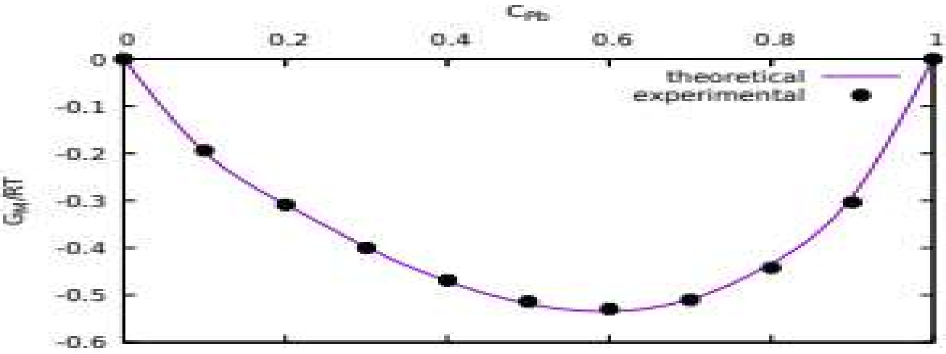

Figure 1: Gibbs free energy of mixing versus bulk concentration of Pb.

Our examination of the binary alloy Hg-Pb is carried out at a set air pressure and fixed temperature of 600 K depending on the alloy's composition. We evaluated various thermodynamic and structural characteristics for compounds generating molten alloys with x = 1 and y = 2 while assuming complexity throughout the experiment. The sections below include descriptions of the study's various findings.

Thermodynamic Properties

We take into account the aforementioned Eqs. (7), (9), (11), and (12) for the analysis of the thermodynamic characteristics. With the use of experimental values in the concentration range (0.1 to 0.9), the interaction energy parameters for the Gibbs free energy of mixing are established by the method of successive approximation for a number of concentrations [34]. The following are the energy parameter's approximations:

$$\frac{\omega}{k_B T} = 2.139,$$
$$\frac{\Delta\omega_{AB}}{k_B T} = -2.264,$$
$$\frac{\Delta\omega_{BB}}{k_B T} = 0.392$$

Since no statistical techniques, such as mean square deviation, were used to determine the best fit values when calculating the interaction energy parameters, the results are regarded as reasonable for analysis and have been taken into account throughout the investigation of various mixing properties. The experimental values given in Fig. 1 and the estimated values of GM/RT accord well. At a Pb concentration of 0.6, the free energy of mixing is theoretically calculated to be at least 0.533RT. The alloy HgPb is weakly interacting at the molten state, according to the calculation of the free energy of mixing. Similar to that, it is categorised as an irregular alloy since it is asymmetric at 0.5 concentration.

The method of successive approximation is used to determine the temperature derivatives of the interaction energy parameters that are required to theoretically calculate the enthalpy of mixing. The approximations of these parameters with the best match are:

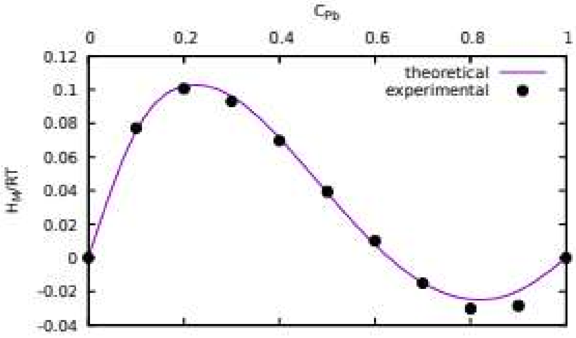

Figure 2: Enthalpy of mixing versus bulk concentration of Pb

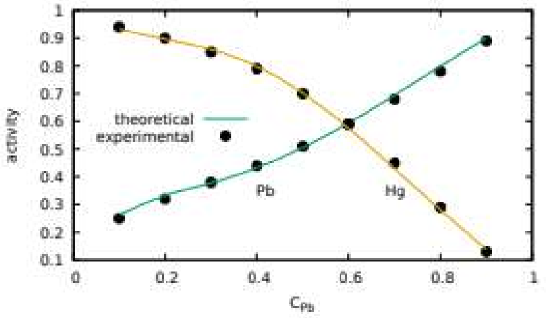

Figure 3: Chemical activity versus bulk concentration of Pb

The parameters so acquired have been taken into account during the investigation of various mixing qualities and are thought to be appropriate for analysis. The experimental values given in Fig. 1 and the estimated values of GM/RT accord well. At a Pb concentration of 0.6, the free energy of mixing is theoretically calculated to be at least 0.533RT. The alloy HgPb is weakly interacting at the molten state, according to the calculation of the free energy of mixing. Similar to that, it is categorised as an irregular alloy since it is asymmetric at 0.5 concentration. The method of successive approximation is used to determine the temperature derivatives of the interaction energy parameters that are required to theoretically calculate the enthalpy of mixing. The approximations of these parameters with the best fit are

$$\frac{1}{k_B}\frac{d\omega}{dT} = 0.767,$$
$$\frac{1}{k_B}\frac{d\Delta\omega_{AB}}{dT} = -0.3128,$$
$$\frac{1}{k_B}\frac{d\Delta\omega_{BB}}{dT} = 0.429$$

In Fig. 2, the relationship between mixing enthalpy and lead concentration is plotted. Below a lead concentration of 0.6, it is positive; beyond this concentration, it is negative. The computed and experimental values of the enthalpy of mixing agree with only minor differences. Chemical activity, a measure of effective concentration in the mixture, can be used to analyse the alloy's divergence from ideal behaviour because its size depends on the interaction of its constituent binary components. The determination of the chemical activity of the elements in the alloy Hg-Pb uses equations (11) and (12). Figure 3 depicts experimental and theoretically calculated values of the chemical activity of the alloy's constituent parts, demonstrating good agreement between the two methods at a temperature of 600 K and for all Pb concentrations.

Microscopic Properties

Experiments involving diffraction on materials are challenging at high temperatures. Therefore, the concentration variations in the long-wavelength limit (SCC (0)) are studied to improve the effectiveness of studying the local organisation of atoms in the binary alloy.

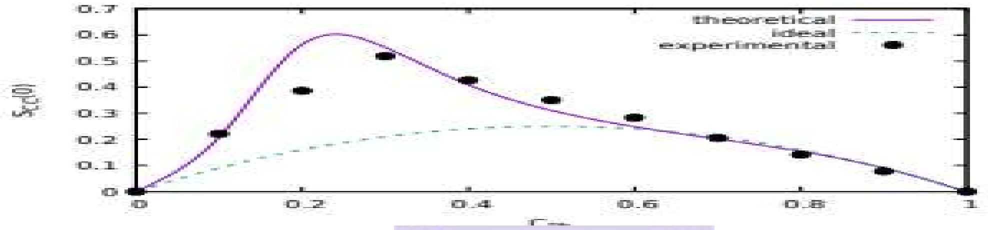

Figure 4: Concentration fluctuation in long-wavelength limit versus bulk concentration of Pb

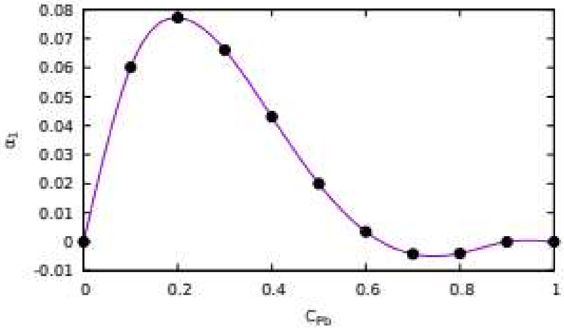

Figure 5: Warren-Cowley short-range order parameter versus bulk concentration of Pb

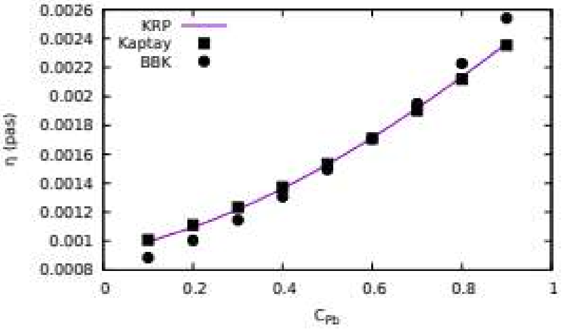

Figure 6: Viscosity versus bulk concentration of Pb

some of the most significant microscopic processes [20, 35]. If SCC (0) Sid CC (0) for any given concentration, the alloy is predicted to form in a complicated manner, and if SCC (0) > Sid CC (0), the alloy is predicted to segregate. Figure 4 displays the graph of the experimental, theoretical, and ideal values of SCC (0) versus concentration of Pb. The alloy has a segregating nature below this concentration of lead, while displaying an ordering nature above this concentration, as shown in the figure, where both the experimental and theoretical values of SCC (0) sit above the ideal value for lead concentration values below 0.6.

One of the most effective parameters for learning about the atom arrangement in liquid alloys is the Warren-Cowley short range parameter (1). The amount of local atom arrangement in the alloys is quantified by this information. Its value ranges from +1 to -1. A segregating nature is shown by the positive value of 1, which is complete for 1 = 1, whereas an ordering nature is indicated by the negative value of 1, which is complete for 1 = 1. In a similar manner, the number 1 = 0 denotes the atoms' haphazard configurations in the liquid mixture. In Fig. 5, where coordination number Z = 10, we calculated the value of 1 as a function of the Pb concentration using Eq. (16). The strong tendency of the alloy to segregate is indicated by the fact that the 1 is positive up to a lead concentration range of 0.6, with peak values at a concentration of 0.2. However, the value of 1 continues to decrease above a lead concentration of 0.6, demonstrating the alloy's ordering tendency.

Viscosity

For the KRP and Kaptay models, the viscosities of each component (Pb and Hg) are necessary for the theoretical calculation of the viscosity of the HgPb alloy at 600 K. These values are derived from Eq. (19) by replacing the metal-specific 0 and values from reference [26]. Enthalpy values for various concentrations are taken from Eq. (9), while each pure metal's activation Gibbs energy is taken from Eq (21). V E is assumed to be zero because no experimental value has been found for it. In actuality, the value of V E for a non-ideal alloy is non-zero, but the contribution of this factor to the calculation of viscosity is very negligible [15]. The comparison of the outcomes from the three models is depicted in Fig. 6. According to the models, as the lead content rises, the liquid alloy's viscosity also rises. The graphic demonstrates that the viscosity calculated by the BBK model deviates very little from the others.

Conclusions based on the models for the concentration dependence of the viscosity of Hg-Pb liquid alloy at temperature 600 K become challenging due to the inability to compare theoretically calculated findings with experimental results.

Surface segregation and surface tension

The densities and surface tension of individual metals for all models necessary at 600 K are computed by utilising the relations presented in reference [26] in order to determine the surface tension of the alloy Hg-Pb. The same interaction parameters and jk used in thermodynamic properties are applied to the compound formation model. The surface concentrations of both metals are now obtained by writing these values along with values for other quantities in Eqs. (23) and (24) and solving them simultaneously. The surface tension is then calculated using each surface concentration of the respective metals. The other models are used in a similar way. For the statistical mechanical technique, the interchange energy is calculated as = 0.699 using Eq. (8). The bulk and partial excess free energies of mixing individual lead and mercury in a liquid state at 600 K are used from reference [34] for the revised derivation of the Butler model. The geometrical constant and the surface excess energy to bulk excess energy ratio (G S, Xs I /Gb, Xs I) are thought to be 1.061 and 0.818, respectively, [33]. Kaptay proposed that the partial molar volume might be replaced by the molar volume of the same component in the event of a minimal or unknown excess molar volume of the combination. In this case, the surface area (S 0 I) of the identical pure component takes the place of the partial surface area (Si) [16,36]. The calculated surface concentrations and surface tension.

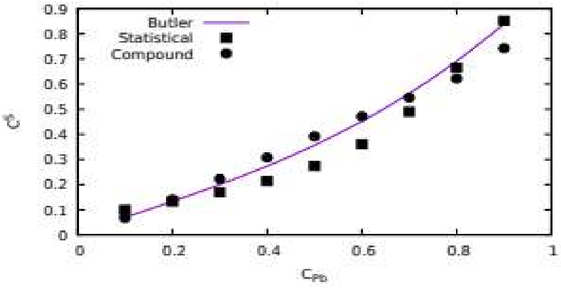

Figure 7: Surface concentration of lead versus bulk Pb concentration

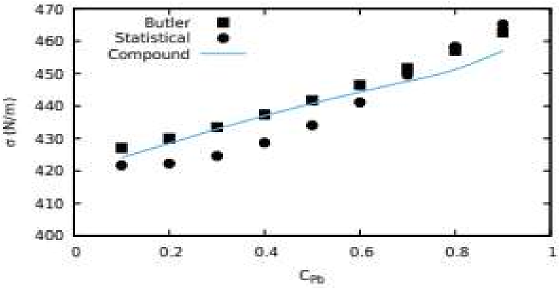

Figure 8: Surface tension versus bulk Pb concentration

According to Fig. 8, the surface tension of the alloy Hg-Pb steadily rises as the bulk concentration of Pb does. Since compound formation is a possibility at higher bulk concentrations of Pb, it is thought that the variation of surface tension in the compound formation model at these higher bulk concentrations of Pb than in the other two models is what led to the consideration of the set of interaction energy parameters. Due to the inclusion of interaction characteristics, the compound formation model is anticipated to perform better than the other two models. However, computed findings cannot be compared because there are no experimental results available.

Conclusions

The current research is a theoretical investigation into the thermodynamic, structural, transport, and surface behaviour of the binary liquid alloy Hg-Pb at 600 K under the presumption that the compound formation model's predicted presence of the HgPb2 complex in the liquid mixture is true. The work provides an explanation for the thermodynamic characteristics' asymmetric behaviour as a function of concentration and an alloy with weak interactions. According to the theoretical analysis, the alloy tends to segregate at lower Pb concentrations, but at higher Pb concentrations at 600 K, it exhibits an ordered nature. Similar to how viscosity does, surface tension also rises as lead concentration does. The surface concentration of each individual metal is then used to compute the surface tension. Similar techniques are applied to the other models. The exchange energy for the statistical mechanical method is determined using Eq. to be = 0.699. (8). For the improved derivation of the Butler model, the bulk and partial excess free energy of mixing individual lead and mercury in a liquid state at 600 K are taken from reference [34]. The surface excess energy to bulk excess energy ratio (G S, Xs I /Gb, Xs I) and the geometrical constant are estimated to be 1.061 and 0.818, respectively [33]. In the case of a minimal or zero partial molar volume, Kaptay suggested that it can be substituted by the molar volume of the same component.

Reference:-

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