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CALCULATION OF THERMODYNAMIC PROPERTIES OF SN-ZN LIQUID ALLOY AT 750 K USING SELF ASSOCIATION MODEL

Dr. M. ANJAN KUMAR , *Associate Professor , Department of CSE*
Viswam Engineering College(Autonomous), Mandanaplli, Andhra Pradesh.

ABSTRACT:
The concentration effect on the free energy of mixing (SM), activity (a), and microscopic properties of a Sn-Zn binary liquid alloy, including the concentration change in the long wavelength limit (Scc) and the Warren-Cowley short range order parameter, is determined using the self-association model. The calculations indicate that the Sn-Zn liquid alloy exhibits homo-coordination or phase separation with mild interaction at 750 K, regardless of concentration.

Keywords: *Metallic materials; Alloys; Hypothetical modeling; Asymmetric.*

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1. INTRODUCTION

Background to research

Alloy metals are composed of two or more elements that have been combined together in such a way that they are difficult to separate. It is composed of two or more metals, or of a metal and anything other than a metal. For example, combining tin (Sn) and zinc (Zn) yields an excellent plating solution. Carbon steel is formed when carbon (C) and iron (Fe) combine. Nonetheless, because many binary solid alloys are formed by cooling them from a liquid state, a broad grasp of how molten alloys work is required. The size factor, electrochemical effect, and electron concentration factors that primarily regulate the solubility of a uniform solid phase do not provide a satisfactory explanation for how liquid alloys behave when mixed. As a result, both experimentalists and philosophers drew a lot of attention. This is why the purpose of this research is to determine the thermodynamic properties of a binary liquid alloy at a certain temperature.

Validation for the research

The alloy chosen for this investigation was chosen because of its capacity to be used in industry and give sufficient testing results. As a result, research is being conducted on the Sn-Zn metal. Zinc (Zn) is found in block D, group 12, period 4, and tin (Sn) is found in block P, group 14, period 5. These chemical and alloy groups are useful in electrical and computer projects. IN this work, we employed self-association models to calculate the thermodynamic properties (free energy of mixing and activity) as well as the microscopic properties (concentration change in the long wavelength limit and Warren-Cowley chemical short-range order parameter).

2.THEORETICAL BACKGROUND

Based on theoretical modeling, binary liquid alloys can be divided into two categories: symmetric alloys and asymmetric alloys. This is evident from the entropy of mixing, concentration variations, free energy of mixing, heat of mixing, and other features of symmetric alloys (such as CuZn, CdAl, NaK, and others) that are symmetrical or nearly so (concentration c=0.5). These alloys are commonly referred to as normal metals.

Asymmetric metals, on the other hand, do not have the same mixing behavior at c=0.5. Most of the focus in recent decades has been on liquid chemical complexes (such as MgBi, CuZn, AgAl, and so on) or their side effects (such as Bi-Zn, Cu-Pb, K-Pb, and K-Ti). In theory, these complex-forming metals have been extensively explored and written about under a variety of names, including regularly related solutions, compound-forming

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solutions, and complex-forming solutions.

When elements A and B are combined, they usually form a binary metal. As a result, an A-B binary answer is generated. Let =Nc and NB=N(1-c) gm moles represent atoms A and B, respectively, in the binary solution. In this case, c is the atomic fraction of the A atoms. It is expected that a certain sort of complex DB will develop, where and v are very small quantities indicating the amount of A and B atoms in the complex. According to the law of atom conservation, if n1 g moles of A atoms, n2 g moles of B atoms, and n3 g moles of DB are formed in the solution, then

$$n_1=Nc-\mu n_3$$
$$n_2=N(1-c)-V n_3 \quad (1)$$
$$n=n_1+n_2+n_3=N-(\mu+v-1)n_3$$

"n" denotes the number of atoms, while "c" is the amount formed when a compound is formed.

Thermodynamic methodology

The thermodynamic technique or methodology is used when looking at the attributes of a combination on a large scale without considering how its atoms behave. To do this, the experimental values of a few factors are employed first, and then these values are entered into a number of appropriate models. The Self Association Model is employed in this scenario. Many properties have been investigated, both microscopically and thermodynamically.

Enthalpy (H): The amount of heat or energy in a thermodynamic system is referred to as its enthalpy. In simple terms, it is as follows:

$$H=U+PV \quad (2)$$

The absolute enthalpy of a system cannot be measured directly. However, variations in temperature (dT), which indicate how much heat is absorbed or lost, can be utilized to calculate changes in enthalpy (H). If you use a calorimeter to determine the specific heat capacity, the following equation can be used to calculate the enthalpy change:

$$\Delta H=\int_{T_1}^{T_2} C_p dT \quad (3)$$

Entropy (S): Entropy is a quantity that indicates how poorly a system operates. One of the most essential concepts in thermodynamics is how heat energy travels inside a system. As scientists, we are more interested in the change in entropy (dS) that occurs during a certain thermodynamic process than in any type of absolute entropy.

$$RT\ln a_K=\left(\frac{\partial G_M}{\partial N_k}\right)_{T,p,N} \quad (4)$$

Gibbs function (G): The Gibbs free energy is calculated by multiplying enthalpy (H) by entropy (S). This is the chemical process's usable energy.

$$G=H-TS \quad (5)$$

Gibbs free energy (Gfe) changes in the following ways in a basic fluid system:

$$(dG)=Vdp-SdT \quad (6)$$

Enthalpy of mixing (HM), entropy of mixing (SM), and their link to Gibbs free energy of mixing (GM) are terms used in alloy systems.:

$$G_M=H_M+TS_M \quad (7)$$

Activity ($a1$): Activity (e): An atom's activity can be calculated using its concentration (c) and activity number (3).

$$aA=c\gamma A \quad (8)$$
$$aB=(1-c)\gamma B \quad (9)$$

To obtain the task, utilize the general phrase bK (k=A,B).

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$$RT\ln a_K = \left(\frac{\partial G_M}{\partial N_k}\right)_{T,p,N} \quad (10)$$

Activity is one thermodynamic function that can be observed directly from an experiment. This can be accomplished using the Knudsen effusion method or the electromotive force methodology. As a result, it can be used to verify the accuracy of theoretical statements.

Changes in concentration at the long wavelength limit [dLc(0)]: The concentration factor is Scc(q) is at the long wavelength limit in a binary combination and can be represented as one of the following:

Concentration fluctuation in the long wavelength limit [Scc(0 Using the Gibbs free energy G in statistical mechanics, it is simple to calculate the mean square fluctuation in concentration, which is represented by (c)2.

$$S_{cc}(0)=N\langle(\Delta c)^2\rangle \quad (11)$$

Using the Gibbs free energy G in statistical mechanics, it is simple to calculate the mean square fluctuation in concentration, which is represented by (c)2,

$$\left\langle(\Delta c)^2\right\rangle = \frac{k_B T}{\left(\frac{\partial^2 G}{\partial c^2}\right)_{T,p,N}} \quad (12)$$

Small-angle diffraction tests could be used to directly determine c(0), but this would be a far more difficult experimental problem that has never been addressed.

When a perfect solution exists and the Gibbs free energy of mixing (GM),

$$G_M = cInc+(1-c)In(1-c) \quad (13)$$

$S_{cc}(0)$, Therefore, becomes an ideal value $S_{cc}^{id}(0)$. This is of great interest to visualize the degree of interaction in a mixture of the alloy.

$$S_{cc}^{id}(0) = c(1-c) \quad (14)$$

Short-range order parameter (α): In solids and liquids, how well are atoms and molecules ordered? This is frequently described using the Warren-Cowley short-range order parameter 1 for the first-neighbor shell. This organized sense is just temporary, like between atoms. The 1. covers any case in which there is a variation on a local length scale. These versions depict three different circumstances. 1=0 indicates that the atoms are randomly distributed, 0 indicates that the atoms do not pair up with each other, and 1 >0 indicates that the atoms tend to group together, implying that they pair up with each other. We will utilize statistics to demonstrate that the limiting values of 1 fall within the following range:

$$-\frac{c}{(1-c)} \le \alpha_1 \le 1, c \le 0.5 \quad (15)$$

$$-\frac{(1-c)}{c} \le \alpha_1 \le 1, c \ge 0.5 \quad (16)$$

The connection shifts to -1 1 at d=0.5. This suggests that the mixtures are all the same. The potential worth,

$$\alpha_1^{\min} = -1 ,$$

However, this demonstrates 1 1 the entire order of A-B pairs in the melt.,

$$\alpha_1^{\max} = 1$$

Demonstrates that the melt has been entirely separated, giving the closest neighbors the appearance of atoms.

3.THEORETICAL MODELS

The difficulty in determining values for various high-temperature mixing features emphasizes the importance of researching parameters such as GM and 1. Furthermore, the necessity to describe how alloys act compels us to develop theories that evolve throughout time. There are numerous models, including the Percus-Yevick (PY)

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hard sphere model, the Self-Association Models the quasi-chemical mode (addressed next), and others.
Quasi-chemical model: Because alloys produce compounds when they are solid, it was assumed that there might be chemical complexes Pb in the liquid state. A and B are the atoms that make up a binary mixture in the fundamental version of the quasi-chemical equation. These are represented by the atom pairs NDB and NBB, and the interchange energy () between them is equal to the number of atom pairs that do not match.

$$\frac{4N_{AANBB}}{N_{AB}^{2}}=\eta^{2} \tag{17}$$

The first shell coordination number is z, and =(zkNT). When is not zero, the mixing free energy is written as

$$G_M = G_M^{id} + G_M^{xs} \tag{18}$$

Where G_M^{xs} *and* G_M^{xs} is ideal and excess Gibbs free energy of mixing respectively

$$G_M^{id} = RT\left\{c\ln c+(1-c)\ln(1-c)\right\} \tag{19}$$

And,

$$G_M^{xs} = RT\left\{c\ln\gamma_A+(1-c)\ln\gamma_B\right\} \tag{20}$$

The concentration of A and B atoms in the alloy are c and $(1-c)$ respectively while the activity coefficient γ_A *and* γ_B are

$$\gamma_A=\left\{\frac{\beta-1+2c}{c(1-\beta)}\right\}^{\frac{1}{2}Z}=\left(\frac{\phi_1}{c\phi_2}\right)^{\frac{1}{2}Z} \tag{21}$$

$$\gamma_B=\left\{\frac{\beta+1-2c}{(1-c)(1-\beta)}\right\}^{\frac{1}{2}Z}=\left(\frac{\phi_3}{(1-c)\phi_2}\right)^{\frac{1}{2}Z} \tag{22}$$

$$\beta=\left\{1+4c(1-c)(\eta^2-1)\right\}^{\frac{1}{2}} \tag{23}$$

The expression for the entropy of mixing (S_M) can easily be obtained from equation (18) and by using c, R, T, ω, γ_A, , etc.

$$S_M=-\left(\frac{\partial G_M}{\partial T}\right)_p \tag{24}$$

Then obtain,

$$S_M = S_{id} + S_0 + S_1, \tag{25}$$

$$S_{id}=-R\left\{c\ln c+(1-c)\ln(1-c)\right\}, \tag{26}$$

$$S_0=-\frac{1}{2}Rz\left\{c\ln\gamma_A+(1-c)\ln\gamma_B\right\}, \tag{27}$$

$$S_1=-\frac{8Rc^2(1-c)^2\eta^2}{\phi_1\phi_2\phi_3}\left\{\frac{1}{K_B}\frac{d\omega}{dT}-\frac{\omega}{K_BT}\right\} \tag{28}$$

Now by applying equation (18) and (25), we will have the heat of mixing (H_M=G_M+TS_M)

$$\frac{H_M}{RT}=-\frac{8c^2(1-c)^2\eta^2}{\phi_1\phi_2\phi_3}\left\{\frac{1}{K_B}\frac{d\omega}{dT}-\frac{\omega}{K_BT}\right\} \tag{29}$$

However, in this situation, equation (29) equals equiatomic composition (d=0.5).

$$\frac{H_M}{RT}=-0.5\left\{1+\exp\left(\frac{\omega}{zK_BT}\right)\right\}^{-1}\times\left\{\frac{1}{K_B}\frac{d\omega}{dT}-\frac{\omega}{K_BT}\right\} \tag{30}$$

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Equation 18 can also be used to calculate the concentration change (0) at q=0 (long wavelength limit).

$$S_{cc}(0)=\frac{RT}{\left(\frac{\partial^2 G_M}{\partial c^2}\right)_{T,P,N}}=\frac{c(1-c)}{1+\frac{1}{2}z(1-\beta)/\beta} \quad (31)$$

Finally, the foregoing equation (17) can be utilized to derive the Warren-Cowley formula for the first coordination shell's short-range order parameter,

$$\alpha_1=\frac{\beta-1}{\beta+2} \quad (32)$$

Surprisingly, when 0, 1, and 0 are present, atoms that do not belong together want to group together. When >0, however, >1 ensures that 1>0, and similarly, there is a preference for like atoms to be the closest neighbors, which leads to alloy segregation.

4.METHODS AND COMPUTATION

The self-association model (SAM)

In 1992, Singh and Sommer developed the Self Association Model to investigate the thermodynamic properties of liquid metals that do not mix properly.

The expression for the Gibbs free energy of mixing: The mixing Gibbs free energy expression looks like this: A variety of factors influence the alloy's free energy of mixing. Here are a few examples:

The atom amounts are as follows: c for atoms A and (1 - c) for atoms B.

The ordered energy is denoted by =, and the exchange energy is denoted by.

The self-associate count is as follows: $n=\square/v$

The mixing free energy, SM, can be written as

$$G_M=RT[c\ln c+(1-c)\ln(1-c)+c\ln(1-\beta)+\ln\gamma]+c(1-c)\gamma W \quad (33)$$

Where $\beta=1-1/n, \gamma=1/(1-c\beta)$

The activity of the components: What the component performs is as follows: The experiment allows you to obtain precise readings of this critical quantity. People believe that the sizes of activities are defined by the connections between system components, which in turn determine the bond energies. As a result, it appears likely that measuring the activities of a set of comparable systems will, at the very least, contribute to the development of a foundation for behavior correlation, which can subsequently be used to extrapolate the behavior of more complicated systems. The behavior of a part in a solution can also indicate how likely it is to separate from the solution.

You can find this using the general formula in Equation (8).

$$RT\ln a_K=\left(\frac{\partial G_M}{\partial N_k}\right)_{T,p,N}$$

If we substitute 33 for 8 in the previous equation, we get the following activities:

$$\ln a_A=\ln\left(c\gamma(1-\beta)\right)+(1-c)\gamma\beta+(1-c)^2\gamma^2\frac{W}{RT} \quad (34)$$

And,

$$\ln a_B=\ln\left(c\gamma\right)+c(1-\beta)\gamma(1-n)+nc^2(1-\beta)\gamma^2\frac{W}{RT} \quad (35)$$

The enthalpy of mixing: This understanding stems from the relationship between thermodynamics and mixing enthalpy.

$$H_M=G_M-T\left(\frac{\partial G_M}{\partial T}\right)_p \quad (36)$$

As a result, the enthalpy of mixing HA will be

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$$H_M = c(1-c)\gamma W - c(1-c)\gamma T\frac{\partial W}{\partial T} + RT^2 c(1-c)\gamma\left[\frac{\beta}{1-\beta} - c\gamma\frac{W}{RT}\right]\frac{\partial\beta}{\partial T} \quad (37)$$

The entropy of mixing: This is given as

$$S_M = R\left[c\ln c + (1-c)\ln(1-c)\right] + R(c\ln n - \ln\gamma) - c(1-c)\gamma\frac{\partial W}{\partial T} + RTc(1-c)\gamma\left[\frac{\beta}{1-\beta} - c\gamma\frac{W}{RT}\right]\frac{\partial\beta}{\partial T} \quad (38)$$

The concentration-concentration fluctuation in the long wavelength limit: Long wavelengths limit changes in concentration: In this manner, use equations (33) and (34) or (35) (34) or (35) in this way

$$S_{cc}(0) = RT\left(\frac{\partial^2 G_M}{\partial c^2}\right)^{-1}_{T,P,N} = (1-c)a_A\left(\frac{\partial a_A}{\partial c}\right)^{-1}_{T,P,N} = ca_A\left[\frac{\partial a_A}{\partial(1-c)}\right]^{-1}_{T,P,N} \quad (39)$$

We will then have

$$S_{cc}(0) = \frac{c(1-c)}{1-c(1-c)g(n,W)} \quad (40)$$

Where,

$$g(n,W) = \frac{zn^2\left(\frac{W}{RT}\right) - (n-1)^2\left[c+n(1-c)\right]}{\left[c+n(1-c)\right]^3} \quad (41)$$

The short-range order parameter: This is the small range order parameter: The Warren-Cowley short-range order parameter 1 can be written as follows:

$$\alpha_1 = \frac{s-1}{s(Z-1)+1} \quad (42)$$

Where

$$S = \frac{S_{cc}(0)}{c(1-c)} \quad (43)$$

Z is the coordination number.

5.RESULTS AND ANALYSIS

The thermodynamic properties and microscopic functions of the Sn-Zn binary liquid alloy are determined using the programming language C++. This is done to make computations easier to execute so that they do not need to be done manually. One of C++'s numerous advantages is its support for object-oriented (OO) programming concepts in general and type-independent (generic) programming. This applies even to highly typed languages. When compared to the experimental values across the entire concentration range of 0.0 to 1.0, the calculated value roughly approximates the latter. The American Society of Metals (ASM) provided the experimental data on the temperature-dependent fluctuations of the interaction components.

Deductions from the value of ordering energy parameter, W/RT for Sn-Zn liquid Alloy at RT 750 K Throughout the computation, this value remains constant. A positive value of W shows that the attraction between dissimilar atoms (Sn-Zn) does not outweigh the attraction between identical atoms (Sn-Sn or Zn-Zn). As a result, liquid Sn-Zn alloys have a tendency to split. Deductions from the Gibbs free energy of mixing, GM/RT for Sn-Zn alloy at 750 K Computational concepts and the Gibbs Graph The estimated and measured free energies for mixing (VMAL) and concentration (CZn) show a strong correlation, indicating a high degree of similarity (Figure 1). There may be a small distinction between this and the statement "rising from the entropy of mixing."

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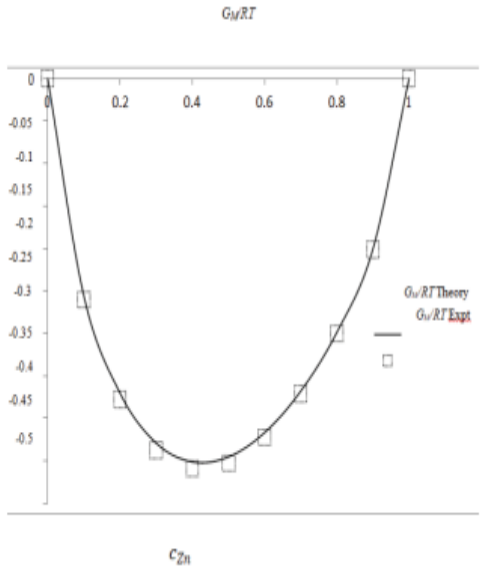

Figure 1: This graph depicts the Gibbs free energy of mixing (GM/RT) vs content (baT) in a Sn-Zn alloy at 750 K. The straight line represents the experimental values, whereas the square boxes show the approximated values..

Deductions from the activity (a) for Sn-Zn alloy at 750 K The activity of the Sn-Zn liquid was calculated using Equation 33. Figure 2 shows an activity diagram that connects the real and calculated numbers.

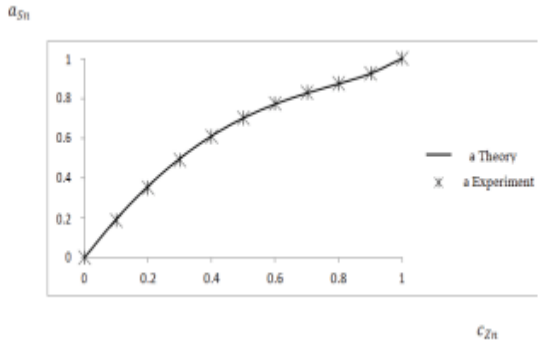

Figure 2: At 750 K, the thermodynamic activity graph of Sn-Zn alloy shows the temporal variation in concentration (Ce i). The hook represents the experimental numbers, while the solid line represents the expected values. Deductions from the microscopic functions-concentration fluctuation, $Scc(0)$ and short-range order parameter, α1 for Sn-Zn alloy at 750 K Some findings about the Sn-Zn metal at 750 K were reached using the short-range order parameter (1) and the concentration fluctuation parameter (Lbc(0)).

$$S_{cc}(0) > S_{cc}^{id}(0)$$

Examining the values of Lbc(0) and 1 is one method for determining the properties and degree of segregation in binary liquid metals. What amount of exhibits the ability of the Sn-Zn alloy in question to separate. After learning the symbol, one can quickly derive the local configurations of the atoms (particularly, Sn and Zn) that make up the mixture (refer to the Short-range Order Parameter). The normalized form of the measure (1) offers information about the atomic local order strength. Figure 3 also displays the estimated, ideal, and measured values of Lbc (0). The calculated and measured values of c(0) for any concentration range are invariably greater than the ideal values. As seen in Figure 4, every combination has one or more 1 values that are greater than zero. Based on the values of Scc(0) and 1, it is possible to conclude that the liquid Sn-Zn alloy at 750 K acts as a segregation system.

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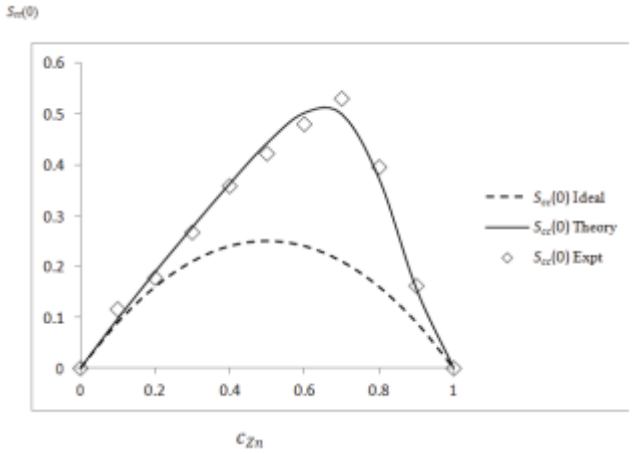

Figure 3: The relationship between Sn-Zn metal concentration (Lbc(0)) and concentration (Cai) at 750 K. The straight line indicates computed values, the diamonds experimental values, and the dotted line ideal values..

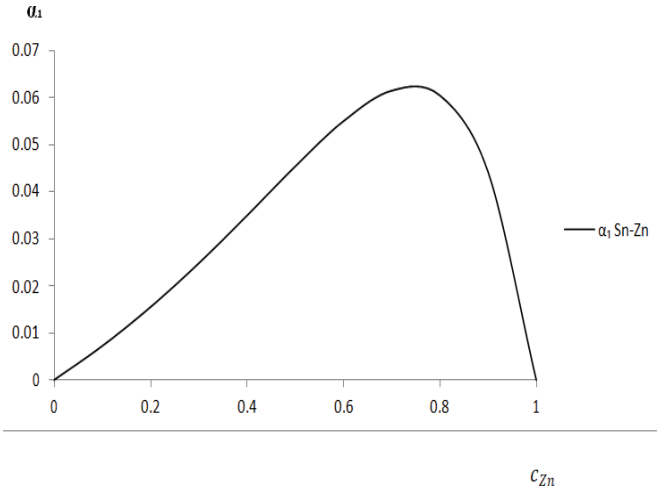

Figure 4: The Warren-Cowley short-range order parameter, aab, for the Sn-Zn metal at 750 K was discovered by observing its fluctuation with concentration.

6.CONCLUSION

The self-association model was used to explore the free energy of mixing, activity, concentration fluctuations in the long wavelength limit, and the Warren-Cowley chemistry short-range order parameter of a liquid Sn-Zn alloy. The simulations revealed that the alloy has a moderate degree of interaction and a substantial proclivity for phase separation or the formation of homo-pairs. It shows a propensity for pairing elements that are similar in nature, specifically Sn-Sn and Zn-Zn .

REFERENCES

1. Zumdahl, S.S., 1993. Introductory chemistry textbook (3rd Ed). D.C. Health and Company, Canada.
2. Prasad, L.C., et al., 1988. Correlation between bulk and surface properties of AgSn Liquid Alloys. J Phys Chem B, 102(6), pp. 921-926.
3. Awe, O.E., et al., 2005. Thermodynamic investigations of Bi-Cd, In-Pb, and Ni-Pd liquid alloys. Int J Mat Res, 96(1).
4. Singh, R.N., et al., 1987. Thermodynamics properties molten Li-Mg alloy. Can J Phys, 145(3), pp. 358-364.
5. Singh, R.N., 1987. Short-range order and concentration fluctuations in binary molten alloys. Canadian Journal of Physics, 65(3), pp. 309-325.
6. Guggenheim, E.A., 1952. Mixtures; the theory of the equilibrium properties of some simple classes of mixtures, solutions, and alloys. Oxford University Press, Oxford. Singh, R.N., et al., 1992. Z. Metallkd, 83, pp. 553.

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7. Singh, R.N., et al., 1992. Temperature dependence of the thermodynamic functions of strongly interacting liquid alloys. J Phys CondenS Matter, 4(24), pp. 5345-5358.
8. Singh, R., et al. 1992. Segregation and immiscibility in liquid binary alloys. Rep Prog Phys, 60(1), pp. 57-150.
9. Adhikari, D., et al., 2013. Thermodynamic, structural and transport properties of molten Copper-Thallium alloys. International Journal of Physical and Mathematical Sciences, 7(5), pp. 792-797.
10. Hultgren, R., et al., 1973. Selected values of the thermodynamic properties of binary alloys. Metals Park, OH: American society for testing and materials, pp. 1435.

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