International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

Correlation Between Thermodynamic and Electronic Properties of Liquid Al-Au Alloys at 1338K

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ABSTRACT

The mixing behaviour of liquid aluminium–gold (Al-Au) alloys at 1338K has been investigated as a function of composition using the quasi-lattice model (QLM). The model is employed to evaluate key thermodynamic properties, including Gibbs free energy of mixing, entropy of mixing, enthalpy of mixing, activity, concentration fluctuations $S_{cc}(0)$, short-range order parameter are analysed within the framework of QLM to assess the degree of chemical ordering in Al-Au liquid alloy at 1338K. Furthermore, the electronic and electrical properties of the Al-Au system are examined by correlating resistivity with thermodynamic and structural parameters. The calculated resistivity exhibits a pronounced deviation from ideal Nordheim behaviour, with a maximum near the equiatomic composition, indicating significant electron scattering influenced by short-range order and concentration fluctuations. The results reveal that thermodynamic interactions strongly govern both structural organization and electronic transport behaviour. Overall, the study demonstrates that the QLM provides a unified approach to understand the thermodynamic, structural, and electronic properties of liquid Al–Au alloys, confirming the presence of partial chemical ordering at 1338K.

Keywords: *Activity, entropy of mixing, enthalpy of mixing, concentration fluctuation, Gibbs free energy of mixing, electrical resistivity and electronic transport property, Quasi-lattice model.*

1. INTRODUCTION

A comprehensive understanding of the thermodynamic properties of liquid alloys is essential for interpreting the phase stability, atomic ordering, and transport phenomena in metallic systems. In particular, the Al–Au binary system in its molten state near 1338 K exhibits pronounced deviations from ideal solution behaviour due to differences in atomic size, electronegativity, and interatomic bonding. These differences lead to non-linear variations in Gibbs free energy, G_M, enthalpy of mixing, H_M and activity, a, indicating strong heteroatomic interactions and the presence of short-range chemical ordering in the melt [1–3]. Such deviations are closely associated with concentration fluctuations and non-random atomic arrangements in liquid alloys [2,4,5].

The quasi-lattice model (QLM) [1] provides an effective statistical framework for describing these non-ideal effects in liquid alloys. By incorporating interaction parameters and local atomic configurations, the model enables the evaluation of thermodynamic functions such as G_M, S_M, and H_M, along with structural descriptors including

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

concentration fluctuations $S_{cc}(0)$ and short-range order parameters, α [4–7]. These structural quantities, derived from thermodynamic analysis, are essential for the understanding of the microscopic arrangement of atoms in Al–Au melts at 1338 K.

The electronic and electrical properties of liquid alloys are strongly governed by their thermodynamic and structural characteristics. Electrical resistivity in metallic melts arises primarily from electron scattering caused by compositional disorder and atomic-scale inhomogeneities, as described by the classical theories of J. M. Ziman, P. Nordheim, and N. F. Mott [8–10]. In Al–Au liquid alloys, strong thermodynamic interactions promote short-range ordering, which modifies the electronic density of states and reduces random scattering, resulting in deviations from ideal Nordheim behaviour and a composition-dependent resistivity profile [6,11,12].

Recent investigations have further demonstrated that thermodynamic stability, concentration fluctuations, and local atomic ordering collectively influence electronic transport properties in liquid metals, even at elevated temperatures [13–20]. These studies confirm that short-range order persists in liquid Al–Au alloys at 1338 K and plays a critical role in determining macroscopic properties such as electrical conductivity and diffusivity.

Therefore, establishing a direct correlation between thermodynamic functions and electronic transport behaviour is essential for a complete understanding of liquid alloys. In this context, the present work employs the quasi-lattice model to investigate the thermodynamic properties of Al–Au melts at 1338 K and to elucidate their influence on structural ordering and electrical transport behaviour.

2. FORMALISM

2.1 Thermodynamic properties

The thermodynamical variables of compound forming alloy, quasi lattice-model (QLM) is used in statistical mechanics within the formalism of grand partition function [1]. It assumes that the inter-atomic interaction between closest neighbours within a chemical complex differs from that between atoms not belonging to the complex. In QLM, the compound forming alloy of the elements A and B can be treated as a pseudo ternary solution containing A and B atoms and chemical complexes of type $A_\mu B_\nu$ where μ and ν are integers. In a solid forming alloy, there is a natural tendency for such complexes to form at specific stoichiometric compositions given by

$$c_c = \frac{\mu}{(\mu + \nu)}.$$

The mixing properties of complex forming liquid alloys, the presence of these complexes is explicitly considered [10]. Each complex is assumed to be formed by μ atoms of A and ν atoms of B according to equilibrium condition $\mu A + \nu B \rightleftharpoons A_\mu B_\nu$. For a binary molten alloy, the thermodynamic quantity namely the Gibbs free energy of mixing G_M is expressed as [1]

$$G_M = G_M^{XS} + G_M^{id} \quad (1)$$

as $$G_M^{id} = Nk_BT[c\ln c + (1-c)\ln(1-c)] \quad (2)$$

or, $$G_M = G_M^{XS} + Nk_BT[c\ln c + (1-c)\ln(1-c)] \quad (3)$$

where, N indicates the total number of atoms, k_B represents Boltzmann constant and T refers to absolute temperature in Kelvin(K). Here c and (1-c) are concentrations of atom A and B respectively.

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

According to phase diagram [2], Al-Au melts at 1338K exhibit the formation of Al_2Au type complex. Therefore, in present case, we have taken μ=2 and ν=1 to represent the G_M^{XS} as [1]

$$\frac{G_M^{XS}}{RT} = \frac{\omega}{k_BT}\phi(c) + \frac{\Delta\omega_{AB}}{k_BT}\phi_{AB}(c) + \frac{\Delta\omega_{AA}}{k_BT}\phi_{AA}(c) \qquad (4)$$

with,

$$\phi(c) = c(1-c) \qquad (4a)$$

$$\phi_{AB}(c) = \frac{1}{6}c + c^2 - \frac{5}{3}c^3 + \frac{1}{2}c^4 \qquad (4b)$$

$$\phi_{AA}(c) = -\frac{1}{4}c + \frac{1}{2}c^2 - \frac{1}{4}c^4 \qquad (4c)$$

in the above expression, $\omega = Z(\varepsilon_{AB} - \frac{\varepsilon_{AA} + \varepsilon_{BB}}{2})$, is the interchange energy with Z as coordination number and ε_{ij} (where i, j ≡ A, B) corresponds to the bond energies of like pairs (AA and BB) and unlike pairs AB while $\Delta\omega_{ij}$ signifies the interaction parameters associated with the respective atomic interaction.

Equation (3) and (4) yield [4]

$$\frac{G_M}{RT} = \frac{\omega}{k_BT}\phi(c) + \frac{\Delta\omega_{AB}}{k_BT}\phi_{AB}(c) + \frac{\Delta\omega_{AA}}{k_BT}\phi_{AA}(c) + c\ln c + (1-c)\ln(1-c) \qquad (5)$$

The expression (5) represents the analytical formula for G_M of a binary melt.

Among the various thermodynamic quantities, activity is particularly significant because it can be determined from experimental measurements. For the i^{th} component, (i ≡ A, B) in a binary melt, the activity a_i is written as [4]

$$\ln a_i = \frac{G_M}{RT} + \frac{(1-c_i)}{RT}\left(\frac{\partial G_M}{\partial c_i}\right)_{T,P,N} \qquad (6)$$

Equations (5) and (6) provide

$$\ln a_A = \frac{G_M}{RT} + (1-c)\left[\frac{\omega}{k_BT}(1-2c) + \frac{\Delta\omega_{AB}}{k_BT}\left(\frac{1}{6} + 2c - 5c^2 + 2c^3\right) + \frac{\Delta\omega_{AA}}{k_BT}\left(-\frac{1}{4} + c - c^3\right)\right] + \ln\left(\frac{c}{1-c}\right) \qquad (7a)$$

$$\ln a_B = \frac{G_M}{RT} + c\left[-\frac{\omega}{k_BT}(1-2c) - \frac{\Delta\omega_{AB}}{k_BT}\left(\frac{1}{6} + 2c - 5c^2 + 2c^3\right) - \frac{\Delta\omega_{AA}}{k_BT}\left(-\frac{1}{4} + c - c^3\right)\right] - \ln\left(\frac{c}{1-c}\right) \qquad (7b)$$

The equations (7a) and (7b) provide the working expressions for the activities a_A and a_B respectively.

The entropy of mixing, S_M is an important thermodynamic quantity for understanding of the structural characteristics of binary melts. However, since the experimental determination of S_M is often difficult, its theoretical evaluation becomes particularly significant.

For the binary melt, S_M^{XS} is expressed as [1]

$$S_M^{XS} = -\left[\frac{\partial G_M^{XS}}{T}\right]_P \qquad (8)$$

From equations (3) and (8) one can obtain

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

$$\frac{S_M^{XS}}{N} = -\frac{\partial \omega}{\partial T}\phi(c) - \frac{\partial(\Delta\omega_{AB})}{\partial T}\phi_{AB}(c) - \frac{\partial(\Delta\omega_{AA})}{\partial T}\phi_{AA}(c) \quad (9)$$

$$\frac{S_M^{XS}}{R} = -\frac{1}{k_B}\frac{\partial \omega}{\partial T}\phi(c) - \frac{1}{k_B}\frac{\partial(\Delta\omega_{AB})}{\partial T}\phi_{AB}(c) - \frac{1}{k_B}\frac{\partial(\Delta\omega_{AA})}{\partial T}\phi_{AA}(c) \quad (10)$$

The entropy of mixing, S_M of a binary melt can be represented as

$$S_M = S_M^{XS} + S_M^{id}$$

$$S_M = S_M^{XS} - R[c\ln c + (1-c)\ln(1-c)] \quad (11)$$

So, using equation (11), S_M for binary melt is written as

$$\frac{S_M}{R} = -\frac{1}{k_B}\frac{\partial \omega}{\partial T}\phi(c) - \frac{1}{k_B}\frac{\partial(\Delta\omega_{AB})}{\partial T}\phi_{AB}(c) - \frac{1}{k_B}\frac{\partial(\Delta\omega_{AA})}{\partial T}\phi_{AA}(c) - c\ln c - (1-c)\ln(1-c) \quad (12)$$

The equation (12) is employed to evaluate the entropy of mixing, S_M for a binary liquid alloy.

Although, enthalpy of mixing, H_M of a binary melts can be measured experimentally, its theoretical interpretation is crucial for revealing the type and extent of atomic interactions presents between the components of solution.

The thermodynamic quantities, G_M^{XS}, G_M and S_M are interrelated from the fundamental thermodynamic relation as [22]

$$H_M = G_M^{XS} + TS_M^{XS}$$

Using equations (4) and (10) in above equation, one can obtain

$$\frac{H_M}{RT} = \left[\frac{\omega}{k_BT} - \frac{1}{k_B}\frac{\partial \omega}{\partial T}\right]\phi(c) + \left[\frac{\Delta\omega_{AB}}{k_BT} - \frac{1}{k_B}\frac{\partial(\Delta\omega_{AB})}{\partial T}\right]\phi_{AB}(c) + \left[\frac{\Delta\omega_{AA}}{k_BT} - \frac{1}{k_B}\frac{\partial(\Delta\omega_{AA})}{\partial T}\right]\phi_{AA}(c) \quad (13)$$

Equation (13) provides the expression which can be used to evaluate the enthalpy of mixing, H_M/RT for a binary melt.

2.2. Structural properties

The structural parameter known as the concentration fluctuations in a long wavelength limit, $S_{cc}(0)$ is an important quantity for describing the microscopic behaviour of a binary melt. $S_{cc}(0)$ may be represented by [3,5,22]

$$S_{cc}(0) = Nk_BT\left(\frac{\partial^2 G_M}{\partial c^2}\right)^{-1}_{T,P,N} \quad (14a)$$

$$S_{cc}(0) = (1-c)a_A\left(\frac{\partial a_A}{\partial c}\right)^{-1}_{T,P,N} = ca_B\left(\frac{\partial a_B}{\partial(1-c)}\right)^{-1}_{T,P,N} \quad (14b)$$

The values of $S_{cc}(0)$ obtained by substituting the experimental activity data of a_A and a_B into equation (14b) are treated as the experimental estimates of the concentration fluctuation parameter.

For ideal melts,

$$G_M^{id} = RT\sum_i c_i \ln c_i)\ (i \equiv A, B) \quad (15)$$

Equations (14b) and (15) together yield the expression used to calculate the ideal concentration fluctuation, $S_{cc}^{id}(0)$ i.e.

$$S_{cc}^{id}(0) = c(1-c) \quad (16)$$

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
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www.ijarse.com
IJARSE
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It is noteworthy that any departure of $S_{cc}(0)$ from ideal values provides an important information about the structure ordering of melts [3, 22]. A lower value of $S_{cc}(0)$ than ideal $S_{cc}(0)$ indicates the tendency towards ordering meaning that unlike atoms (A-B) preferentially occupy nearest neighbour positions. Conversely, a higher value of $S_{cc}(0)$ than ideal $S_{cc}(0)$ reflects segregation, where like atoms (A-A or B-B) are more likely to be nearest neighbours.

Combining equations (5) and (14a), one obtained

$$S_{cc}(0) = \frac{c(1-c)}{1 - 2\frac{\omega}{k_B T}\phi(c) + \frac{\Delta\omega_{AB}}{k_B T}\phi(c)\phi''_{AB} + \frac{\Delta\omega_{AA}}{k_B T}\phi(c)\phi''_{AA}} \quad (17)$$

with,

$$\phi''_c = -2 \quad (18a)$$

$$\phi''_{AB} = \frac{\partial^2}{\partial c^2}\phi_{AB}(c) = 2 - 10c + 6c^2 \quad (18b)$$

$$\phi''_{AA} = \frac{\partial^2}{\partial c^2}\phi_{AA}(c) = 1 - 3c^2 \quad (18c)$$

In addition to concentration fluctuations, the Warren-Cowley short-range parameter i.e. α_1 is another important structural parameter associated with first coordination shell, of the binary melts [22-23]. This parameter provides the local degree of ordering within the liquid.

Mathematically, α_1 for a binary melt for Z coordination number is expressed as

$$\alpha_1 = \frac{(S-1)}{S(Z-1)+1} \quad \text{where,} \quad S = \frac{S_{cc}(0)}{S_{cc}^{id}} \quad (19)$$

It is notable that the value of Z is commonly taken to be 10 (9)

2.3. Transport property

The atomic diffusivity is a key transport property that helps to explain the microscopic mechanism of mixing in binary melt. It describes the rate at which constituent atoms migrate within the melt and therefore strongly influenced by interatomic interactions and local structural arrangements.

For a binary molten system, the ratio of diffusivity can be expressed in terms of thermodynamic quantities as given in [6, 24]

$$\frac{D_M}{D_{id}} = \frac{S_{cc}^{id}(0)}{S_{cc}(0)} \quad (20)$$

here, D_M signifies the mutual diffusion coefficient for a metallic melt, whereas D_{id} corresponds to the ideal intrinsic diffusion coefficient. The expression for ideal intrinsic diffusion coefficient is given by

$$D_{id} = c_A D_B + c_B D_A \quad (21)$$

In this expression, Di (with i ≡ A, B) signifies the self-diffusion coefficient of component i. Equation (20) suggests that the binary molten alloys can exhibit segregation or chemical ordering depending on the relative magnitude of the relevant diffusion ratio. A value of D_M/D_{id} greater than unity signifies the tendency towards segregation, whereas the value of D_M/D_{id} less than unity indicates ordering nature, corresponding to the predominance of like atoms or unlike atoms respectively.

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

2.4. Electronic and electrical property

The electronic and electrical properties of liquid alloys are strongly influenced by their thermodynamic and structural characteristics. In binary melts, electrical resistivity arises primarily due to electron scattering caused by compositional disorder and atomic scale inhomogeneities. In the case of Al–Au melts at 1338 K, the quasi-lattice model (QLM) provides concentration-dependent thermodynamic quantities such as Gibbs free energy, (G_M) , activity (a_i) (i=A, B) , and the concentration fluctuation parameter $S_{cc}(0)$, which can be directly related to resistivity [1,2,3,4].

Following the classical Nordheim theory of resistivity in alloys, the resistivity ρ of a binary melt can be expressed as [8-10]:

$$\rho(C_{Al}) = \rho_0 C_{Al} C_{Au}[1 + kS_{cc}(0)] \qquad (22)$$

where, C_{Al} and C_{Au} are the mole fractions of aluminium and gold respectively, $S_{cc}(0)$ is the long wavelength concentration fluctuation parameter from QLM analysis, ρ_o is a reference resistivity factor, and k is proportionality constant reflecting scattering strength due to short range order [25-26]. This formulation ensures that the composition dependance of resistivity is properly captured via $C_{Al}C_{Au}$, while the structural ordering is incorporated via $S_{cc}(0)$. The resistivity is expected to show non-linear deviations from ideal behaviour, particularly near compositions where Al-Au atomic complexes form, as predicted by the QLM framework.

3. RESULTS AND DISCUSSIONS

The expressions derived in the structure of QLM have been applied to investigate the thermodynamic and structural properties of molten Al–Au alloys at 1338 K. The observed quantities include the G_M, G_M^{XS}, S_M, and H_M, activity a_i (i=A, B). In addition, Scc(0), α_1, and $\frac{D_M}{D_{id}}$ were also calculated for the system.

3.1. Thermodynamic properties

From equation (3), it follows that the calculation of the required quantity for Al-Au melts at 1338K depends on the interaction parameter ω, $\Delta\omega_{AB}$ and $\Delta\omega_{AA}$ These parameters were estimated using the successive approximation method [27], [28] based on the available experimental data of G_M^{XS} for Al-Au melts at 1338K. The best satisfied values of the interaction parameters are

$$\frac{\omega}{k_B T} = -9.255 \; ; \; \frac{\Delta\omega_{AB}}{k_B T} = 3.200 \quad \text{and} \quad \frac{\Delta\omega_{AA}}{k_B T} = 13.755$$

It is noteworthy that the above interaction parameters were employed thoroughly to compute the thermodynamic, structural, and transport properties of Al–Au melts at 1338 K.

The theoretical results for the relevant thermodynamic functions, G_M and G_M^{XS} plotted as a function of concentration of Al for the Al–Au melt at 1338 K, are compared with the corresponding experimental data [21], as shown in Fig. 1. A very good agreement between theory and experiment is observed in the whole composition range of C_{Al} = 0.1 – 0.9. At all compositions, the values are negative, for G_M with minimum values of -3.722 (theory) and -3.716 (experiment), and for G_M^{XS} with minimum values of -3.029 (theory) and -3.022 (experiment), both occurring at C_{Al}= 0.5. The large magnitude of G_M as well as G_M^{XS} suggest that the interatomic interactions in

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

Al-Au liquid alloys are strong, non-ideal and ordering alloys. Thus, the observed asymmetry in G_M and G_M^{XS} are well explained by quasi-lattice model. Thus, QLM successfully explains that the Al–Au melt at 1338K has a tendency toward the formation of chemical complexes.

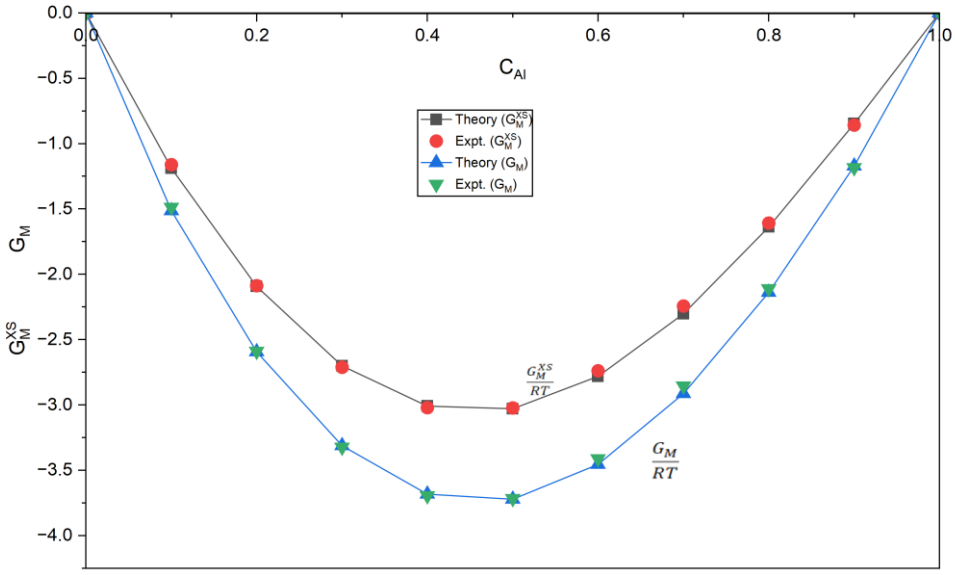

Fig. 1. The $\frac{G_M^{XS}}{RT}$ and $\frac{G_M}{RT}$ versus C_{Al}, for Al-Au melts at 1338K

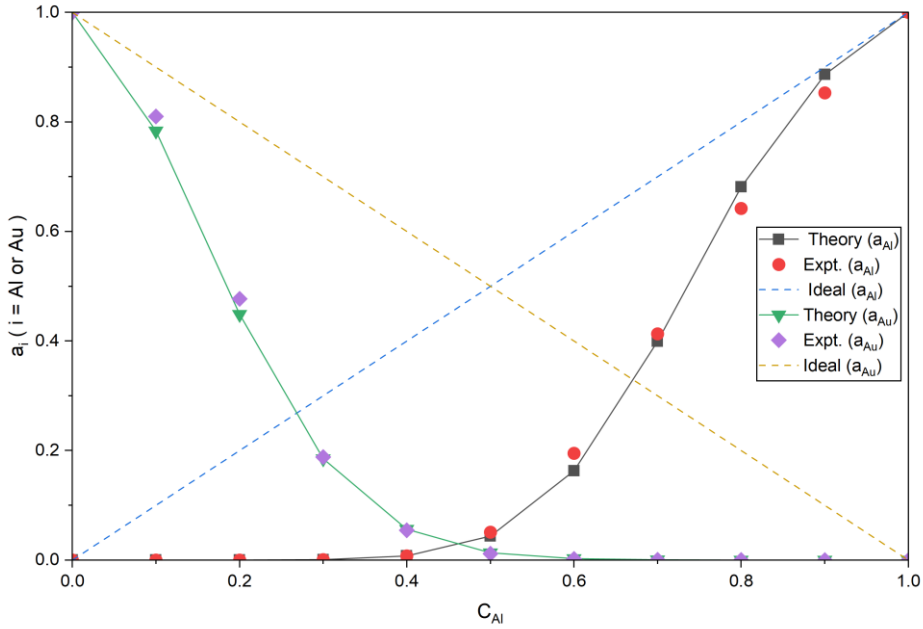

Fig. 2 Activity of Al (a_{Al}) and activity of Au (a_{Au}) versus C_{Al} for Al-Au melts at 1338K

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International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

The activity of Al, a_{Al} and the activity of Au, a_{Au} for Al-Au melts at 1338K were evaluated from equations (7a) and (7b). The comparison between the calculated and experimentally associated values [21] of a_{Al} and a_{Au} for Al-Au melts at 1338K are shown in Fig. 2. The calculated theoretical data are in good agreement with the corresponding experimental data in the entire composition range i.e. $C_{Al} = 0.1$ to 0.9. Both a_{Cu} and a_{Au} show large negative deviations from the ideal solution behaviour, indicating the presence of attractive interactions between the unlike atoms and consequently a strong tendency toward chemical ordering in Al-Au melts at 1338K. The close correspondence between calculated and experimental activities further supports the reliability of the estimated interaction parameter ω, $\Delta\omega_{AB}$ and $\Delta\omega_{AA}$.

The equations (11) and (12) explicitly incorporate the temperature dependence of the interaction parameters ω, $\Delta\omega_{AB}$ and $\Delta\omega_{AA}$. Hence, the evaluations of S_M and H_M, require the determination of the temperature derivatives of these energy parameters. These quantities i.e. $\frac{\partial \omega}{\partial T}$, $\frac{\partial(\Delta\omega_{AB})}{\partial T}$ and $\frac{\partial(\Delta\omega_{AA})}{\partial T}$, were estimated using the successive approximation method [28, 29] in equation (11) to the available experimental data for S_M of Al-Au melts at 1338K. The best optimized values are:

$$\frac{\partial\omega}{\partial T} = -5.947k_B \;\; ; \;\; \frac{\partial\Delta\omega_{AB}}{\partial T} = 8.400k_B \;\; \text{and} \;\; \frac{\partial\Delta\omega_{AA}}{\partial T} = -13.054k_B$$

The estimated values of $\frac{\partial \omega}{\partial T}$, $\frac{\partial(\Delta\omega_{AB})}{\partial T}$ and $\frac{\partial(\Delta\omega_{AA})}{\partial T}$ were subsequently substituted into equation (11) and (12) to evaluate the composition dependency of S_M, and H_M, respectively for Al-Au melts at 1338K.

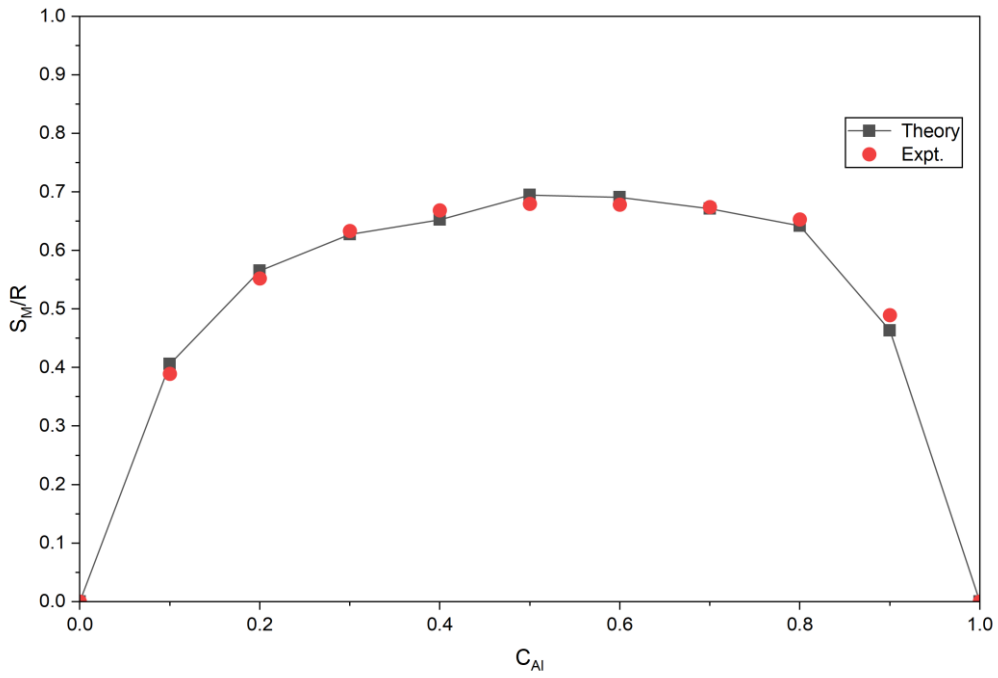

Fig. 3. $\frac{S_M}{R}$ versus C_{Al}, for Al-Au melts at 1338K.

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

The calculated values of S_M obtained from equation (11) of Al-Au liquid alloy at 1338K are shown in Fig. 3, together with the experimental data [21]. The theoretical results are in good agreement with the experimental findings. Both the theoretical and experimental results are positive in the entire composition range of Al. The maximum theoretical value of entropy of mixing, S_M, is found to be 0.695 at $C_{Al} = 0.5$ while the experimental value is 0.680 at $C_{Al} = 0.5$. Therefore, the observed symmetry in $\frac{S_M}{R}$ for molten Al-Au at 1338K is successfully explained by the present theoretical approach.

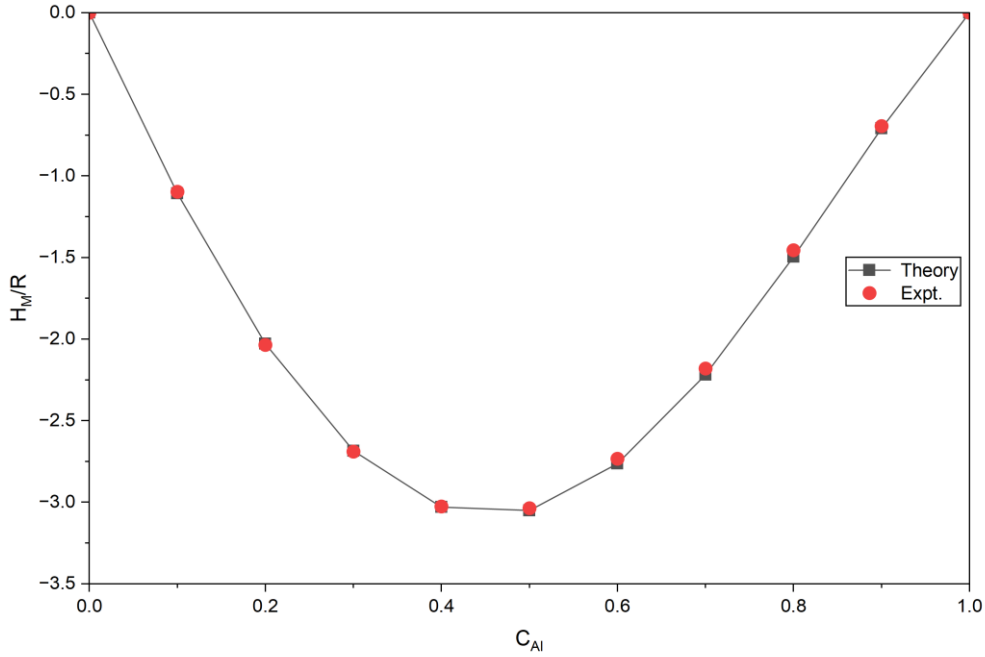

Fig. 4. $\frac{H_M}{RT}$ versus C_{Cd}, for Al-Au melts at 1338K

Equation (12) has been employed to evaluate the enthalpy of mixing, H_M, for molten Al-Au alloys at 1338 K. In order to ensure consistency, the same interaction energy parameters previously determined $\frac{\omega}{k_BT}$, $\frac{\Delta\omega_{AB}}{k_BT}$, and $\frac{\Delta\omega_{AA}}{k_BT}$ along with their corresponding temperature derivatives $\frac{\partial\omega}{\partial T}$, $\frac{\partial\Delta\omega_{AB}}{\partial T}$, and $\frac{\partial\Delta\omega_{AA}}{\partial T}$, have been used in the calculations.

The calculated and experimental values [21] of $\frac{H_M}{RT}$ for molten Al-Au alloys at 1338K are plotted in Fig. 4 as a function of Al concentration. The theoretical results show good agreement with the experimental data. A minimum in $\frac{H_M}{RT}$ occurs at $C_{Al} = 0.5$, where the theoretical value is -3.051 and the experimental value is -3.037. Hence, the symmetric behavior of H_M for Al-Au molten alloys at 1338 K is satisfactorily explained by the present theoretical model i.e. QLM.

3.2. Structural properties

For the Al–Au liquid alloy at 1338 K, the thermodynamic quantities under consideration have been evaluated as a function of Al concentration using equation (16), (17), and (18) using the previously determined model

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

parameters. The calculated values of $S_{cc}(0)$ and ideal values of $S_{cc}(0)$ i.e. $S_{cc}^{id}(0)$ are presented in Fig. 5 together with the corresponding experimental results derived from activity data [21] through Eq. (13b), plotted as a function of Al concentration. The comparison demonstrates very good agreement between theoretical predictions and experimental findings [21].

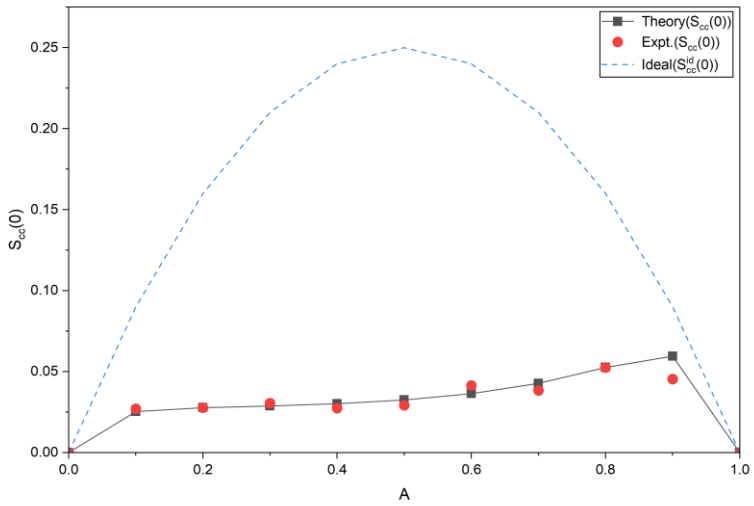

Fig. 5 $S_{cc}(0)$ versus C_{Al} for Al-Au at 1338K

The values of $S_{cc}(0)$ exhibit the large negative deviations from $S_{cc}^{id}(0)$ in the whole concentration range of Al i.e. $S_{cc}(0) < S_{cc}^{id}(0)$, signifies the hetero-coordination, meaning that unlike atoms (Al-Au) preferentially associate as nearest neighbours in A-Au melts at 1338K. The difference between $S_{cc}^{id}(0)$ and $S_{cc}(0)$ i.e. $S_{cc}^{id}(0) - S_{cc}(0)$ is maximum having a value of 0.2175 at $C_{Al} = 0.5$. Again the large negative deviations between $S_{cc}(0)$ and $S_{cc}^{id}(0)$ indicates the complex forming tendency in Al-Au melts at 1338K. Therefore, the present analysis suggests that the Al-Au system at 1338 K behaves as an ordered alloy with a strong preference for Al-Au nearest-neighbour pairing.

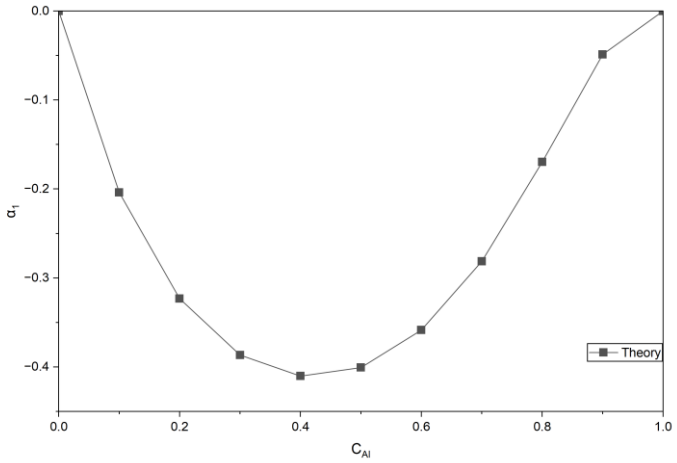

Fig. 6. α_1 versus C_{Al} for Al-Au melts at 1338K

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

The Warren–Cowley short-range order parameter, α_1, [22,23] provides valuable insight into the local atomic arrangement in liquid alloys. A value of α_1 corresponds to a completely random distribution of atoms. The positive values of α_1 indicate segregation (a preference for like-atom pairing), whereas negative values signify chemical ordering, meaning that unlike atoms preferentially occupy nearest-neighbour positions.

Fig. 6 shows the variation of α_1, for Al–Au melts at 1338 K, evaluated using Eq. (19), as a function of Al concentration. Since experimental measurements of α_1 for this system are not available in the literature, a direct comparison with experimental data cannot be made. The calculated results reveal that α_1 remains negative throughout the entire Al composition range from 0.1 to 0.9. The most negative value, -0.4103, occurs at the composition $C_{Al} = 0.4$. The negative sign of α_1 signifies a preference for unlike-atom pairing, indicating chemical ordering in the melt. The negative sign and relatively small magnitude of α_1 indicate that the Al-Au system at 1338 K is a strongly interacting, yet ordered, liquid alloy.

3.3. Transport properties

The diffusivity ratio for the Al–Au melt has been evaluated using Eq. (20) as a function of Al concentration [6, 24]. The calculated values are presented in Fig. 7. It is observed that the diffusivity ratio remains greater than unity over the entire composition range, i.e. 0.1 to 0.9. The maximum value of diffusivity ratio is 7.958, occurs at the composition $C_{Al} = 0.4$, indicating the strongest degree of chemical ordering at this concentration for the Al–Au melt at 1338 K. Again, comparison with experimental data could not be performed because the relevant experimental measurements are not available in the literature.

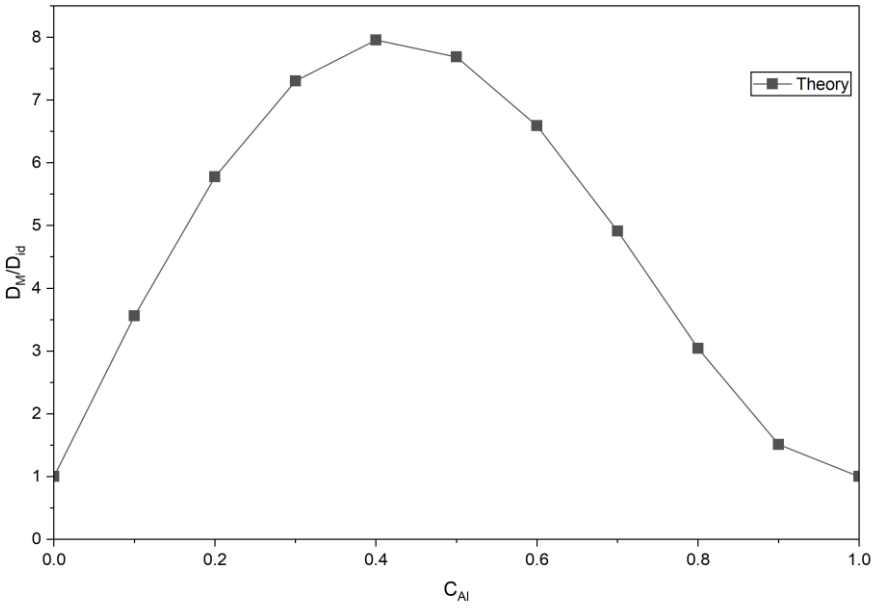

Fig. 7. $\frac{D_M}{D_{id}}$ versus C_{Al}, for Al-Au melts at 1338K

10.5281/zenodo.21616017

International Journal of Advance Research in Science and Engineering
Volume No. 15, Issue No. 07, July 2026
www.ijarse.com
IJARSE
ISSN 2319 - 8354

3.4. Electronic and electrical properties

The electrical resistivity of Al–Au melts at 1338 K are unavailable, in the equation (17) and (22), where ρ_o is a system dependent scaling parameter and k is an empirical parameter for the short-range order on electron scattering, its value is normally obtained by fitting experimental activity data [30]. Here, the phenomenological value of parameter $\rho_o = 50$ and $k = -0.25$ are taken to illustrate the concentration dependence of resistivity within the quasi-lattice model. These parameters are only served as scaling constants and do not represent experimentally determined material constants. Theoretical value of ρ was presented in Fig.8 as a function of C_{Al}. The graph shows that there was a non-ideal composition dependence, peaking near the equiatomic ratio ($C_{Al} = 0.5$) with a maximum value of 12.398 [8-9].

This behaviour clearly deviates from the ideal Nordheim rule and correlates closely with increased concentration fluctuations $S_{cc}(0)$, indicating significant short-range chemical ordering. Such ordering alters electron scattering and the local electronic structure, leading to asymmetric resistivity across the composition range. Near pure components, resistivity approaches zero due to reduced compositional disorder. These findings demonstrate that resistivity in Al–Au melts is strongly governed by thermodynamic interactions and atomic-scale structural fluctuations, which are effectively captured in the framework of the quasi-lattice model linking thermodynamic and electronic transport properties.

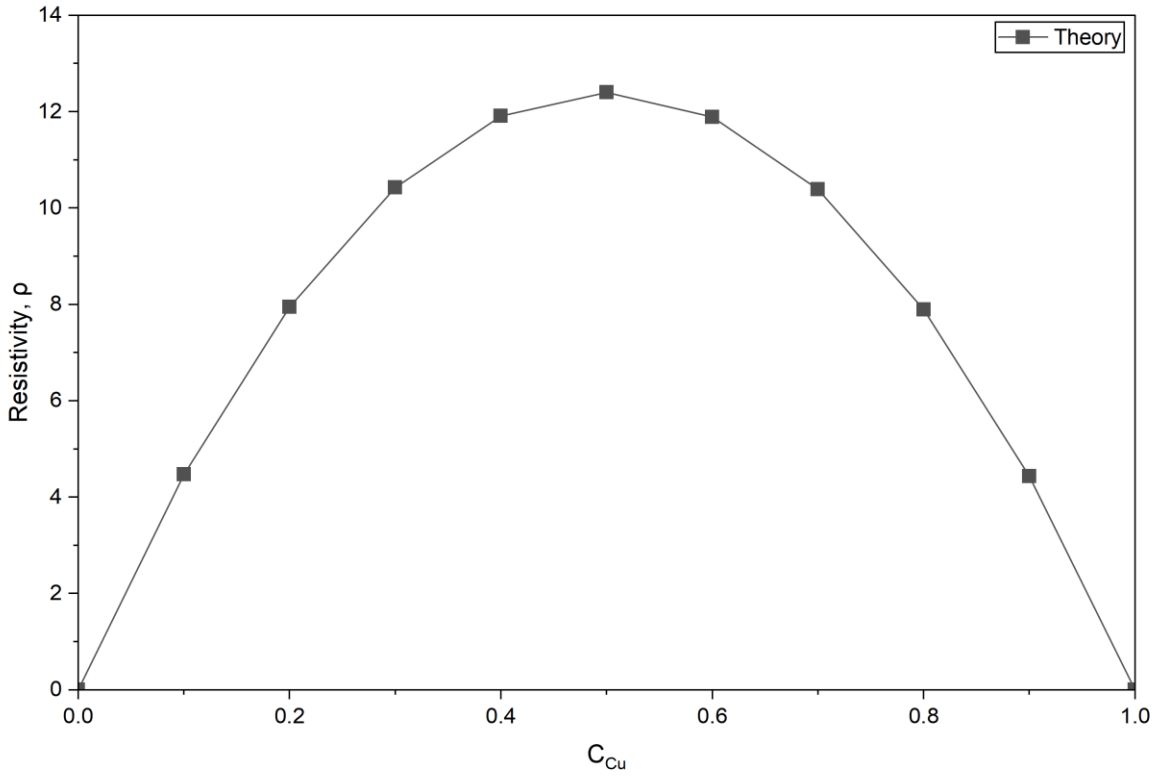

Fig. 8 Resistivity (ρ) versus concentration of Al (C_{Al}) for Al-Au melt at 1338K

10.5281/zenodo.21616017

4. CONCLUSIONS

The quasi-lattice model analysis of Al–Au melts at 1338 K successfully reproduces the thermodynamic (G_M^{XS}, G_M, H_M, S_M and a_i), structural ($S_{cc}(0)$, α_1), transport diffusivity ratio, and electronic/electrical properties (ρ_0) of the Al-Au liquid alloy at 1338K. The key findings include:

- Strong chemical ordering is observed near equiatomic compositions, evidenced by negative α1 and deviations of $S_{cc}(0)$ from ideal values.
- Thermodynamic quantities (G_M^{XS}, G_M, H_M, S_M, a_i) exhibit asymmetry about C_{Al} = 0.5 due to strong heteroatomic interactions.
- Electronic resistivity is strongly influenced by concentration fluctuations and short-range order, with $\rho(C_{al})$ peaking near the equiatomic composition and deviating from ideal Nordheim behaviour.
- The correlation between thermodynamic ordering and electronic transport highlights the predictive power of QLM for analyzing structure-property relationships in liquid alloys at high temperatures.

  Thus, QLM provides a unified framework to connect thermodynamics, structure, transport, and electronic properties in Al–Au melts at 1338 K, facilitating the design and understanding of complex metallic liquids.

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