Effect of temperature on mixing behavior and stability of liquid Al-Fe alloys

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Abstract. A theoretical model based on the assumption of compound formation in binary liquid alloy has been used to investigate the thermodynamic properties (free energy of mixing, enthalpy of mixing and entropy of mixing), microscopic properties (concentration fluctuation in long wavelength limit and chemical short range order parameter), surface properties (surface tension and surface composition) and dynamic properties (viscosity and diffusion coefficient). All the properties of Al₂Fe binary melt have been measured using the same energy parameters configured for experimental values of free energy of mixing. The energy parameters are detected as independent of concentration, but depend on temperature. The findings are well consistent with the experimental standards.

Keywords: Bulk properties; Ordering; Surface tension; Positive deviation

1. INTRODUCTION

The development of lightweight, energy-efficient materials is critical for mitigating the global energy crisis [1]. Aluminum alloys are intensively researched in the automotive and aerospace sectors as test specimens, structural components, and massive metal surfaces. Aluminum alloys are the most often utilized light alloys for structural component weight reduction. At room temperature, these materials are often distinguished by their low density, high thermal conductivity, and good corrosion resistance [2–5]. Because of the extent to which its microstructure may be changed, the Al - Fe alloy system is particularly appealing for aeronautical constructions [6]. Al-Fe alloys have good oxidation properties, a high melting point, and a cheap material cost, making them an economically attractive material for industrial use [7,8]. Al-Fe alloys are also significant in powder metallurgy and spray forming [7,9]. They are the primary components of metal-matrix composites. Additionally, by changing the composition and thermal treatments of Al-Fe alloys, especially when coupled with additional elements like Mg, Si, Cu, and Zn, stronger Al-Fe alloys can be produced [10]. When the thermodynamic characteristics of a binary liquid alloy deviate significantly from ideality, the theoretical models used to analyze it provide vital information. These deviations induce asymmetry in thermodynamic characteristics away from equiatomic composition. The asymmetry in the thermodynamic characteristics of binary melt is mostly due to the size effect [11] and the electronegativity difference [12]. The size ratio (≈1.4) and electronegativity difference (≈0.22) for Al - Fe liquid alloy are too small to produce significant asymmetry in thermodynamic characteristics. The phase diagram [13] shows that the Al - Fe alloy has many stable phases, including Al₁₃Fe₂, which has a complex end – center monoclinic structure, Al₁₃Fe₅, which has an end – center orthorhombic structure, AlFe, which has an ordered bcc (B₂) structure isotypic with CsCl, AlFe₃, which has an ordered bcc (D₀₃)}
structure isotypic with BiF$_3$, and Al$_2$Fe having a complex rhombohedral structure. Among these phases, the presence of Al$_3$Fe complex in the liquid state has been considered in this investigation, and its thermodynamic and microscopic characteristics at 1873 K have been calculated using the complex formation model [14]. The Moelwyn–Hughes method [15] has been used to investigate the viscosity of the selected alloy, whereas the Prasad model [16,17] was used to investigate the surface characteristics. Due to the lack of long-range atomic order, researching the characteristics of alloys in liquid form is challenging. As a result, theorists have used several models [18–24] to better explain the characteristics of binary liquid alloys. Theoreticians have previously studied the Al$_3$Fe alloy in its liquid form at a constant temperature of 1873K [12]. The energetics of Al$_2$Fe alloy at various temperatures have been investigated in this study utilizing a complex formation model [14]. To demonstrate the correctness of this technique in thermodynamic and structural description of the provided binary system, the results are examined and compared with published data [25].

2. Formulation

2.1 Thermodynamic Properties

To investigate the mixing behavior of Al - Fe compounds, the complex formation model has been used. According to this model, the Al-Fe alloy will be a ternary combination of three species: Al atoms, Fe atoms, and the chemical complex Al$_2$Fe, all of which will be in chemical equilibrium with one another. Conformal solution is another name for this ternary combination. $N_{Al} = x$ number of Al atoms and $N_{Fe} = (1 - x)$ number of Fe atoms make up the total number of atoms in the provided binary system, which equals $N = N_{Al} + N_{Fe}$. The thermodynamic characteristics of components Al and Fe are altered when they are combined to produce a binary Al-Fe solution. Because of compound formation in the melt, the quantity of free atoms will decrease. For $n_1$ g, $n_2$ g and $n_3$ g atoms of Al, Fe and Al$_2$Fe respectively,

\[ n_1 = x - 2n_3 \]
\[ n_2 = 1 - x - n_3 \] (1)

After mixing, the total number of atoms is

\[ n = n_1 + n_2 + n_3 = 1 - 2n_3 \] (2)

The free energy loss due to compound formation is given by $-n_3 \psi$; the complex formation energy is denoted by $\psi$; and the ternary mixture mixing free energy is denoted by $G'$. Then the binary mixture’s free energy of mixing may be expressed as [14],

\[ G_M = G' - n_3 \psi \] (3)

In the case of the ternary ideal solution,

\[ G' = \frac{RT}{n} \sum_{i=1}^{3} (n_i \ln n_i) \] (4)

Where the implications of the size differences in the mixture are not to be neglected and the interaction between species is limited, but not zero, the zeroth approximation of regular solutions [26] or conformal solution approximation [27] must be valid. In this approximation, $G'$ in terms of interaction energy parameter, $V_{ij}$, can be expressed as,

\[ G' = \frac{RT}{n} \sum_{i=1}^{3} (n_i \ln n_i) + \frac{1}{n} \sum_{i<j}^{3} n_i n_j V_{ij} \] (5)

The free energy of mixing for compound forming and regular binary alloys is now expressed as

\[ G_M = \frac{RT}{n} \sum_{i=1}^{3} (n_i \ln n_i) + \frac{1}{n} \sum_{i<j}^{3} n_i n_j V_{ij} - n_3 \psi \] (6)

The equilibrium state at a particular pressure and temperature may be used to calculate the value of $n_3$. 


Substituting $G_M$ from equation 6 and doing some algebraic calculations, we get

$$\ln\left(n_1 n_2^2 n_1^{-1} n_2^{-1}\right) + \chi = \frac{\psi}{RT}$$

Which is the equilibrium equation, where

$$\chi = \left(\frac{2n_1n_2}{n} - 2n_2 - n_1\right) \frac{V_{12}}{nRT} + \left(\frac{2n_3n_2}{n} - n_3 + n_2\right) \frac{V_{23}}{nRT} + \left(\frac{2n_3n_3}{n} - 2n_3 + n_1\right) \frac{V_{13}}{nRT}$$

The heat of mixing $H_M$ can be expressed as follows [14]:

$$H_M = G_M - T\frac{\partial G_M}{\partial T}$$

Using the value of $G_M$ from equation 6, we obtain

$$H_M = -n_1 \left[\psi - T\left(\frac{\partial \psi}{\partial T}\right)_p\right] + \frac{1}{n} \sum_{i<j} n_i n_j \left[n_i - \frac{1}{n} \sum_{j<i} n_j \frac{\partial V_{ij}}{\partial T}\right]$$

The entropy of mixing expression, $S_M$, may be written as

$$S_M = \frac{(H_M - G_M)}{T} = n_3 \frac{\partial \psi}{\partial T} - R \left(\frac{3}{n} \sum_{i<j} n_i \ln \frac{n_i}{n} - \frac{1}{n} \sum_{i<j} n_i n_j \frac{\partial V_{ij}}{\partial T}\right)$$

### 2.2 Structural Properties

Any variation from the ideal value $S_{cc}^{id}(0)$ is crucial in understanding the nature of ordering and phase separation in molten alloys, therefore the concentration fluctuation at the long wavelength limit is of great importance. The free energy of mixing is linked to concentration variation at long wavelength limits by the formula [28],

$$S_{cc}(0) = RT \left(\frac{\partial^2 G_M}{\partial \chi^2}\right)^{-1}$$

Differentiating $G_M$ twice with respect to $x$

$$\frac{\partial^2 G_M}{\partial \chi^2} = RT \sum_{j=1}^{3} \left(\frac{n_j^2}{n} - \frac{n_j^2}{n}\right) + \frac{2n}{RT} \sum_{i < j} V_{ij} \left(\frac{n_i}{n} + \frac{n_j}{n}\right)^{-1}$$

$$S_{cc}(0) = \sum_{i=1}^{3} \left(\frac{n_i^2}{n} - \frac{n_i^2}{n}\right) + V_{ij} \left(\frac{n_i}{n} + \frac{n_j}{n}\right)^{-1}$$

In terms of composition, the prime on the $n$'s refers to their first derivative. By using the following formula, the theoretically predicted values of $S_{cc}(0)$ may be compared to observed values computed from constituent element activity at different compositions.

$$S_{cc}(0) = x_{Fe} a_{Al} \left(\frac{\partial a_{Al}}{\partial \chi_{Al}}\right)^{-1} = x_{Al} a_{Fe} \left(\frac{\partial a_{Fe}}{\partial \chi_{Fe}}\right)^{-1}$$

$S_{cc}^{id}(0)$ represent the ideal value as,

$$S_{cc}^{id}(0) = x_{Al} x_{Fe}$$
In the following equation, \( \alpha \) indicates Warren – Cowely chemical short range order parameter which measures the degree of local order within the binary melt [29,30].

\[
\alpha_i = \frac{s - 1}{s(z - 1) + 1}
\]

(17)

In equation 17, \( z \) is coordination number.

2.3 Transport Properties

The molten alloy’s mixing behavior can even be examined at the fundamental level in terms of diffusion coefficient. With the aid of Darken’s equation [31], the mutual diffusion coefficient \( (D_M) \) of binary liquid alloys may be described in terms of activity \( (a_i) \) and self- diffusion coefficient \( (D_i) \) of individual component.

\[
D_M = x_iD_i \frac{d\ln a_i}{dx_i}
\]

(18)

with \( D_M = x_{Al}D_{Fe} + x_{Fe}D_{Al} \)

Where \( D_{Al} \) and \( D_{Fe} \) are the self – diffusion coefficients of Al and Fe respectively. In terms of \( S_{cc}(0) \), the ratio of mutual diffusion coefficient \( (D_M) \) to self – diffusion coefficient \( (D_i) \) can be expressed as

\[
\frac{D_M}{D_i} = \frac{S_{cc}(0)}{S_{cc}(0)}
\]

(19)

The microscopic mixing behavior of liquid alloys may also be described in terms of viscosity. The Moelwyn – Hughes equation for liquid alloy viscosity is

\[
\eta = (x_{Al}\eta_{Al} + x_{Fe}\eta_{Fe}) \left[ 1 - 2x_{Al}x_{Fe} \frac{H_M}{RT} \right]
\]

(20)

Here \( \eta_i \) is the viscosity of individual elements Al and Fe. This value can be optimized for required temperature \( (T) \) as [32],

\[
\eta_i = \eta_{i0} \exp \left( \frac{E}{RT} \right)
\]

(21)

Here \( \eta_{i0} \) is a constant in the unit of viscosity and \( E \) is the activation energy.

2.4 Surface Properties

The surface characteristics of the liquid solution reveal metallurgical phenomena including crystal development, wounding, gas absorption, and gas bubble nucleation [33]. The surface tension equations provided by Prasad et al., [16, 17], have been simplified using the zeroth approximation as

\[
\tau = \tau_{Al} + \frac{k_BT}{\xi} \ln \frac{x_{Al}^s}{x_{Al}} + \frac{\psi}{\xi} \left[ \rho(x_{Fe}^s)^q + (q - 1)x_{Fe}^2 \right]
\]

(22)

\[
\tau = \tau_{Fe} + \frac{k_BT}{\xi} \ln \frac{x_{Fe}^s}{x_{Fe}} + \frac{\psi}{\xi} \left[ \rho(x_{Al}^s)^q + (q - 1)x_{Al}^2 \right]
\]

(23)

Where \( \tau_i \) represents the surface tensions of pure Al and Fe, \( x_i \) and \( x_i^s \) denote the bulk and surface concentrations of alloy components while \( p \) and \( q \) represent the coordination fractions. These are the fraction of an atom’s nearest neighbors generated within its own layer and those created by the next layer. The connection between the coordination fractions \( p \) and \( q \) is \( p + 2q = 1 \). For present
calculation, we assume the closed packed structure for which the \( p \) and \( q \) values are 0.5 and 0.25 respectively.

The mean atomic surface area (\( \xi \)) of the compound can be expressed in terms of component surface area (\( \xi_i \)) as,

\[
\xi = \sum x_i \xi_i \tag{24}
\]

Here

\[
\xi_i = 1.102 \left( \frac{\Omega_i}{N_{Av}} \right)^{2/3} \tag{25}
\]

Where \( \Omega_i \) is the component \( i \)'s molar volume and \( N_{Av} \) is the Avogadro’s number. Equations (22) and (23) may be solved for \( x_i \) as the function of \( x_c \) and hence surface tension compositional dependency can be examined.

3. RESULTS AND DISCUSSION

3.1 Thermodynamic Properties

The order energy values for the Al–Fe liquid phase were calculated using known experimental data on thermodynamic characteristics [25] as well as phase diagram information [13]. The mixing functions, i.e. the Gibbs free energy and the enthalpy of mixing (figure 1), are negative for all compositions and have a flat minimum of -1.4770 and -1.2775 at equiatomic composition, \( x_c = 0.5 \), showing the compositional site of an energetically favorable compound, the Al – Fe. The preferred configurations of Al and Fe component atoms facilitate the production of Al2Fe complexes (\( \mu=2 \) and \( \nu=1 \)) in liquid alloys. All calculations were performed at \( T = 1873 \) K, taking into account the Al - Fe phase diagram [13] and the existence of the liquid phase across the entire concentration range. At \( T = 1873 \) K, the interaction energy parameters \( \psi \), \( V_{12} \), \( V_{13} \) and \( V_{23} \) as well as their temperature derivatives, were calculated using the Gibbs energy of mixing, \( G_M \), of liquid Al - Fe alloys and the enthalpy of mixing, \( H_M \) [25]. The interaction energy parameters' values were tweaked to produce concentration dependences of \( G_M \) that closely matched the thermodynamic data. \( V_{12} = -3.095RT \), \( V_{13} = -0.851RT \), \( V_{23} = -1.970RT \) and \( \psi = 2.552RT \) are the estimated interaction energy parameters for liquid Al - Fe alloys, and they remain constant throughout all computations. The number of complexes, \( n_3 \), was calculated using equations (8-9) and equations (1-2). The concentration dependence of the equilibrium values of chemical complexes, \( n_3 \), reaches a maximum value of around 0.261 at the compound forming composition, \( x_c = 0.667 \).

If energy parameters are assumed to be temperature independent, the values of \( H_M \) and \( S_M \) are found to be in poor agreement with the experiment. As a result, we looked at how these parameters changed with temperature to see how heat and entropy of formation changed with observed values [25]. At \( T = 1873K \), the temperature-dependent energies are \( \partial V_{12} / \partial T = 0.980R \), \( \partial V_{13} / \partial T = 2.591R \), \( \partial V_{23} / \partial T = 2.984R \) and \( \partial \psi / \partial T = 0.212R \). Equations (11) and (12) have been used to calculate the enthalpy of mixing, \( H_M \) and the entropy of mixing, \( S_M \) and have been compared to existing experimental data [25]. A comparison of the anticipated values of \( H_M \) and \( S_M \) computed at \( T = 1873 \) K with published data of liquid Al - Fe alloys reveals a reasonable agreement (figure 1).

The temperature-dependent fluctuation of interaction energy parameters can be written as

\[
V_{ij}(T_R) = V_{ij}(T) + (T - T_R) \frac{\partial V_{ij}}{\partial T} \tag{26}
\]
Here $T_e = 2073K, 2273K, 2473K$ and $2673K$

Equation (26) was used to derive the interaction energy parameters at $2073K$, $2273K$, $2473K$, and $2673K$ using the values of interaction energy parameters at $1873K$ and their temperature derivatives (figure 2). Table 1 shows the optimized values of interaction parameters at elevated temperatures.

![Figure 1.](image1.png)  
**Figure 1.** Gibb’s free mixing energy ($G_M/RT$), heat of mixing ($H_M/RT$) and entropy of mixing ($S_M/RT$) vs. concentration of aluminum ($x_{Al}$) in the liquid Al - Fe alloy at $1873K$.

![Figure 2.](image2.png)  
**Figure 2.** Temperature (T) effects on the interaction parameters ($V_{ij}$ and $\psi$)

| Parameter/ $T$ | $2073K$ | $2273K$ | $2473K$ | $2673K$ |
|---------------|---------|---------|---------|---------|
| $V_{12}/RT$   | -2.702  | -2.378  | -2.106  | -1.875  |
| $V_{13}/RT$   | -0.519  | -0.245  | -0.016  | 0.179   |
| $V_{23}/RT$   | -1.492  | -1.098  | -0.768  | -0.487  |
| $\psi/RT$     | 2.326   | 2.140   | 1.984   | 1.852   |

The linear fit $V_{ij}(T) = a + bT$ for the temperature dependence of interaction energy parameters is excellent. Table 2 summarizes the $a$ and $b$ values for interaction parameters.

| Coefficients | $V_{12}$ | $V_{13}$ | $V_{23}$ | $\psi$ |
|--------------|----------|----------|----------|--------|
| $a$ (Joule)  | -63456.4 | -53599.2 | -77144.3 | 36438.8|
| $b$ (Joule K$^{-1}$) | 8.14772 | 21.5416 | 24.8090 | 1.76257|

Equation (6) is used to obtain the variation of $G_M$ with temperature using these interaction parameters at various temperatures (figure 3). When temperature rises from $1873K$ to $2673K$, the maximum value of $G_M/RT$ at equiatomic composition increases from $-1.4770$ to $-1.0947$, indicating a phase separation tendency at higher temperatures.
3.2 Structural Properties

Concentration fluctuations in the long-wavelength limit, \( S_{cc}(0) \), and chemical short-range order parameter, \( \alpha_{1} \), as functions of bulk concentration, have been used to investigate the ordering processes in the Al - Fe liquid phase. Equations (14) and (16) are used to derive the \( S_{cc}(0) \) values and the values that characterize ideal mixing \( S_{cc}^{id}(0) \) in weak approximation. Figure 4 plots these values along with the observed values from equation (15) using activity data. At \( x_c = 0.5 \), the largest difference between theoretical and ideal concentration fluctuations in the long-wavelength limit is 0.1519. This means that \( x_c \) is the concentration at which the chemical can form [28]. As can be observed, \( S_{cc}(0) \) is lower than \( S_{cc}^{id}(0) \), showing that chemical order exists across the whole concentration range. With increasing temperature, the value of \( S_{cc}(0) \) decreases, reducing the gap between ideal and theoretical values, indicating the tendency of similar atom pairing, leading to homo co-ordination (figure 5). As the temperature rises, the solution approaches its optimum state. At \( T \approx 7788K \), the regular solution becomes fully ideal, and \( S_{cc}(0) \) is defined by the equation (16). The negative values of the Warren–Cowley parameter, \( \alpha_{1} \), over the whole concentration range support this conclusion (figure 4). The phase separating tendency is supported by the variation of \( \alpha_{1} \) with temperature, as evidenced by the variation of free energy of mixing with temperature.

![Figure 3. Temperature effects on \( G_M/RT \) with respect to bulk composition of Al.](image)
3.3 Transport Properties

The viscosities of the constituent elements, $\eta_i$, and the related activation energies at a fixed temperature were obtained from the literature [32]. Equation (21) is used to optimize these values for the temperature of research. Equation (20) is then used to calculate the viscosity of the liquid Al – Fe alloy at 1873K. Figure 6 depicts the viscosity's compositional dependence as well as the ideal value. Over the whole compositional range, the obtained viscosities are higher than ideal values. Up to $x_{Al} = 0.4$, the positive departure from ideality grows at which the deviation is maximum ($= 0.001866$) but sharply decreases below $x_{Al} = 0.7$. The plot of $\eta$ at different temperature with respect to $x_{Al}$ (figure 7.) shows that there is decreasing tendency of $\eta$ as temperature increases.

At the fundamental level, the mixing tendency of the liquid alloy is investigated by determining the ratio of mutual and intrinsic diffusion coefficients ($D_{M} / D_{a}$). $D_{M} / D_{a} > 1$ denotes the likelihood of compound formation; $D_{M} / D_{a} < 1$ denotes phase separation; and $D_{M} / D_{a} = 1$ denotes the solution's ideality. The values of $D_{M} / D_{a}$ are found to be positive and greater than unity throughout the compositions using equation (19) (figure 6). At the equiatomic composition, the maximum value ($=2.5475$) occurs. The theoretical examination of the presence of chemical order in the liquid state of Al-Fe alloy at 1873 K is now even clearer. Figure 8 shows that when the temperature raises, the amount of $D_{M} / D_{a}$ decreases. The maximum difference ($=0.6098$) in $D_{M} / D_{a}$ values for the temperatures 2673K and 1873K at equiatomic composition, $x_{Al} = 0.5$ again support high ordering tendency at that composition.

**Figure 4.** Concentration fluctuation at long wavelength limit ($S_{cc}(0)$) and chemical short range order ($\alpha_1$) vs. concentration of aluminum ($x_{Al}$) in the liquid Al - Fe alloy at 1873K.

**Figure 5.** Temperature effects on $S_{cc}(0)$ and chemical short range order ($\alpha_1$) of liquid Al - Fe alloy with respect to bulk composition of Al.
Figure 6. The mutual-to-intrinsic diffusion coefficient ratio ($D_{M}/D_{D}$) and viscosity ($\eta$) vs. concentration of aluminum ($x_{Al}$) in the liquid Al - Fe alloy at 1873K.

Figure 7. Temperature effects on viscosity ($\eta$) of liquid Al - Fe alloy with respect to bulk composition of Al.

Figure 8. Temperature effects on the mutual-to-intrinsic diffusion coefficient ratio ($D_{M}/D_{D}$) of liquid Al - Fe alloy with respect to bulk composition of Al.
3.4 Surface Properties

The Prasad model [16,17] was used to compute the surface composition, \( x_{Al}^s \), and surface tension, \( \tau \), of liquid Al-Fe alloy as functions of bulk composition at various temperatures (T = 1873K, 2073K, 2273K, and 2473K). The surface composition values, \( x_{Al}^s \), with regard to bulk concentration of Al, have been numerically solved using the expression derived by subtracting equation (23) from equation (22) (figure 9). Aluminum surface concentration in Al-Fe alloys is observed to rise as the bulk concentration of Al increases. The surface composition of Al deviates from ideality in a positive way. The surface compositions vs. concentration values were then utilized in the same equations to calculate the surface tension (figure 9). The same interaction energy parameters, surface coordination fractions \( (p = 0.5 \) and \( q = 0.25 \)), mean atomic surface area, and surface tension data of pure components are used in both sets of equations (equations 24-25). The surface tensions of pure components at given temperatures, as well as the essential inputs for calculating mean atomic surface area and pure component element densities at fixed temperatures, were obtained from the literature [32]. Using the following formulas, these values have been evaluated at working temperature (T).

\[
\rho_i(T) = \rho_i^0 + (T - T_i^0)\Delta \rho_i
\]
\[
\tau_i(T) = \tau_i^0 + (T - T_i^0)\Delta \tau_i
\]

The following figures show the surface concentration values and surface tensions at various temperatures.

\[\text{Figure 9.}\] Surface concentration of aluminum \((x_{Al}^s)\) and surface tension \((\tau)\) vs. bulk concentration of aluminum \((x_{Al})\) in the liquid Al - Fe alloy at 1873K.

\[\text{Figure 10.}\] Compositional dependence of surface concentration of aluminum \((x_{Al}^s)\) and surface tension \((\tau)\) in liquid Al - Fe alloy at different temperatures.

For the component metals of the alloys, \(\Delta \rho_i\) and \(\Delta \tau_i\) denote temperature coefficient of density and surface tension, respectively. Figure 10 shows the estimated surface concentration values for molten Al - Fe alloys at 1873 K and various temperatures. With increasing temperature, the surface concentration likewise decreases. The decreasing tendency of surface concentration with rise in temperature from 1873K to 2673K is maximum (=0.1310) at \(x_{Al} = 0.1\) and minimum (=0.0060) at \(x_{Al} = 0.9\). This implies the decreasing tendency of surface composition with respect to temperature, increases with decrease in bulk composition \(x_{Al}\).
Furthermore, as shown in figure 9, the surface tension isotherm derived by the CFM for the regular solution deviates negatively from that calculated by the ideal solution model \( \gamma_{\text{ideal}} = \gamma_{Al}x_{Al} + \gamma_{Fe}x_{Fe} \) with regard to surface composition of Al. This strongly suggests that liquid alloys with negative excess Gibbs energy in the bulk have negative surface tension departures from their ideal solution [34]. Figure 10 shows the surface tensions of Al–Fe alloys as a function of Al content at various temperatures. The surface tension of the alloy has been found to decrease as the temperature rises. At temperatures ranging from 1873K to 2673K, the difference in surface tension values is greatest (=0.2732) at \( x_{Al} = 0.9 \) and smallest (=0.0217) at \( x_{Al} = 0.1 \). This means that as the bulk composition of Al increases, \( \gamma_{2673K} - \gamma_{1873K} \) increases as well.

4. CONCLUSIONS

Different theoretical models have proven effective in explaining the thermodynamic, microscopic, transport, and surface characteristics of Al-Fe alloys. At all concentrations, the theoretical study of thermodynamic characteristics reveals a propensity for dissimilar atom pairing or ordering in liquid Al - Fe alloys. The energy parameters are found to be negative, suggesting that the component elements are attracted to one another. The interaction parameters are also discovered to be temperature dependent and concentration independent. With the exception of the formation energy parameter, the negativity of the rest of the interaction parameter diminishes as temperature increases. At all temperatures investigated, symmetry is seen in the free energy of mixing and the heat of mixing. For entropy of mixing, however, asymmetry is found about \( x_{Al} = 0.2 \). The CSRO and concentration fluctuation studies reveal that there is a propensity for hetero co-ordination in liquid Al - Fe alloy. Viscosity isotherms show a positive divergence from Roult's law. At all compositions, the ratio of diffusion coefficients, \( D_M / D_d > 1 \), shows that there is a tendency for complex formation across the entire range of concentrations. The surface tension of the liquid alloy decreases as the bulk concentration of Al in the alloy increases at all temperatures studied. The surface tension of the Al-Fe alloy is found to be less than that of ideal solution. In the setting of varying temperatures, as the temperature of the investigation rises, it falls. Metals with lower surface tension tend to segregate on the surface of molten alloys, according to this research. The compound formation propensity of Al – Fe liquid alloy diminishes as temperature increases, according to temperature variation researches of all characteristics.

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