Complex formation of sodium-mercury alloy at molten state

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Abstract
Thermodynamic properties of compound forming binary liquid sodium-mercury alloy at temperature 673 K have been analyzed as a function of concentration by considering $\text{NaHg}_2$ complex using quasi chemical approximation. The surface tension of the alloy has been studied by the compound formation model, Butler equation as improved by Kaptay, and Statistical mechanical approach. The mixing behavior of the alloy is studied in detail with more emphasis on the interaction energy parameters between neighboring atoms of the alloy. The study provides the information of moderately interacting as well as ordering nature on the entire range of concentration of the liquid alloy and the computed theoretical thermodynamic data are in good agreement with the corresponding experimental data at 673 K. The surface tension of the alloy computed predicts deviation from the ideal case.

1. Introduction

In metallurgical science, alloys are considered superior to individual metals due to their high mechanical strength, chemical resistance, and heat resistance. The formation of an alloy is due to the interaction and structural rearrangement of constituent atoms so that the chemical properties of each constituent element are repressed and new properties are evolved. Most of the alloys are far away from the ideal solution and show the micro-inhomogenous atomic arrangement and hence are difficult to realize as compared to the crystals. The mixing property of the alloy is mainly governed by the electrochemical effect, size of atoms and the concentration of constituent elements so that atoms of individual elements either tend to align showing self-coordinated tendency or a strong ordering tendency \cite{1}. Thus the understanding of the mixing behavior of metals forming alloys has been of great interest to metallurgists and physicists. However, materials remained uninvestigated due to experimental difficulties and time constraints. In order to solve such problems, different theoretical models have been developed.

Alloys are widely used in industries as commercial materials and hence studied extensively in solid-state. The properties of the initial melt of mixing play a vital role in the formation of alloys. Various properties of the alloys in the liquid state are studied in metallurgy as well as for the discovery of new materials for high-temperature application.

Among the various alloys, sodium mercury alloy (sodium amalgam) is of great interest to researchers \cite{2–8} where most of the studies are focused on thermodynamic properties at specified temperatures. It is used as a strong reducing agent in reactions. It is also used in the design of high-pressure sodium lamps where sodium and mercury produce the proper color and electrical characteristics respectively. The production of alkali and chlorine by electrolysis process with liquid mercury as a cathode is considered to be one of the important applications of sodium amalgam \cite{9}.

There are a number of solid intermetallic compounds of sodium amalgam. Balej \cite{4} has suggested sodium concentration in the liquid amalgams below 18\%, viz: $\text{NaHg}_{10}$, $\text{NaHg}_{15}$, $\text{NaHg}_{5}$, $\text{NaHg}_{7}$, $\text{NaHg}_{9}$, $\text{NaHg}_{10}$, $\text{NaHg}_{12}$, and $\text{NaHg}_{14}$. Similarly, mercury and sodium form a congruently melting compound in the form of $\text{NaHg}_4$ (mp. 626 K) \cite{9}. It shows negative deviation from Raoult’s law and also shows anomalous behavior that...
some of its equilibrium mixing properties such as free energy of mixing, enthalpy of mixing, entropy of mixing, and concentration fluctuation in long-wavelength limit at 673 K are asymmetric at equiatomic composition. The alloys showing such behavior are usually known as compound forming binary alloys at one or more defined compositions [10].

The present work aims to study Na – Hg alloy theoretically to determine concentration-dependent thermodynamic properties at 673 K assuming NaHg₂ complex in the melt by using quasi chemical approximation [11] and study of surface tension by the compound formation model developed by Novakovic et al in which connection between surface and bulk properties has been developed through the grand partition functions[12] by the consideration of interaction energy parameters as that of the aforementioned method. Due to lack of experimental data, we intend to compare surface tension thus obtained with other two models: the Butler model as improved by Kaptay [13] and the Statistical approach [14].

The model used in the study assumes an alloy as a pseudo ternary mixture of X atoms, Y atoms, and XₙYₙ group of atoms (μ and ν are small integers) of an energetically favored compound forming alloys all in chemical equilibrium with each other. The equilibrium properties of mixing binary alloy are governed by short-range atomic interaction energies φₓₓ, φᵧᵧ and φₓᵧ for XX, YY, and XY atomic pairs respectively [15]. Based on the pairing of atoms of the constituent elements, the alloys can be classified into two main categories, segregating where like atoms tend to be the nearest neighbor and the compound forming alloys (ordering) where unlike atoms tend to be the nearest neighbor.

The thermodynamic properties such as free energy of mixing, chemical activity, heat of mixing, and entropy of mixing, provide the information on the interaction, stability, and bonding strength among the constituent atoms of alloy whereas information on the structural ordering of atoms in binary alloys in the liquid state is provided by the quantitative analysis of microscopic functions., the concentration fluctuations in the long-wavelength limit (Sₓₓ(0)), short-range order parameter (cₓ₁) [16]. The surface tension is one of the important thermophysical properties studied in metallurgy to get the information of surface property of liquid alloy and is important in the casting process for getting different devices for better mechanical performance. Further, surface segregation, which mainly refers to the inequality in concentration between the surface and that of bulk materials of the alloy, is one of the important factors of the alloy which is to be studied in metallurgical science. The reason for this inequality is the difference in surface energy between the constituent elements of the alloy where the element with smaller surface energy has the tendency to segregate on the surface [17].

The organization of this paper is as follows. In section 2, the expressions required for the calculation are presented. In section 3, the result and general discussion of Na-Hg alloy are presented. Finally, the conclusions are presented in section 4.

2. Theoretical basis

2.1. Thermodynamical functions

Consider a binary alloy of N number of atoms with elements X and Y. The model (QCA) considers the existence of chemical complexes XₙYₙ where

\[ \mu X + \nu Y = XₙYₙ \]  

With this consideration, grand partition function in terms of configurational energy ‘E’ is simplified and excess free energy of mixing \( G_M^{XS} \) at temperature T is expressed as

\[ G_M^{XS} = Nk_B T \int_0^c Y dc \]  

Where \( Y \) is ratio of activity coefficient of element \( x \) to \( y \), \( c \) is the concentration of X atoms.

After simple mathematical calculation [11] the solution of equation (2) is given below.

\[ G_M^{XS} = N[\theta ω + \theta xy \Delta ωxy + \theta xx \Delta ωxx + \theta yy \Delta ωyy] \]  

Where \( \theta = C(1 - C) \) and \( \theta_j;k’s (j,k = X, Y) \) are the simple polynomials in C depending on the values of X and Y, \( \theta (=Ze_xy - (φₓₓ/2 + φᵧᵧ/2)) \) is interchange energy, \( \Delta ω_j;k (=Zφ_j;k) \) are interaction energy parameters and Z is coordination number.

For \( X = Na, Y = Hg, \mu = 1, ν = 2 \), the values of \( \theta_j;k’s \) are found to be [11]

\[ \theta xy(C) = \frac{1}{6} C + \frac{2}{3} C^2 + \frac{1}{2} C^3 \]  
\[ \theta xx(C) = 0 \]
\[ \theta_{YY}(C) = -\frac{1}{4}C + \frac{1}{2}C^2 - \frac{1}{4}C^4 \]  

(6)

The Free energy of mixing for the complex alloy is given by

\[ G_M = G^{\text{SS}}_M + G^{\text{deal}}_M \]
\[ = G^{\text{SS}}_M + RT[C \ln C + (1 - C) \ln (1 - C)] \]
\[ = N[\theta \omega + \theta_{XY} \Delta \omega_{XY} + \theta_{XX} \Delta \omega_{XX} + \theta_{YY} \Delta \omega_{YY}] \]
\[ + RT[C \ln C + (1 - C) \ln (1 - C)] \]

(7)

Here \( \theta_{XX} \) is taken zero because according to the model, for \( \mu = 1 \), the probability of \( X \) and \( X \) (or \( XX \)) pair to be part of the complex is zero so that the coefficient of \( \Delta \omega_{XY} \) in equation (7) also tends to zero. If there are not complexes in the alloy then \( \Delta \omega_{XY} \) is zero. In such case, the above equation takes the form as,

\[ G_M = N\theta \omega + RT[C \ln C + 1 - C \ln (1 - C)] \]

(8)

The heat of mixing is found out by using standard thermodynamic relation:

\[ H_M = G_M - T \left( \frac{dG_M}{dT} \right)_p \]
\[ = N \left[ \theta \left( \omega - T \frac{d\omega}{dT} \right) + \theta_{XY} \left( \omega_{XY} - T \frac{d\omega_{XY}}{dT} \right) + \theta_{XX} \left( \omega_{XX} - T \frac{d\omega_{XX}}{dT} \right) + \theta_{YY} \left( \omega_{YY} - T \frac{d\omega_{YY}}{dT} \right) \right] \]

(9)

The standard thermodynamic relation for the entropy of mixing is

\[ S_M = \frac{H_M}{T} - \frac{G_M}{T} \]

(10)

The activity of the constituent elements in the alloys is determined from following standard thermodynamic relation.

\[ RT \ln a_j(j = X, Y) = G_M + (1 - C) \left( \frac{\partial G_M}{\partial C_j} \right)_{T,P,N} \]

(11)

By solving equations (7) and (11), the theoretical values of activities of each component are given as follows,

\[ RT \ln a_X = \frac{G_M}{RT} + \frac{1}{k_BT} (1 - 2C) \omega + \theta'_{XY} \Delta \omega_{XY} + \theta'_{XX} \Delta \omega_{XX} + \theta'_{YY} \Delta \omega_{YY} + \ln \frac{C}{1 - C} \]

(12)

\[ RT \ln a_Y = \frac{G_M}{RT} - \frac{C}{k_BT} (1 - 2C) \omega + \theta'_{XY} \Delta \omega_{XY} + \theta'_{XX} \Delta \omega_{XX} + \theta'_{YY} \Delta \omega_{YY} + \ln \frac{C}{1 - C} \]

(13)

Where \( \theta'_{XY}, \theta'_{XX} \) and \( \theta'_{YY} \) are concentration derivatives of \( \theta_{XY}, \theta_{XX} \) and \( \theta_{YY} \) respectively.

2.2. Microscopic functions

The concentration fluctuation in long-wavelength limit for the alloy is derived from standard relation as [18].

\[ S_{CC}(0) = RT \left[ \frac{\partial^2 G_M}{\partial C^2} \right]^{-1}_{T,P,N} \]

(14)

The value of \( S_{CC}(0) \) can be obtained by using observed activities as

\[ S_{CC}(0) = C_X a_X \left[ \frac{\partial a_X}{\partial C} \right]^{-1}_{T,P,N} = C_Y a_Y \left[ \frac{\partial a_Y}{\partial C} \right]^{-1}_{T,P,N} \]

(15)

Where \( C_X (= C) \) and \( C_Y (= 1 - C) \) are concentrations of elements \( X \) and \( Y \) respectively. The values of \( S_{CC}(0) \) obtained from equation (15) are called experimental values.

Solving equations (7) and (14), the theoretical value of \( S_{CC}(0) \) is found as follows.

\[ S_{CC}(0) = \frac{C(1 - C)}{1 + (1 - C) \left[ -2 \frac{\omega}{k_BT} + \theta''_{XY} \frac{\omega_{XY}}{k_BT} + \theta''_{XX} \frac{\omega_{XX}}{k_BT} + \theta''_{YY} \frac{\omega_{YY}}{k_BT} \right]} \]

(16)

Where \( \theta''_{jk} \) is the second derivative of \( \theta_{jk} \) with respect to concentration.

The Warren–Cowley short-range order parameter [19, 20] is related to concentration fluctuation in the long-wavelength limit as,
\[ \alpha_i = \frac{L - 1}{L(Z - 1) + 1} \]  

(17)

Where,

\[ L = \frac{S_{CC}(0)}{S_{CC}^0(0)} \]  

(18)

2.3. Surface tension

The surface tension is considered as an important factor in metallurgy for the processes such as molten-metal processing, fusion-welding, soldering, etc. in which liquid alloy or metal is involved. It concerns the problems related to the surface and interface in the liquid metal process [21, 22]. The interfacial motion caused by the surface tension of liquid plays a major role in many industrial phenomena and hence the surface and interfacial behavior of liquid metals are considered to have importance in metallurgical processes for solidification, controlling the processes of welding and casting [23].

In the present work, we try to study the surface tension of Na–Hg alloy at 673 K by using three different models: compound formation model improved Butler equation and Statistical mechanical approach.

2.3.1. Compound formation model

The model assumes the compound forming tendency in the binary liquid alloy in the form of short-ranged volume elements due to the formation of intermetallic compound \((X_n Y_m)\) in the melt like that of a compound forming tendency in solid-state. The equation of surface tension \(\sigma\) at temperature \(T\) is given below.

\[
\sigma = \sigma_X + \frac{K_B T}{\rho} \ln \frac{C_X^S}{C_X} + \frac{\omega}{\rho} \left[ p(\varphi^S - \varphi) - q\varphi \right] + \frac{\Delta \omega_{XY}}{\rho} \left[ p(\varphi_{XY}^S - \varphi_{XY}) - q\varphi_{XY} \right] - \frac{\Delta \omega_{YY}}{\rho} \left[ p(\varphi_{YY}^S - \varphi_{YY}) - q\varphi_{YY} \right] 
\]

(19)

\[
\sigma = \sigma_X + \frac{K_B T}{\rho} \ln \frac{C_X^S}{C_X} + \frac{\omega}{\rho} \left[ p(f^S - f) - qf \right] + \frac{\Delta \omega_{XY}}{\rho} \left[ p(f_{XY}^S - f_{XY}) - qf_{XY} \right] + \frac{\Delta \omega_{YY}}{\rho} \left[ p(f_{YY}^S - f_{YY}) - qf_{YY} \right] 
\]

(20)

Where \(\sigma_X, C_X^S (j = X, Y)\) are surface tensions and surface concentration of pure component X and Y respectively. Similarly \(\varphi, f, \varphi_{XY}, \varphi_{YY}\) and \(f_{XY}, f_{YY}\) are bulk concentration functions and \(\varphi^S, f^S, \varphi_{XY}^S, f_{XY}^S\) and \(\varphi_{YY}^S, f_{YY}^S\) are surface concentration functions. \(p\) and \(q\) are surface coordination fractions that indicate the fraction of the number of nearest neighbors of an atom within its own layer and adjoining layers respectively and are related as \(p + 2q = 1\). For a closed packed crystal, \(p = 1/2\) and \(q = 1/4\). \(\rho\) is the mean surface area of the alloy and is calculated by:

\[ \rho = \sum_j C_j \rho_j \]  

(21)

with the surface area of each component \(\rho_j\) is given as [12]:

\[ \rho_j = 1.012 \left( \frac{V_j}{N_{Av}} \right)^{\frac{2}{3}} \]  

(22)

Where \(V_j\) is the molar volume of pure metal and \(N_{Av}\) is Avogadro’s number.

For \(\mu = 1\) and \(\nu = 2\), the bulk concentration functions are:

\[ \varphi = C^2 \]  

(23)

\[ \varphi_{XY} = \frac{1}{6} + 2(1 - C) - 6(1 - C)^2 + \frac{16}{3}(1 - C)^3 - \frac{3}{2}(1 - C)^4 \]  

(24)

\[ \varphi_{YY} = -\frac{1}{4} + (1 - C) - \frac{1}{2}(1 - C)^2 + (1 - C)^3 - \frac{3}{4}(1 - C)^4 \]  

(25)

\[ f = (1 - C)^2 \]  

(26)

\[ f_{XY} = -(1 - C)^2 + \frac{10}{3}(1 - C)^3 - \frac{3}{2}(1 - C)^4 \]  

(27)
The surface concentration functions $\varphi^S$, $\varphi^S_{jk}$, $f^S$ and $f^S_{jk}$ are obtained from equations (23) to (28) by replacement of bulk concentration $C$ by surface concentration $C^S$.

2.3.2. Improved butler equation

It is the layered interface concept that assumes the existence of a monoatomic layer (called surface monolayer) at the surface of a liquid as a separate phase and is in thermodynamic equilibrium with the bulk phase. The equation for binary liquid alloy at temperature $T$ is given as:

$$\sigma = \frac{A^0_j}{A_j} \sigma_j + \frac{RT}{A_j} \ln \frac{C^S_j}{C^0_j} + \frac{G^S_{X,S} - G^0_{X,S}}{A_j}$$

Where $A^0_j$ is the molar surface area of pure liquid metal, $A_j$ is the partial molar surface area of component $i$ respectively. $G^S_{X,S}$ and $G^0_{X,S}$ are the partial excess free energy of mixing in the surface and bulk of constituent components of the alloy, respectively.

The molar surface area of each pure component $j$ is given as [24].

$$A^0_j = g(V_j)^{2/3}(N_{\text{At}})^{1/3}$$

Where $g$ is geometrical constant and is given as,

$$g = \left(\frac{3f_v}{4}\right)^{2/3} \pi^{1/3}$$

Where $f_v$ and $f_s$ are volume packing fraction and surface packing fraction respectively. Their values are based on the crystal structure type of every pure component of the alloy. For liquid metal the values of $f_v$ and $f_s$ are 0.66 and 0.906 respectively [24].

2.3.3. Statistical mechanical approach

This method is also based on the layered structure concept near the interface and assumes a surface monolayer, as well as the layer just below the surface layer that bridges the surface monolayer to the bulk solution [25]. The model relates the surface tension to thermodynamic properties through interchange energy ($\omega$) and activity coefficients ($\gamma_j$) between the elements of the alloy. The equation at temperature $T$ is given as below.

$$\sigma = \sigma_j + \frac{k_B T}{\rho} \ln \frac{C^S_j}{\gamma_j C_j} + \frac{[p(1 - C^S_j)^2 + q(1 - C_j)^2]}{\rho} \omega$$

3. Results and discussion

3.1. Thermodynamic properties

The properties of binary liquid alloys depend on temperature, concentration, and pressure. The study of the binary alloy Na – Hg was carried out as a function of the concentration of the alloy at fixed atmospheric pressure and a temperature 673 K. For the calculations of thermodynamic as well as structural properties of liquid alloy by quasi chemical approximation, the main work is to calculate the interchange energy ($\omega$) and interaction energy parameters ($\Delta \omega_{jk}$). During the calculation of parameters, no any statistical method like mean square deviation is applied in order to decide the best fit so that the parameters used here are considered as reasonable for the study. For the sake of consistency, the same theoretical parameters have been considered throughout the calculations of other mixing properties. The different results thus obtained from the study are outlined in the section below.

We utilized equations (7), (9), (10), (11), and (12) for the analysis of the thermodynamic property. For the free energy of mixing, the interaction energy parameters are determined by successive approximation method for a couple of concentrations, following the stoichiometry of the NaHg$_2$ by the help of experimental values in the concentration range (0.1 to 0.9) [26]. The approximate values of the parameters are as follows.

$$\omega = \frac{k_B T}{-10.524}$$

The plot of free energy of mixing versus concentration of sodium ($C_{Na}$) is shown in figure 1. The computed and experimental values of $G_{Na}/RT$ are in good agreement. The theoretical value of free energy of mixing is minimum 1.102RT at 0.4 concentration of Na. The theoretical calculation of free energy of mixing shows that...
the alloy Na – Hg in the liquid state is moderately interacting and hence the tendency of compound formation is not so strong.

The deviation from the ideal behavior of alloy can be explained by chemical activities, a measure of effective concentration in the mixture, as its magnitude depends on the interaction of constituent binary components of the alloy. Equations (12) and (13) are used for the theoretical calculation of the chemical activity of constituent elements of alloy Na – Hg. Figure 2 shows the observed and theoretical value of the chemical activity of the alloy. There is good agreement between experimental and theoretical value of activities of Na and Hg in the alloy at 673 K for all concentrations of Na.

For the theoretical determination of heat of mixing, temperature derivatives of interaction parameters are required which are obtained by successive approximation method. The best fit values of parameters are

$$\frac{1}{k_B} \frac{d\omega}{dT} = -2.097, \quad \frac{1}{k_B} \frac{d\Delta\omega_{AB}}{dT} = 8.971, \quad \frac{1}{k_B} \frac{d\Delta\omega_{BB}}{dT} = -19.105$$

The plot of heat of mixing versus concentration of sodium ($C_{Na}$) is shown in figure 3. It is found that the heat of mixing is more negative at 0.4 concentration of sodium. The computed and experimental values of $H_M/RT$ are in good agreement.
Using equations (7) and (9), the entropy of mixing \((S_M)\) is computed. Energy parameters used in Gibb’s free energy and heat of mixing of the alloy are used consistently throughout our calculation. The plot of entropy of mixing \((S_M/R)\) versus concentration of sodium is shown in figure 4 for both theoretical and observed values. From the figure, it is observed that theoretical values are in reasonable agreement with observed values.

3.2. Microscopic properties

One of the important functions for the study of nature of atomic order of the binary liquid is considered as the concentration fluctuations in the long-wavelength limit \(S_{CC}(0)\) because it removes difficulties in the diffraction experiment [18]. For a given concentration if \(S_{CC}(0) < S_{id}^{cc}(0)\), then complex formation tendencies are expected while \(S_{CC}(0) > S_{id}^{cc}(0)\) points to the segregating tendencies. The experimental and theoretical values of \(S_{CC}(0)\) at different concentrations of sodium are obtained from equations (15) and (16) respectively. The plot of experimental and theoretical along with ideal values of \(S_{CC}(0)\) versus concentration of Na \((C_{Na})\) is shown in figure 5.
It is clear from the figure that the theoretical value of lies below the ideal value of $S_{CC}(0)$ throughout the whole range of concentration of lead which is the good signature of ordering in the alloy.

The Warren–Cowley short-range order parameter ($\alpha_1$) is another most powerful parameter to provide information on the local arrangement of the atoms in the molten alloys. Actually, it quantifies the degree of chemical order in the liquid alloys whose value lies between $-1$ to $+1$. The negative value of $\alpha_1$ is an indication of the ordering nature of the alloy, which is complete for $\alpha_1 = -1$. The value $\alpha_1 = 0$ is the indication of the random distribution of the atoms in the mixture and similarly, positive values of $\alpha_1$ is the indication of segregating nature, which is complete for $\alpha_1 = 1$. The value of $\alpha_1$ has been computed as a function of the concentration of Na using equation (17). For this, we take coordination number $Z = 10$. The plot of theoretical values of $\alpha_1$ versus concentration of Na (C$_{Na}$) is shown in figure 6. From the figure, it is observed that the value of $\alpha_1$ is negative throughout the whole range of concentration of sodium with maximum negative at 0.4 concentration of sodium which signifies the strong tendency of ordering nature of the alloy.

3.3. Surface tension

To calculate the surface tension of Na – Hg alloy the densities and surface tension of individual metals for all models required are calculated at 673 K by using relations given in reference [27].
For the unknown or negligible excess molar volume of the alloy, the partial molar volume is replaced by the molar volume of the pure component in the case of the improved Butler model and hence the partial surface area \( (A_j) \) of each component is definitely replaced by surface area \( (A_j^0) \) of the same pure component \([13, 28]\). The bulk and partial excess free energy of mixing of individual sodium and mercury in a liquid state at 673K are taken from reference \([26]\). The geometrical structure factor and ratio of surface excess energy to the bulk excess energy \( (\omega / \omega_{bulk}) \) are considered 1.061 and 0.818 \([24]\) respectively. Now writing these values to both metals in equation \((17)\) and solving them simultaneously, we first obtain surface concentrations of both metals, and then using each surface concentration of corresponding metals, the surface tension is obtained. Similar method is applied for the other two models as well.

For the statistical model, the interchange energy \( (\omega = -9.564 k_B T) \) obtained from equation \((7)\) is used since this method is not based on the complex of the alloys. Similarly, for the compound forming model, the same interaction energy parameters \( \omega \) and \( \omega_{jk} \) are used as in thermodynamic properties. The computed values of surface concentrations and surface tensions from different models are compared in figures 7 and 8 respectively.

Figure 7 shows the surface concentration increases with increasing bulk concentration of \( \text{Na}(C_{Na}) \) in all three models. The computed values of surface concentration suggest the segregation tendency of Na atoms to the surface but the segregation is more at higher bulk concentration of Na. This further suggests that at lower
bulk concentration of Na, the two different atoms of the alloy involve in the formation of chemical complexes or intermetallic compounds: possibly NaHg$_2$.

In figure 8, the surface tension of Na–Hg alloy decreases gradually with an increase in the bulk concentration of Na and is almost negatively deviated from the ideal value. In the compound formation model, the interaction energy parameters are considered which is the case of uniform deviation from the ideal one.

4. Conclusion

The present study is the theoretical analysis for the understanding of thermodynamic, structural, and surface behavior of binary liquid Na–Hg alloy at 673 K, under the assumption of the existence of NaHg$_2$ complex in the liquid mixture by quasi chemical approximation. The study explains the asymmetry behavior of the thermodynamic properties as a function of concentration. The theoretical study shows that the alloy exhibits ordered tendencies that become weaker with increasing temperature. It is noticed that segregating tendencies are not to be found in the bulk alloy for any concentrations. The sodium atoms segregate more on the surface at higher concentrations of sodium. The surface tension is negatively deviated from the ideal value.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Conflicts of interest

The authors declare no conflict of interest.

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