

## Thermodynamic, Structural and Surface Properties of Liquid Al-Sr Alloy at Different Temperatures

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### Abstract

Thermodynamic functions like excess Gibbs free energy of mixing ( $\Delta G_M^{XS}$ ) and activity ( $a$ ) of liquid Al-Sr alloy were studied in the temperature range 1323-1623 K in the frame work of Redlich-Kister (R-K) polynomial. The compositional and temperature dependence of structural functions like concentration fluctuation in long wavelength limit ( $S_{CC}(0)$ ), Warren-Cowley short range order parameter ( $\alpha_1$ ) and ratio of mutual to intrinsic diffusion coefficients ( $D_M/D_{id}$ ) were computed and analysed using the same approach. The surface tension ( $\sigma$ ) and surface segregation ( $x_i^S$ ) tendencies of the atoms in the liquid mixture were computed and studied using Butler's model. Present investigations revealed that association tendency among the atoms of metallic mixture gradually decreased with increase in temperature.

*Keywords:* self-association, ordering nature, ideal mixing, surface concentration, bulk phase.

### Introduction

The knowledge of mixing properties of liquid alloys plays an important role in the fabrication of new materials with reliable characteristics. The thermodynamic and structural properties of initial melt of the alloys provide information about the types of preferable associations among the constituent atoms, called 'pseudomolecules' or 'clusters' or 'complexes' (Yadav, Jha, and Adhikari 2015). Further, they help to obtain information related to the existence of different stable complexes, their respective stoichiometric compositions or mole fractions and melting temperatures resulting from the solidification of melts. Similarly, the knowledge of surface properties is crucial to understand the physical processes like wettability, crystal growth, nucleation, gas absorption, etc. (Yadav, Jha, and Adhikari 2016). Hence, thermodynamic (Dhungana, Yadav, and Adhikari 2020; Flory 1942; Gohivar et al. 2021; Jordan 1970; Sah, Adhikari, and Yadav 2023; Wang, Jin, and Du 2003; Yadav 2023a, 2023b; Yadav et al. 2016), structural (Bhatia and Hargrove 1974; Gohivar et al. 2021; Ruppertsberg and Reiter 1982; Yadav 2023b, 2023a; Yadav et al. 2016) and surface (Butler 1932; Kaptay 2015; Yadav 2023b; Yadav et al. 2016) properties of binary liquid alloys have been studied by several researchers employing different approaches.

### Literature Review

In this regard, a few of mixing properties of liquid Al-Sr alloy were estimated and analyzed at different or higher temperatures on the basis of different theoretical models. Consequently, the thermodynamic properties of the system have been studied by many researchers (Alcock and Itkin 1989; Chartrand and Pelton 1994; Liang et al. 2014; Srikanth and Jacob 1991; Wang et al. 2003; Yi et al. 2020; Zhong et al. 2004) and recently, Yi et al. (Yi et al. 2020) have presented a brief review of literature related to the system. They calculated the phase diagrams and thermodynamic properties of the Al-Si-Sr ternary system and constituent Al-Si, Si-Sr and Al-Sr

subsystems. For the purpose, they optimised the linear temperature-dependent (T-dependent) parameters of excess Gibbs free energy of mixing ( $\Delta G_M^{XS}$ ) for Si-Sr, and those of Al-Sr and Al-Si were taken from the literature. The optimised self-consistent linear T-dependent parameters of  $\Delta G_M^{XS}$  for Al-Sr system presented by Zhong et al. (2004) (Zhong et al. 2004) were considered in the present study. The thermodynamic properties, such as  $\Delta G_M^{XS}$  and activities ( $a_{Al}$  and  $a_{Sr}$ ), and structural properties, such as  $S_{CC}(0)$ , short range order parameter ( $\alpha_1$ ) and ratio of diffusion coefficients ( $D_M/D_{id}$ ) were calculated using Redlich-Kister (R-K) polynomial (Gohivar et al. 2021; Redlich and Kister 1948; Yadav 2023b). Butler's model (Butler 1932; Kaptay 2015; Yadav 2023b) was used to calculate the surface characteristics of the alloy, such as surface tension and tendency of surface segregation of atoms. The above mentioned properties of the system were investigated at temperatures 1323 K, 1423 K, 1523 K and 1623 K.

## Materials and Method

### Thermodynamic and structural functions

In the framework of R-K polynomial, the expression for  $\Delta G_M^{XS}$  of the binary system can be given as (Dhungana et al. 2020; Gohivar et al. 2021; Redlich and Kister 1948; Yadav 2023b)

$$\Delta G_M^{XS} = x_i x_j \sum_{\varphi=0}^n L_{\varphi} (x_i - x_j)^{\varphi} \quad (1)$$

where  $x_i$  and  $x_j$  ( $=1 - x_j$ ) are the mole fractions of components A (=Al) and B (=Sr) of the A-B type liquid alloy.  $L_{\varphi}$  are the linear T-dependent coefficients of R-K polynomial and can be expressed in the form as

$$L_{\varphi} = a_{\varphi} - b_{\varphi} T \quad (2)$$

Herein,  $a_{\varphi}$  and  $b_{\varphi}$  are enthalpy part ( $\Delta H_M$  in J mol<sup>-1</sup>) and entropy part ( $\Delta S_M^{XS}$  in J mol<sup>-1</sup>K<sup>-1</sup>) of  $\Delta G_M^{XS}$ . Eq. (2) is equivalent to the standard thermodynamic relation as  $\Delta G_M^{XS} = \Delta H_M - T \Delta S_M^{XS}$ . With the help of Eq. (2), Eq. (1) can be extended as (Dhungana et al. 2020; Gohivar et al. 2021)

$$\Delta G_M^{XS} = x_i x_j \sum_{\varphi=0}^n (a_{\varphi} - b_{\varphi} T) (x_i - x_j)^{\varphi} \quad (3)$$

The Gibbs free energy of mixing ( $\Delta G_M$ ) can be related to  $\Delta G_M^{XS}$  as

$$\Delta G_M = \Delta G_M^{XS} + RT(x_i \ln x_i + x_j \ln x_j) \quad (4)$$

where  $R$  (in Jmol<sup>-1</sup>K<sup>-1</sup>) real gas constant and  $T$  (in K) is absolute temperature. The partial excess Gibbs free energy ( $\Delta G_i^{XS}$ ) of each component in the metallic solution can be given as

$$\Delta G_i^{XS} = \Delta G_M^{XS} + \sum_{j=1}^2 (\delta_{ij} - x_j) \frac{\partial \Delta G_M^{XS}}{\partial x_j} \quad (5)$$

where  $\delta_{ij}$  is Kronecker delta symbol and for  $i = j$ ,  $\delta_{ij} = 1$  and for  $i \neq j$ ,  $\delta_{ij} = 0$ . Using Eq. (3) in Eq. (5), the relations for  $\Delta G_i^{XS}$  ( $i=Al$ ) and  $\Delta G_j^{XS}$  ( $j=Sr$ ) can be obtained as

$$\Delta G_i^{XS} = x_j^2 \sum_{\varphi=0}^n L_{\varphi} [(1 + 2\varphi)x_i - x_j] (x_i - x_j)^{\varphi-1} \quad (6)$$

$$\text{and } \Delta G_j^{XS} = x_i^2 \sum_{\varphi=0}^n L_{\varphi} [x_i - x_j(1 + 2\varphi)] (x_i - x_j)^{\varphi-1} \quad (7)$$

The activities ( $a_i$  and  $a_j$ ) of the atoms in the liquid alloy then can be calculated by using the relations (Yadav 2023b, 2023a)

$$a_i = x_i \exp\left(\frac{\Delta G_i^{XS}}{RT}\right) \quad (9)$$

$$\text{and } a_j = x_j \exp\left(\frac{\Delta G_j^{XS}}{RT}\right) \quad (10)$$

Knowledge of structural functions aids comprehension of the local arrangement of atoms in a liquid mixture. Among them, the concentration fluctuation in long wave length limit ( $S_{CC}(0)$ )

can be expressed in terms of  $\Delta G_M$  by standard relations (Bhatia and Hargrove 1974; Yadav 2023a; Yadav et al. 2016)

$$S_{CC}(0) = RT \left( \frac{\partial^2 \Delta G_M}{\partial x_1^2} \right)_{T,P}^{-1} \quad (11)$$

Using Eqs. (3) and (4) in Eq. (11) and putting  $\varphi = 0, 1$  and  $2$ , one can obtain (Gohivar et al. 2021)

$$S_{CC}(0) = \frac{RT}{\left[ -2L_0 + (-12x_i + 6)L_1 + (-48x_i^2 + 48x_i - 10)L_2 + \frac{RT}{x_i x_j} \right]} \quad (12)$$

The ideal value of  $S_{CC}(0)$  can be obtained using the relation  $S_{CC}^{id}(0) = x_i x_j$  (13)

Another structural function, Warren-Cowley short range order parameter ( $\alpha_1$ ) for binary liquid alloy is calculated using the expression (Cowley 1950; Ruppertsberg and Reiter 1982; Yadav 2023a; Yadav et al. 2016)

$$\alpha_1 = \frac{S-1}{S(Z-1)+1} \text{ with } S = \frac{S_{CC}(0)}{S_{CC}^{id}(0)} \quad (14)$$

where  $Z (=10)$  is coordination number.

### Surface properties

In surface properties, surface tension ( $\sigma$ ) of the system and surface concentrations ( $x_i^S$ ) of its components were estimated on the basis of Butler model (Butler 1932; Kaptay 2008, 2015, 2016; Yadav et al. 2016). The expression of  $\sigma$  for the binary liquid alloy can be given as

$$\sigma = \sigma_i^0 + \frac{RT}{A_i} [\ln x_i^S - \ln x_i] + \frac{\Delta G_{s,i}^{xs} - \Delta G_i^{xs}}{A_i} \quad (15)$$

where  $\sigma_i^0$  ( $i = 1, 2$ ) is the surface tension,  $A_i$  is the molar surface area and  $x_i^S$  and  $x_i$  are the surface and bulk concentrations of atom  $i$  in the surface phase and bulk phase of the liquid alloy respectively.  $\Delta G_{s,i}^{xs}$  is the surface partial excess Gibbs's free energy of component  $i$  in the liquid mixture. The expression relating  $\Delta G_i^{xs}$  and  $\Delta G_{s,i}^{xs}$  is given as

$$\Delta G_{s,i}^{xs} = \beta \Delta G_i^{xs} \quad (16)$$

where  $\beta$  is constant and  $\beta = 0.8181$  (Kaptay 2008, 2015; Yadav 2023b) is taken for calculations in present work. The molar surface area of the atom  $i$  is calculated by the relation

$$A_i = 1.00 (V_i^0)^{2/3} (N_A)^{1/3} \quad (17)$$

where  $V_i^0$  is the molar volume of pure atom  $i$  and  $N_A$  is the Avogadro's number. The molar volume ( $V_i^0$ ) of pure atom  $i$  is calculated by taking the ratio of its mass ( $m_i$ ) and density ( $\rho_i^0$ ) at required temperature ( $T_K$ ). The temperature dependence expressions of  $\sigma_i^0$  and  $\rho_i^0$  can be given as (Brandes and Brook 2013)

$$\sigma_i^0 = \sigma_0 + (T_K - T_0) \frac{d\sigma}{dt} \text{ and } \rho_i^0 = \rho_0 + (T_K - T_0) \frac{d\rho}{dt} \quad (18)$$

where  $\sigma_0$  and  $\rho_0$  are the surface tension and density of the pure atom  $i$  at its melting temperature,  $T_0$  is the melting temperature of the pure atom and  $\frac{d\sigma}{dt}$  and  $\frac{d\rho}{dt}$  are the temperature derivative terms of surface tension and density respectively.

### Results and discussion

The knowledge of  $\Delta G_M^{xs}$  provides insight into the strength of interaction between complex atoms in alloys. The values of  $\Delta G_M^{xs}$  have been estimated throughout the whole concentration range at 1323-1623 K using Equations (1-3) and the parameters displayed in Table 1. The T-dependent plots of  $\Delta G_M^{xs}$  for fixed composition ratios are displayed in Figure 1. The optimum negative value of  $\Delta G_M^{xs} = -11.3735 \text{ kJmol}^{-1}$  at  $x_{Al} = 0.6$  and 1323 K, being its melting

temperature. Thus, the system is found to be asymmetric in terms of  $\Delta G_M^{xs}$  and weakly interacting in nature. The negative values of  $\Delta G_M^{xs}$  gradually decrease with increase in temperature of the system above its melting temperature, Figure 1. As a result, the system's tendency to produce compounds gradually declines at high temperatures.

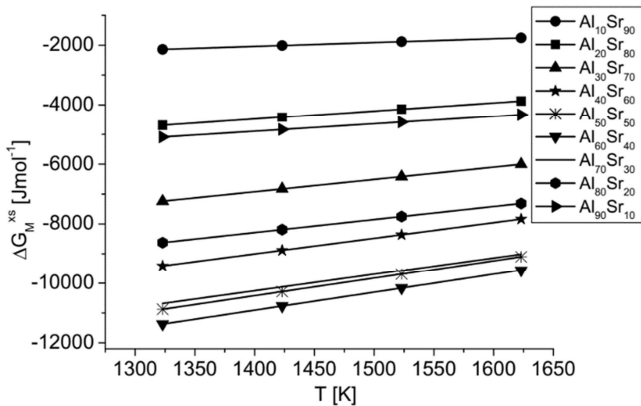
**Table 1:**

*Self-consistent parameters for  $\Delta G_M^{xs}$  (Zhong et al. 2004)*

$L_\phi$ [ $\text{Jmol}^{-1}\text{K}^{-1}$ ]
$L_0 = -74839 + 23.686 * T$
$L_1 = -31790 + 8.549 * T$
$L_2 = +10683 - 4.130 * T$

**Figure 1:**

*Computed values of  $\Delta G_M^{xs}$  for Al-Sr liquid alloy at different temperatures.*

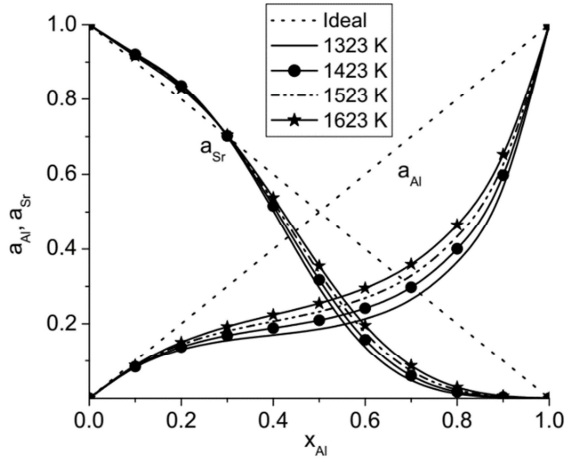


Activity of binary liquid alloy is an important function that gives knowledge related to the stability of the complexes formed. The partial excess Gibbs free energies of elements Al ( $\Delta G_{Al}^{xs}$ ) and Sr ( $\Delta G_{Sr}^{xs}$ ) of the liquid mixture have been calculated using Equations (6) and (7), and parameters of Table 1. These values are then used in Equations (9) and (10) to estimate the activities of components Al ( $a_{Al}$ ) and Sr ( $a_{Sr}$ ) at different compositions and temperatures. The obtained values are displayed as a function of concentration in Figure 2.

The estimated values of  $a_{Al}$  demonstrate negative deviations from ideal values at all compositions at the melting temperature, 1323 K (Figure 2). But those of  $a_{Sr}$  deviate negatively from ideal values in the range  $x_{Al} > 0.2$  whereas show positive deviation in the rest of the concentrations ( $x_{Al} < 0.2$ ). These results indicate that the system shows a compound-forming tendency in the former concentration range and a demixing tendency in the later concentration range. The activities of both components rise steadily as their bulk concentrations increase. Furthermore, the values of  $a_{Al}$  are observed to gradually grow and approach ideal values as the system's temperature increases. The values of  $a_{Sr}$  gradually increase in the range  $x_{Al} > 0.2$  and decrease in the range  $x_{Al} < 0.2$  at elevated temperatures, Figure 2. The present investigations show that strength of interaction between the atoms of the complexes of the system gradually decrease when its temperature is increased beyond melting temperature. Moreover, the system showed ideal mixing behaviour at higher temperatures, as expected.

**Figure 2:**

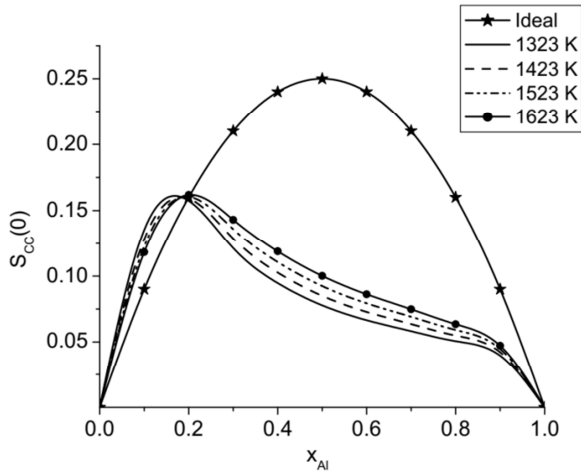
Composition-dependent values of  $a_{Al}$  and  $a_{Sr}$  in Al-Sr liquid alloy at different temperatures.



To gain deeper insight into the interacting nature of the system, the structural functions have been determined and studied. The values of  $S_{CC}(0)$  have been determined using Equations (12) and (13) and the parameters in Table 1. The computed values of  $S_{CC}(0)$  along with its ideal values ( $S_{CC}^{id}(0)$ ) at different temperatures are displayed in Figure 3.

**Figure 3:**

Computed values of  $S_{CC}(0)$  for Al-Si liquid alloy versus  $x_{Al}$  at different temperatures.



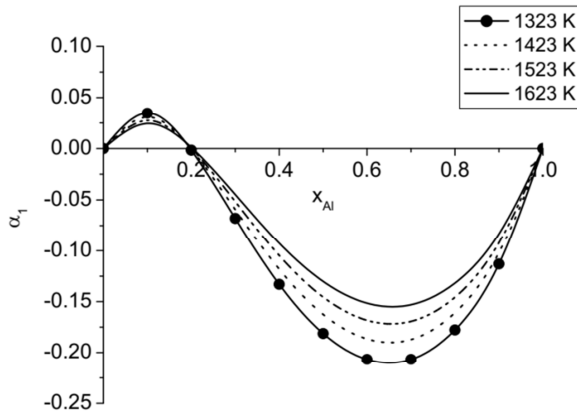
At a given temperature and concentration, if  $S_{CC}(0) < S_{CC}^{id}(0)$ , then hetero-atomic pairing or compound forming tendency or ordering nature in the liquid alloy is expected. Under the same conditions, if  $S_{CC}(0) > S_{CC}^{id}(0)$ , then homo-atomic pairing or self-association or segregating nature in the system is expected (Sah et al. 2023; Yadav 2023b; Yadav et al. 2016). The perusal of Figure 3 shows that the computed values of  $S_{CC}(0) < S_{CC}^{id}(0)$  in the concentration range  $x_{Al} > 0.2$  and  $S_{CC}(0) > S_{CC}^{id}(0)$  for  $x_{Al} < 0.2$  at all preferred temperatures. Thus, the system

shows ordering nature in the former concentration range and segregating nature later. These results are in accordance with those obtained from the investigation of activity above. Additionally, the system shows transformation of phase from segregating to ordering at  $x_{Al} = 0.2$ . The computed values  $S_{CC}(0)$  gradually get closer to ideal values at higher temperatures.

The previous results can be enhanced by studying the Warren-Cowley short range order parameter ( $\alpha_1$ ). The values of  $\alpha_1$  are calculated using Equation (13) with the aid of estimated values of  $S_{CC}(0)$  and are plotted in Figure 4.

**Figure 4:**

*Compositional and temperature dependence of  $\alpha_1$  for Al-Sr liquid alloy.*



The values of  $\alpha_1$  can be less than zero, greater than zero and zero depending upon the nature of alloy. For constrained conditions (given temperature and composition), if  $\alpha_1 < 0$ , then it indicates hetero-atomic pairing tendency, if  $\alpha_1 > 0$ , then it indicates homo-atomic pairing tendency, and if  $\alpha_1 = 0$ , then it indicates ideal mixing tendency of the liquid alloy. From Figure 4, it is observed that the computed values of  $\alpha_1 < 0$  in  $x_{Al} > 0.2$  and  $\alpha_1 > 0$  in  $x_{Al} < 0.2$ . Moreover, the positive and negative values of  $\alpha_1$  get closed to zero at higher temperatures indicating the similar results as predicted by the thermodynamic and other structural functions above.

**Table 2:**

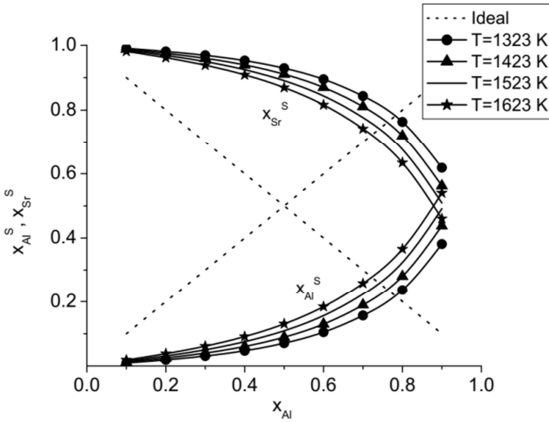
*Input parameters for surface tension (Brandes and Brook 2013)*

Atom	$T_0$ [K]	$\rho_0$ [kgm <sup>-3</sup> ]	$d\rho/dT$ [kgm <sup>-3</sup> K <sup>-1</sup> ]	$\sigma_0$ [Nm <sup>-1</sup> ]	$d\sigma/dT$ [Nm <sup>-1</sup> K <sup>-1</sup> ]
Al	933	2385	-0.35	0.914	-0.00035
Sr	1043	2370	-0.26	0.303	-0.00010

The surface tensions ( $\sigma_{Al}$  and  $\sigma_{Sr}$ ) and volumes ( $V_{Al}$  and  $V_{Sr}$ ) of pure atoms Al and Sr of the system have been calculated with the aid of Equation (18) and input ingredients of Table 2. The volume of each element of the liquid alloy gradually rises as the temperature ascended. The surface tension of each pure component gradually decreases at elevated temperatures (Figure 5).

**Figure 5:**

Surface tensions ( $\sigma_{Al}$  and  $\sigma_{Sr}$ ) and volumes ( $V_{Al}$  and  $V_{Sr}$ ) of Al and Sr at different temperatures.



The surface tension ( $\sigma_{Al-Sr}$ ) and surface concentrations ( $x_{Al}^S$  and  $x_{Sr}^S$ ) of atoms in the metallic solution have been determined using Equations (15)-(18) and input ingredients from Table 2. The computed values  $x_{Al}^S$  and  $x_{Sr}^S$  are displayed in Figure 6 and those of  $\sigma_{Al-Sr}$  are plotted in Figure 7.

**Figure 6:**

Temperature and composition dependent values of  $x_{Al}^S$  and  $x_{Sr}^S$  in Al-Sr liquid alloy.

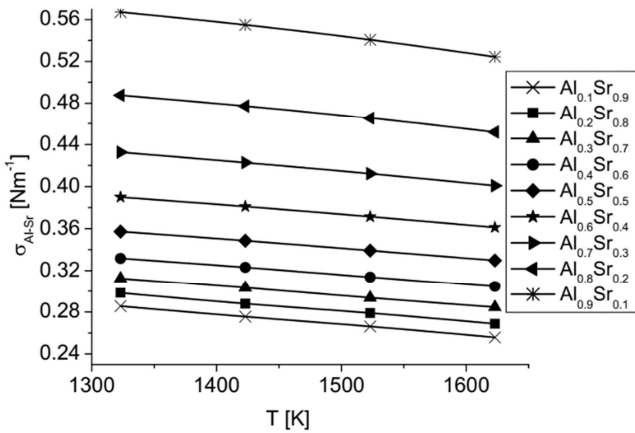
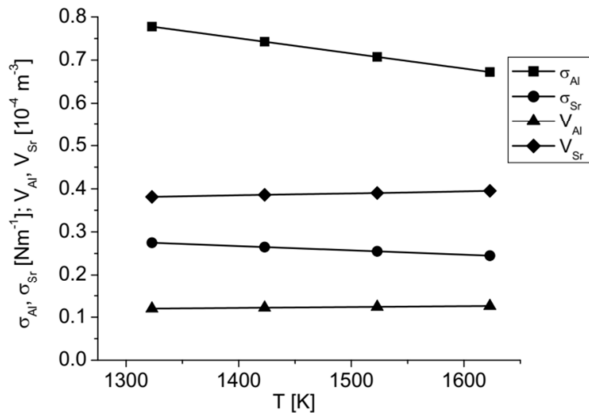


Figure 6 indicates that the value of  $x_{Sr}^S$  is found to be more than the bulk concentration of Sr, while  $x_{Al}^S$  is found to be smaller than the respective bulk concentration at elevated temperatures. These findings demonstrate that the atoms of Sr segregate in the surface phase whereas those of Al remain in the bulk phase of the liquid mixture because the surface tension of the former is found to be lower than that of the latter. Moreover, with the increase in temperature of the system both  $x_{Al}^S$  and  $x_{Sr}^S$  get closure to their respective ideal values (Figure 6). Figure 7 indicates that the surface tension of the liquid alloy reduces steadily as the temperature increased. This could be attributed to a drop in the system's cohesive energy, with the predicted results.

**Figure 7:** Temperature dependence of  $\sigma_{Al-Sr}$  of Al-Sr liquid alloy.

### Conclusion and Recommendations

The greatest compound formation tendency of the Al-Sr liquid alloy was observed at its melting temperature of 1323 K. However, the respective tendency steadily lessened as the system's temperature increased. The Sr atoms separated in the surface phase, while the Al atoms remained in the bulk phase of the system. As the temperature increased, the system's surface tension progressively dropped. The thermodynamic, structural, and surface properties all indicated the similar findings. The present investigations can be further extended to calculate to explain the structural and mechanical stabilities, electronic properties and transport properties of the system using first principle calculations.

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