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Exploration of Stability for SnTl Liquid Alloys at Various Temperatures

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Abstract

The quasi-lattice theory (QLT) is employed for the prediction of the temperature and concentration reliance of the thermophysical behavior of the molten SnTl alloys. The analytical expressions are used to calculate the Gibbs free energy of mixing, activity, enthalpy of mixing and entropy of mixing of molten SnTl alloys at 723 K. The model parameters i.e. size ratio and order energy parameter are estimated using the experimental data of the free energy of mixing for molten SnTl system at 723 K. The theoretical data of the thermodynamic functions are in excellent harmony with the correlated experimental data. The theoretical data of the structural properties like concentration fluctuations are also in well harmony with the experimental values for molten SnTl system at 723 K. Further, the optimization procedure is adopted to explain the Gibbs free energy of mixing, activity, concentration fluctuations, short-range order parameter, excess stability function, surface tension, surface concentration, surface concentration fluctuations, diffusivity ratio and viscosity at various temperatures for SnTl system. For the analysis of the surface properties and transport properties of the alloys, Butler model and Moelwyn-Hughes model are employed in the substructure of quasi-lattice theory. The present study explores that the stability and the segregating behavior of molten SnTl system decrease with the upgradation of the temperature from 623 K to 1000 K. Further, the theoretical findings suggest that there may be transition of segregation to ordering at temperature about 1914. 15 K.

Keywords: Quasi-lattice theory; Gibbs free energy of mixing; excess stability function; surface tension; viscosity

1. Introduction

The Tin-Thallium system is an important lead free solder alloy having wide potential applications in electronic industry. It is well known that Sn is the most important constituent in binary solders e.g. SnTl, SnAl, SnIn, SnAg, SnSb etc and Sn-based multi-component system e.g. SnCdTl, BiSnTl, BiCdTl. The SnTl system is utilized in ceramic compounds and as semiconductors [1, 2]. The phase diagram [3] displays the symmetric character of free energy of mixing, G_M , excess free energy of mixing, G_M^{XS} , entropy of mixing, S_M and enthalpy of mixing H_M ; and asymmetry in S_M^{XS} at $c_{Sn} = 0.5$ for SnTl melts at 723 K. Again, G_M^{XS} and H_M are positive in composition range, $c_{Sn} = 0.1$ to 0.9 for SnTl melts at 723 K. This is an indication of segregating nature of SnTl melts at 723 K. Further, there exists SnTl complex in SnTl system at 723 K. In spite of the interesting characteristics and having potential technological and industrial applications, the data on thermophysical properties of SnTl system are scarce in the literature. However, some attempts have been made [4,5,6] to explore theoretically the thermodynamic functions like G_M , S_M and H_M ; microscopic functions like $s_{CC}(0)$ and α_1 ; surface properties like surface concentration, c_i^S and surface tension, σ and transport properties like diffusivity, D and viscosity, η for SnTl melts at 723 K. Awe et al [6] applied quasi-lattice theory to explain G_M , $s_{CC}(0)$, $\frac{D_M}{D_{id}}$ and η of SnTl melts at 723K. Nonetheless, explanation of the stability function for SnTl melts is not available in the literature. Therefore, SnTl melt is a suitable candidate for present investigation.

The stability is a very important parameter which determines whether or not two metals will mix to form an alloy. The factors affecting the stability of a binary liquid alloy include the temperature, concentration and structure of the alloy. In present research work, the aim is to explain the stability of the segregating alloys in SnTl at different temperatures. The excess stability function, E^{XS} introduced by Darken [7] is related to $s_{CC}(0)$ which can be explained in terms of G_M and activity of the alloy [8]. Thus, $s_{CC}(0)$ is a powerful microscopic property to explain the stability of the binary melts. It is necessary to state that the stability is reciprocal to $s_{CC}(0)$.

The quantity, $s_{CC}(0)$ is a very salient parameter to explore the behavior of liquid alloys [9,10] at microscopic level. It is important to state that $s_{CC}(0) < C(1-C)$ i.e. $s_{CC}^{id}(0)$ stands for ordered alloys in which unlike atoms (A-B) linked together as the nearest neighbors. On the contrary, if $s_{CC}(0) > C(1-C)$ then like atoms (A-A or B-B) interact as the closest neighbors and the system is segregating in nature.

The present theoretical investigation is devoted for the exploration of the bulk, surface and transport properties as well as stability of SnTl melts at different temperatures. It is notable that for the understanding of the stability of binary melts, E^{XS} is a very convenient parameter [7]. The positive value of E^{XS} stands for the ordering behavior of alloy. Similarly, the negative value of E^{XS} advocates the segregation in the alloy and $E^{XS} = 0$ represents the ideal alloy [11]. Since E^{XS} is directly related to $s_{CC}(0)$ and the experimental measurement of $s_{CC}(0)$ is problematic [12], therefore, $s_{CC}(0)$ requires theoretical analysis. It is earlier mention that $s_{CC}(0)$ is directly linked to the thermodynamic functions like G_M and activity of the alloy i.e. $s_{CC}(0)$ can be determined by the second derivative of G_M with respect to composition as well as the differentiation of activity with respect to concentration of the alloy. The stability of binary liquid alloys depends significantly on the size ratio of the constituent atoms of the alloys [12]. Taking in view of the effect of size ratio on the stability function of the alloy, the quasi-lattice theory, QLT [12] is applied to analyze the stability of liquid alloys. In QLT, the coupled effect of entropic and enthalpic contributions and size ratio are taken into the consideration for the understanding of the mixing behavior of binary melts. Therefore in present investigation, the composition dependence of G_M , G_M^{XS} , activity and $s_{CC}(0)$ of SnTl melts at a specified temperature has been explored by QLT. The model parameters have been further employed to assess the composition and temperature reliance of G_M , G_M^{XS} , activity and $s_{CC}(0)$ of SnTl melts at different temperatures in the light of

optimization procedure [11, 12, 13, 14]. The QLT model is successfully employed to explore the thermodynamic behavior of several binary melts namely AgCu, AlZn, AlSn, SnZn, CdZn, NaK etc [5,6, 11,12,13,14,15,16,]. However, the limited work is available in the literature [11,13,14] regarding the theoretical explanation of the thermodynamic behavior of the binary melts at various temperature on employing QLT. In literature, the theoretical analysis of the stability of binary liquid alloys like HgNa, HgK, AlIn, BiZn, CdGa, AlAu, AgGe, BiCd etc at a specified temperature [18,19,20] are available. However, least information is available regarding the stability of binary melts at different temperatures [11,12, 13,14]. Therefore in present work, an attempt has been made to explore the stability of the SnTl melts at different temperatures on using optimization procedure in the substructure of QLT. The microscopic property like SRO, α_1 [21,22] for SnTl melts at different temperatures has also been explored. Again, Butler model [23] is utilized to discuss the surface properties of SnTl melts at different temperatures in the framework QLT. Further, the transport properties of SnTl melts at various temperatures are also analyzed in the light of Moelwyn-Hughes [24].

2. Formalism:

The excess stability function, E^{XS} [7] for a binary melt can be determined from the relation

$$E^{XS} = \frac{\partial^2 G_M}{\partial C^2} - \frac{RT}{C(1-C)} \quad (1)$$

where, G_M represents the free energy of mixing of binary melts A-B, C and (1-C) are concentrations of atoms A and B respectively, R is the molar gas constant and T is the absolute temperature (in Kelvin) of the alloy.

The microscopic function i.e. concentration fluctuations, $s_{CC}(0)$ may be represented by [8]

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

Equations (1) and (2) provide

$$E^{XS} = \frac{RT}{s_{CC}(0)} - \frac{RT}{C(1-C)} \quad (3)$$

$$\text{where, } C(1-C) = s_{CC}^{id}(0) \quad (4)$$

From equation (3), it is evident that $\frac{E^{XS}}{RT}$ is less than zero, more than zero or equal to zero provide that $s_{CC}(0) > s_{CC}^{id}(0)$, $s_{CC}(0) < s_{CC}^{id}(0)$ or $s_{CC}(0) = s_{CC}^{id}(0)$ respectively. Thus, the negative value of $\frac{E^{XS}}{RT}$ represents segregating alloys, the positive value of $\frac{E^{XS}}{RT}$ refers to the ordering alloys and $\frac{E^{XS}}{RT} = 0$ exhibits ideal solution [11].

Equation (1) indicates that for the estimation of E^{XS} , the theoretical data of G_M for the binary liquid alloy are required. In present case, the quasi-lattice theory (QLT) [12, 25] is employed to study the concentration dependence of G_M for a binary liquid alloy at specified temperature. The QLT model is useful to analyze the thermodynamic and structural functions of the molten binary system [12] on employing the combined influence of size ratio in conjunction with the energetic contribution and entropic effect.

2.1 Bulk Properties i.e. G_M , S_M , a_i ($i=A,B$), H_M , $S_{CC}(0)$ and α_1 of the binary melts at a given temperature

Let one mole of a molten binary system having n_A and n_B atoms of A and B respectively i.e. $N_A = N C$ and $N_B = N(1-C)$ where $C_A = C$ and $C_B = 1-C$, the compositions of the constituents A and B respectively. Again it is assumed that the component atoms A and B of the molten binary solution are different in shape and size (i.e. volume) so that there is existence of short-range interaction between the atoms. In the framework of QLT [12, 25], on applying the entropic and enthalpic effects in the limit $Z \rightarrow \infty$ where Z refers to the coordination number, the G_M of a molten binary system is given by

$$\frac{G_M}{RT} = C_A \ln(1-\beta) + C_B \ln \beta + C_A \beta W \quad (5)$$

$$\text{with } \beta = \frac{\gamma C_B}{C_A + \gamma C_B} \quad (6)$$

where, T = temperature (in K) of the system, R = molar gas constant, K_B = Boltzmann constant, W = order energy parameter, $\gamma = \frac{V_B}{V_A} (V_A < V_B)$ i.e. the size ratio and ω = the interchange energy given by

$$\omega = \varepsilon_{AB} - \left(\frac{\varepsilon_{AA} + \varepsilon_{BB}}{2} \right) \quad (7)$$

where, ε_{ij} ($i=A$ and $j=B$) refers to $(i-j)$ bond strength.

It is notable that the first two terms on R. H.S. of equation (5) offer the entropic effect and third term indicates enthalpic contribution to G_M of the molten A-B solution.

The G_M^{XS} of A-B solution is given by

$$\frac{G_M^{XS}}{RT} = \frac{G_M}{RT} - \frac{G_M^{id}}{RT} = \frac{G_M}{RT} - (C_A \ln C_A + C_B \ln C_B) \quad (8)$$

where, G_M^{id} = the ideal free energy of mixing.

Now the activities a_A and a_B of the species A and B of the A-B solution are represented respectively by [12]

$$RT \ln a_A = G_M + a_A C_B \left(\frac{\partial G_M}{\partial C_A} \right) \quad (9a)$$

$$RT \ln a_B = G_M + a_B C_A \left(\frac{\partial G_M}{\partial C_B} \right) \quad (9b)$$

Equations (5) and (9) provide

$$\ln a_A = \ln(1-\beta) + \beta \left(\frac{\gamma-1}{\gamma} \right) + \beta^2 W \quad (10a)$$

$$\ln a_B = \ln \beta - (1-\beta)(\gamma-1) + W\gamma(1-\beta)^2 \quad (10b)$$

The S_M for A-B mixture is represented by [12]

$$\frac{S_M}{R} = \left[C_B \ln \beta + C_A \ln(1-\beta) + C_B \beta \left(W + \frac{\partial W}{\partial T} \right) \right] \quad [\text{using equation (5)}] \quad (11)$$

The H_M of a binary mixture is given by [12]

$$H_M = G_M + TS_M$$

Equations (5) and (11) yield

$$\frac{H_M}{RT} = -C_A \beta T \left(\frac{\partial W}{\partial T} \right) \quad (12)$$

The structural behavior like $s_{CC}(0)$ and α_1 [9, 10, 26] are helpful to achieve the information linked to the nature and degree of atomic arrangement in the molten binary system. Since the second derivative of G_M with respect to the concentration determines $s_{CC}(0)$ of the binary melts hence equations (2) and (5) provide

$$s_{CC}(0) = \frac{C_A C_B}{1 - C_A C_B \{f(\gamma, W)\}} \quad (13)$$

$$\text{with } f(\gamma, W) = \left[\frac{\{2\gamma^2 W - (\gamma - 1)^2 (C_A + \gamma C_B)\}}{(C_A + \gamma C_B)^3} \right] \quad (14)$$

Again, $s_{CC}(0)$ in terms of activity may be expressed as [8, 26]

$$s_{CC}(0) = C_B a_A \left(\frac{\partial a_A}{\partial C_A} \right)_{T,P,N}^{-1} = C_A a_B \left(\frac{\partial a_B}{\partial C_B} \right)_{T,P,N}^{-1} \quad (15)$$

It is remarkable that $s_{CC}(0)$ obtained from equation (15) is treated as the experimental data of $s_{CC}(0)$ for a binary solution.

For $W = 0$ and $\gamma = 1$, $f(\gamma, W) = 0$ (via equation (14)) due to which equation (13) provides $s_{CC}^{id}(0) = C_A C_B = C(1 - C)$. Again, equation (14) expresses that $f(\gamma, W) < 0$, when $W = 0$ and $\gamma > 1$ hence equation (13) gives $s_{CC}(0) < s_{CC}^{id}(0)$ showing the ordering nature of the binary system. Further, $s_{CC}(0) < s_{CC}^{id}(0)$ if $f(\gamma, W) < 0$ for $W < 0$ and all values of γ and the system refers to the ordering nature. Also, $f(\gamma, W) > 0$ if $W > 0$ due to which $s_{CC}(0) > s_{CC}^{id}(0)$ indicating segregating nature of the system [12].

Now SRO, α_1 [21, 22] in the first neighbor shell of the melt is represented by [9]

$$\alpha_1 = \frac{(S-1)}{S(Z-1)+1} \quad \text{with } S = \frac{s_{CC}(0)}{s_{CC}^{id}(0)} \quad (16)$$

where, Z = coordination number = 10 (taken during calculations).

It is informative that $\alpha_1 > 0$ and $\alpha_1 < 0$ stand for segregation and ordering respectively in the binary melts while $\alpha_1 = 0$ suggests the random mixing in the binary solution [12].

2.2 Surface properties: C_i^s , σ and $s_{CC}^s(0)$ of the binary solution

The σ of a binary melt in the framework of Butler model [23] may be expressed as

$$\sigma = \sigma_A + \left(\frac{\tilde{G}_A^{E,s} - \tilde{G}_A^{E,b}}{S_A} \right) + \frac{RT}{S_A} \ln \left(\frac{C_A^s}{C_A} \right) \quad (17a)$$

$$= \sigma_B + \left(\frac{\tilde{G}_B^{E,s} - \tilde{G}_B^{E,b}}{S_B} \right) + \frac{RT}{S_B} \ln \left(\frac{C_B^s}{C_B} \right) \quad (17b)$$

where $\sigma_i(i=A,B)$ = the surface tension of i^{th} constituent of the binary melts, $\tilde{G}_i^{E,b}$ = partial excess free energy of i^{th} constituent in the bulk and $\tilde{G}_i^{E,s}$ = partial excess free energy of i^{th} constituent at the surface, s_i = molar surface area of the component i of the binary melts, c_i and c_i^s = bulk and surface concentrations respectively of i^{th} component.

Now s_i is expressed as [27]

$$s_i(i=A,B) = 1.091 V_i^{\frac{2}{3}} N_A^{\frac{1}{3}} \quad (18)$$

where N_A = Avogadro's number and V_i = atomic volume of i^{th} constituent of the binary melts.

Now, $\tilde{G}_i^{E,b}$ is expressed as [12]

$$\tilde{G}_i^{E,b} = RT \ln \gamma_i \quad \text{with} \quad \gamma_i = \frac{a_i}{c_i}(i=A,B) \quad (19)$$

where, γ_i = activity coefficient of the component of i in the bulk.

The $\tilde{G}_i^{E,b}$ and $\tilde{G}_i^{E,s}$ are related as [28]

$$\tilde{G}_i^{E,s} = \lambda \tilde{G}_i^{E,b} \quad (20)$$

with $\lambda = \frac{Z^s}{Z}$ [29] where, Z^s = surface coordination number. It is pointed out that the value of λ lies between 0.50 to 0.84 [30].

The $s_{CC}^s(0)$ is one of the important properties used to study the arrangement of atoms at the surface of a binary melt.

Mathematically, $s_{CC}^s(0)$ may be expressed as [31]

$$s_{CC}^s(0) = \frac{C_A^s C_B^s}{\left[1 + \frac{Z^s}{2\lambda^s (1-\lambda^s)} \right]} \quad (21)$$

$$\text{with } \lambda^s = \left[1 + 4 C_A^s C_B^s \left\{ \exp \left(\frac{2W}{Z^s K_B T} \right) - 1 \right\} \right]^{-\frac{1}{2}} \quad (22)$$

$$\text{where, } C_A^s C_B^s = s_{CC}^{id,s}(0) \quad (23)$$

known as ideal surface concentration fluctuations.

2.3 Transport Properties: Diffusivity ratio, $\frac{D_M}{D_{id}}$ and Viscosity, η

The diffusivity and viscosity are the transport properties applied for the understanding of the mixing behavior of a binary solution at microscopic level. The $\frac{D_M}{D_{id}}$ for a binary melt is expressed as [12]

$$\frac{D_M}{D_{id}} = \frac{s_{CC}^{id}(0)}{s_{CC}(0)} \quad (24)$$

where D_M and D_{id} = mutual diffusion coefficient of binary melts and diffusion coefficient of an ideal solution respectively. In terms of self-diffusion coefficient of constituents A and B i.e. D_A and D_B , D_{id} is expressed as

$$D_{id} = C_A D_B + C_B D_A \quad (25)$$

From equation (24), it is clear that $\frac{D_M}{D_{id}} > 1$ for ordered alloys [32] and $\frac{D_M}{D_{id}} < 1$ refers to segregating alloys [12].

The viscosity is helpful to describe the interatomic interactions between the constituents of a binary solution. In the framework of Moelwyn- Hughes approach [24], the viscosity of a binary solution is represented as

$$\eta = \eta_{id} \left[1 - C_A C_B \left(\frac{2\omega}{K_B T} \right) \right] \quad (26)$$

where, η_{id} = viscosity of the ideal solution which is expressed as

$$\eta_{id} = C_A \eta_A + C_B \eta_B \quad (27)$$

where, η_A and η_B = viscosities of pure components A and B respectively.

The heat of mixing, H_M is also be represented by [12]

$$\frac{H_M}{RT} = -C_A C_B \frac{\omega}{K_B T} \quad (28)$$

Equations (25) and (27) provide

$$\eta = (C_A \eta_A + C_B \eta_B) \left(1 - 2 \frac{H_M}{RT} \right) \quad (29)$$

It is clear that the magnitude of η depends upon the sign of $\frac{H_M}{RT}$. For segregating alloys, $\frac{H_M}{RT}$ is positive hence η is small while for ordered alloys η is large because $\frac{H_M}{RT}$ is negative.

2.4 Optimization procedure

Optimization procedure [11,12,13] plays vital role for the exploration of thermophysical behaviour of a binary solution at various temperatures where experimental measurement is difficult. For this, Redlich-Kister (R-K) polynomials are used to provide a suitable set of model parameters. R-K polynomials represent the concentration and temperature dependence of G_M^{XS} [12, 13] as

$$G_M^{XS}(C,T) = C(1-C) \sum_{l=0}^m K_l(T) (2C-1)^l \quad (30)$$

$$\text{where, } K_l(T) = A_l T + B_l T + C_l T + \ln T + D_l T^2 \quad (31)$$

The coefficient $K_l (l=0,1,2,3,\dots)$ depends on temperature same to the temperature dependence of G (i.e. free energy of mixing). The free energy of mixing, G may be represented as

$$G = A + BT + CT + \ln T + DT^2 + ET^{-1} \quad (32)$$

The partial excess free energy for the constituents A and B may be expressed as [12, 15]

$$G_A^{XS} = (1-C)^2 \sum_{l=0}^m K_l(T) [(1+2l)C - (1-C)] (2C-1)^{l-1} \quad (33a)$$

$$G_{M,B}^{XS} = (1-C)^2 \sum_{l=0}^m K_l(T) [(1+2l)C - (1-C)] (2C-1)^{l-1} \quad (33b)$$

The G_M^{XS} of a binary alloy is given by

$$G_M^{XS} = C G_A^{XS} + (1-C) G_B^{XS} \quad (34)$$

The activity coefficient, γ_i and partial excess free energy of i^{th} component ($i \equiv A, B$) are related as

$$G_i^{XS} = RT \ln \gamma_i \quad (i \equiv A, B) \quad (35)$$

The activity of i^{th} component, a_i ($i \equiv A, B$) can be represented by

$$a_i = \gamma_i C_i \quad (36)$$

3. Results and Discussions

3.1 Bulk Properties: G_M , a_i ($i \equiv A, B$), S_M , H_M , $S_{CC}(0)$, α_i and E^{XS} for SnTl melts at 723 K

The investigative equation (5) for G_M shows that for the computation, the values of model parameters γ and W are required.

The size ratio, $\gamma \left(= \frac{V_{TL}}{V_{Sn}} \right)$ is determined on using the values of V_{Sn} and V_{Tl} at 723 K. For this, the values of V_{Sn} and V_{Tl} at corresponding melting points [33] are utilised in the relation given below

$$V_i(T) = V_i(T_m) [1 + \alpha_i (T - T_m)] \quad (37)$$

where, $i (= Sn, Tl)$, T_m = melting temperature (in K), $T = 723$ K and α_i = coefficient of thermal expansion of the component i in the liquid state. The value of γ is found to 1.07. It is necessary to state that the value of γ may be slightly altered in order to achieve the better results [13, 34]. The parameter W can be ascertained by successive approach method [16, 35] on employing the experimental data of G_M in equation (5).

The reasonable values of γ and W are

$$\gamma = 1.125 \text{ and } W = 0.719$$

The reasonable values of γ and W are applied in equations (5) and (8) to obtain the values of $\frac{G_M}{RT}$ and $\frac{G_M^{XS}}{RT}$ respectively for SnTl melts at 723 K in terms of the concentration of Sn. Fig.1 includes the concentration dependence of theoretical data along with the correlated experimental data [3] of $\frac{G_M}{RT}$ and $\frac{G_M^{XS}}{RT}$ for SnTl melts at 723 K. It is clear that the theory and experiment display the well agreement. At each composition, G_M^{XS} exhibits positive value in the concentration region, $C_{Sn} = 0.1$ to 0.9. This favours to state that SnTl melts at 723 K possess segregating character. The maximum values of $\frac{G_M^{XS}}{RT}$ are observed at $C_{Sn} = 0.5$ i.e. 0.1886 (Theory) and 0.1894 (Experiment). Again, the values of $\frac{G_M}{RT}$ are observed minimum at $C_{Sn} = 0.5$ i.e. -0.5046 (Theory) and -0.5042 (Experiment). Thus, the present theoretical study successfully explains the symmetric behaviour of SnTl melts at 723 K in terms of G_M and G_M^{XS} .

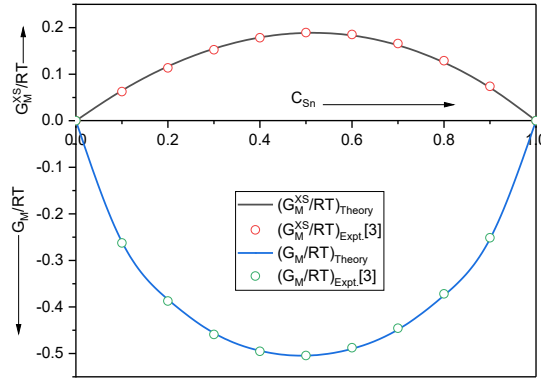


Fig.1 G_M^{XS}/RT and G_M/RT versus C_{Sn} for SnTi melts at 723 K

The equations (10a) and (10b) are employed to obtain the theoretical data of a_{Sn} and a_{Ti} respectively for SnTi melts. It is necessary to clarify that the values of γ and W are taken same so that the consistency is maintained. The theoretical values of a_{Sn} and a_{Ti} for SnTi melts at 723 K in terms of concentration of Sn i.e. $C_{Sn} = 0.1$ to 0.9 are displayed in Fig.2. For comparison, the correlated experimental data [3] are also included in Fig.2. The theory and experiment exhibit excellent harmony. Again, the positive departures of a_{Sn} and a_{Ti} from linearity show the segregating nature of SnTi melts at 723 K. This provides the validity to the model parameters γ and W so that they may be utilized for further calculations of the properties of SnTi alloys.

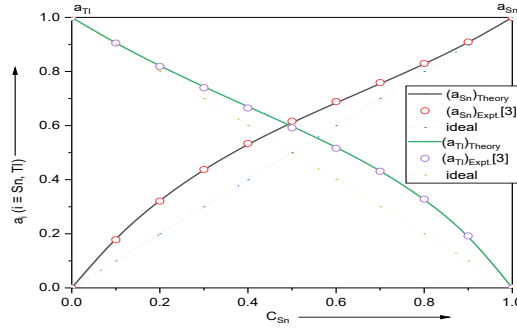


Fig. 2 $a_i (i \equiv \text{Sn, Ti})$ versus C_{Sn} for SnTi melts at 723 K

It is informative that the numerous structural information can be received by the thermodynamic functions like S_M and H_M . The entropy is the characteristics useful to measure the haphazard mixing of atoms (or molecules) in an ideal solution and orderly mixing nature of non-ideal solution. Again, the enthalpy of mixing directly leads to the knowledge of the bonding character in the liquid. Therefore in present investigation, S_M and H_M for SnTi melts at 723 K have been theoretically explored.

Equations (11) and (12) show that the calculations of S_M and H_M for a binary melt require the value of $\frac{\partial W}{\partial T}$. The method of successive approximation [13, 16] is employed on using the experimental data of S_M for SnTi melts at 723 K in equation (11). The reasonable value of $\frac{\partial W}{\partial T}$ for SnTi melts at 723 K is determined as

$$\frac{\partial W}{\partial T} = -0.0006 K^{-1}$$

Fig. 3 shows the concentration dependence of $\frac{S_M}{R}$ and $\frac{H_M}{RT}$ with respect to the composition of Sn for SnTl melts at 723 K. The correlated experimental data [3] are also introduced in Fig.3 for comparison. A well agreement is noticed between theory and experiment. In whole range of composition $c_{Sn} = 0.1$ to 0.9, $\frac{S_M}{R}$ is positive with maximum values $\frac{S_M}{R} = 0.6194$ (Theory) and 0.6188 (Experiment) both at $c_{Sn} = 0.5$. This explains the symmetric behaviour of S_M in SnTl melts at 723 K. The $\frac{H_M}{RT}$ - c isotherm reveals that SnTl melt at 723 K is a segregating alloy because at each composition, $\frac{H_M}{RT}$ is positive. However, a minor departure is observed between the theory and experiment i.e. the maximum values of $\frac{H_M}{RT} = 0.1150$ (Theory) at $c_{Sn} = 0.54$ and 0.1191 (Experiment) at $c_{Sn} = 0.6$.

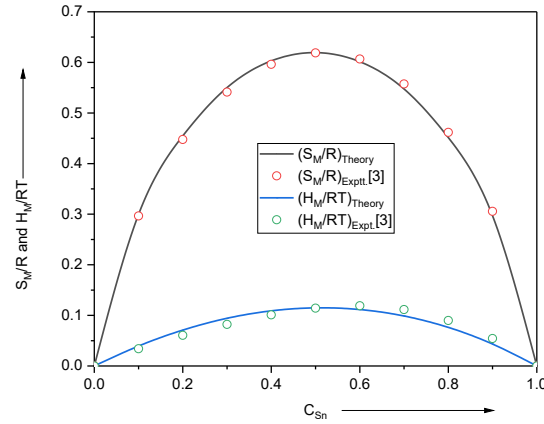


Fig. 3 S_M/R and H_M/RT versus c_{Sn} for SnTl melts at 723 K

The concentration dependence of $s_{CC}(0)$, α_1 and E^{XS} of SnTl melts at 723 K are analyzed with the help of equations (13) and (14); (16) and (3) respectively. It is notable that α_1 and E^{XS} can be interpreted in terms of $s_{CC}(0)$ for binary melts. Therefore, $s_{CC}(0)$ for SnTl melts at 723 K is determined using the equations (13) and (14). In view to maintain the consistency, same values of model parameters are utilized for the computation of $s_{CC}(0)$.

Fig. 4 displays the theoretical and experimental [3] values of $s_{CC}(0)$ for SnTl melts at 723 K. There exists excellent harmony between the theory and experiment. At each concentration of Sn, the $s_{CC}(0) > s_{CC}^{id}(0)$ which discloses that at 723 K, the SnTl system is a segregating alloy. The $s_{CC}(0)$ - c isotherm illustrates that $s_{CC}(0)$ possesses maximum value at $c_{Sn} = 0.5$ i.e. 0.401 (Theory) and 0.402 (Experiment). Therefore, SnTl system at 723 K shows symmetry in terms of $s_{CC}(0)$. It is pointed out that the maximum value of $s_{CC}(0) - s_{CC}^{id}(0)$ is 0.1506 at $c_{Sn} = 0.5$ which is close to 0.1487 [6].

The concentration dependency of α_1 for SnTl melts at 723 K is also presented Fig.4. Obviously, the magnitude of α_1 is positive at each concentration which confirms the segregating behavior of SnTl melts at 723 K. The magnitude of α_1 is smaller which refers to weakly interacting nature of SnTl melts at 723 K.

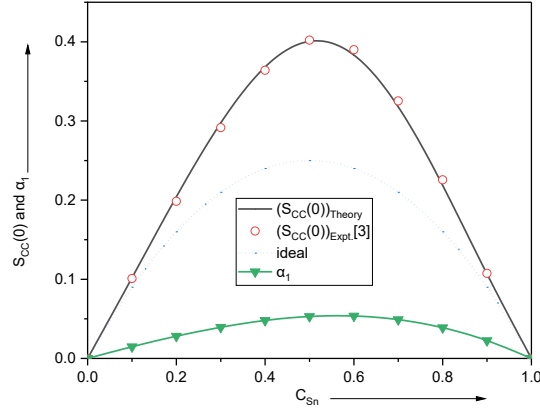


Fig. 4 $S_{CC}(0)$ and α_1 versus C_{Sn} for SnTl melts at 723 K

The equation (3) is utilized to determine the E^{XS} of SnTl melts at 723 K as a function of composition of Sn . The theoretical data of $\frac{E^{XS}}{RT}$ for SnTl melts at 723 K are presented in Fig. 5. It is obvious that $\frac{E^{XS}}{RT}$ is negative at each

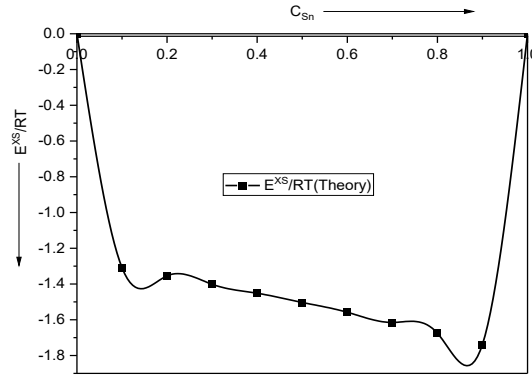


Fig. 5 E^{XS}/RT versus C_{Sn} for SnTl melts at 723 K

concentration in region $C_{Sn} = 0.1$ to 0.9 . This is a manifestation of the segregating nature of SnTl melts at 723 K [11].

3.2 Results for G_M^{XS} , activity, $S_{CC}(0)$, α_1 and E^{XS} of SnTl melts at various temperatures

In recent years, optimization procedure is found to be a very important tool [11, 12, 13, 14, 15, 16] to explain the thermophysical properties of binary melts like AlSn, ZnSn, AgCu, AlZn etc on using the theoretical thermodynamic data and polynomial expressions. The optimized coefficients for given binary melt are evaluated by least square method and these coefficients are further used to predict the thermophysical properties of binary melts at various

temperatures. It is remarkable that optimization procedure is very helpful in the cases for which no experimental data are available in the literature.

The optimization procedure in conjunction with QLT is utilized to predict the theoretical findings of G_M^{XS} for SnTl melts at various temperatures. The concentration dependence of the partial excess free energy of both the components i.e. $A=Sn$ and $B=Tl$ can be determined at various temperatures from equations (33a) and (33b) respectively. For this, optimized coefficients A_l, B_l, C_l and D_l are required to know the values of $K_l (l=0,1,2,3)$ from equation (30). The equation (31) can be used to ascertain the values of $K_l (l=0,1,2,3)$ by using data of G_M^{XS} for SnTl melts at different temperatures are needed. Thus, for the exploration of the thermophysical properties of SnTl melts at different temperatures, the data of G_M^{XS} for SnTl melts at different temperatures. Since, the experimental data of G_M^{XS} are not available in the literature for SnTl alloys at different temperatures, hence the theoretical data of G_M^{XS} are employed as suggested earlier [12].

For the computation of G_M^{XS} at different temperatures, the values of model parameters at different temperatures for SnTl melts are required. The value of $W(T)$ at desired temperature can be obtained by the relation [13,16].

$$W(T)=W(T_0)+\frac{\partial W}{\partial T}(T-T_0) \quad (38)$$

$$T_0 = 723 \text{ K}$$

T= desired temperature in K

$$\frac{\partial W}{\partial T}=-0.0006K^{-1}$$

$$W(T_0)=0.719$$

It is remarkable that the change in size ratio, γ is found to be negligibly small [13, 16] with the change in the temperature under consideration. Thus, during entire calculations, γ is kept constant for SnTl melts as taken earlier [13, 14, 16]. The values of W estimated at 623 K, 723 K, 823 K and 923 K are listed in **Table 1**.

Table 1 Values for interaction energy parameter

Temperature T (K)	Energy parameter (W)
623	0.779
723	0.719
823	0.660
932	0.600

Obviously, the value of interaction energy parameter W declines with the rise in temperature which is similar to earlier findings [13,14, 16].

Equations (33) and (34) are utilised to determine $\frac{G_M^{XS}}{RT}$ at 623 K, 723 K, 823 K and 923 K for SnTl melts relative to $c_{Sn} = 0.1$ to 0.9. Again, equations (30) and (31) are utilized to estimate the optimized coefficients, A_l, B_l, C_l and D_l ($l = 0, 1, 2$ and 3) with the help of least square method, which are illustrated in **Table 2**. It is remarkable that once A_l, B_l, C_l and D_l are known, they are frequently used to determine the optimized values of thermodynamic functions at any temperature.

Table 2: Optimized coefficients for SnTl melts

Values of l	$A_l(Jmole^{-1})$	$B_l(Jmole^{-1}K^{-1})$	$C_l(Jmole^{-1}K^{-1})$	$D_l(Jmole^{-1}K^{-2})$
0	-3.25963×10^{-9}	10.0905284	-1.364×10^{-12}	- 0.005281834
1	4.7512×10^{-9}	0.59468983	1.33×10^{-11}	- 0.000310696
2	-1.08639×10^{-9}	0.03506356	-2.682×10^{-12}	- 1.83016×10^{-5}
3	-1.68238×10^{-8}	0.00206374	-4.507×10^{-11}	-1.07656×10^{-6}

The equations (33a), (33b) and (34) are employed to ascertain the concentration dependence of $\frac{G_M^{XS}}{RT}$ at 623 K, 723 K, 850 K and 1000 K for SnTl melts which are presented in Fig. 6.

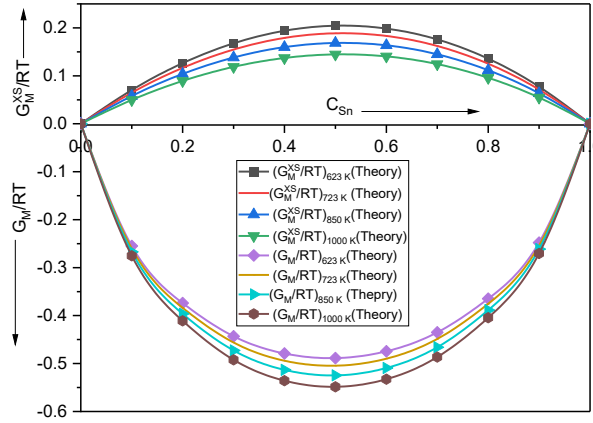


Fig. 6 G_M^{XS}/RT and G_M/RT versus c_{Sn} for SnTl melts at 623 K, 723 K, 850 K and 1000 K

Fig.6 shows that at each temperature and concentration, $\frac{G_M^{XS}}{RT}$ possesses positive value in the concentration region $c_{Sn} = 0.1$ to 0.9, indicating the segregating characteristics of SnTl melts in the temperature region from 623 K to 1000 K. Again, the segregation of SnTl melts decreases due to rise in temperature because the $\frac{G_M^{XS}}{RT}$ exhibits degradation with the elevation of temperature. Further the symmetries in G_M^{XS} remains maintained in the temperature region,

623-1000 K because the value of $\frac{G_M^{XS}}{RT}$ is maximum at $c_{Sn} = 0.5$ i.e. 0.2045 at 623 K, 0.1886 at 723 K, 0.1686 at 850 K and 0.1450 at 1000 K.

The theoretical values of a_{Sn} and a_{Tl} on using equations (35) and (36) for SnTl melts at 623 K, 723 K, 850 K and 1000 K are depicted Fig. 7 in terms of composition of Sn. In the region of temperature from 623 K to 1000 K, both a_{Sn} and a_{Tl} express to the positive deviations from ideal mixing which corresponds to segregation in SnTl melts due to enhancement of temperature. Further, the decrease in the positive deviations of a_{Sn} and a_{Tl} is comparatively small which indicates that there is small decrease in the magnitude of a_{Sn} and a_{Tl} if temperature is increased from 623 K to 1000 K.

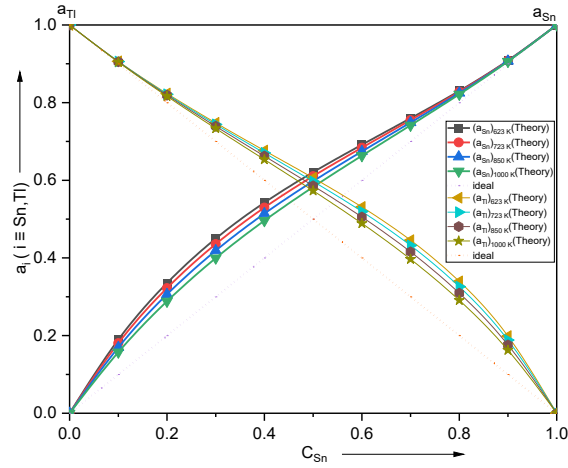


Fig.7 a_i ($i \equiv \text{Sn, Tl}$) versus c_{Sn} for SnTl melts at 623 K, 723 K, 850 K and 1000 K

3.3 Results for $s_{CC}(0)$, α_1 and E^{XS} for SnTl at different temperatures

Equation (15) is employed to achieve the values of $s_{CC}(0)$ for SnTl melts at 623 K, 723 K, 850 K, 1000 K on using the theoretical data of a_{Sn} and a_{Tl} at the undertaken temperatures. Again, the equations (16) and (3) are utilized to predict the concentration dependence of α_1 and E^{XS} respectively for SnTl melts at 623 K, 723 K, 850 K and 1000 K on employing the theoretical data of $s_{CC}(0)$.

For SnTl melts, the theoretical data of $s_{CC}(0)$ at 623 K, 723 K, 850 K and 1000 K are presented in Fig.8. The experimental data of $s_{CC}(0)$ at 723 K [3] also included in Fig. 8 illustrate excellent harmony and have maximum values i.e. 0.401 (Theory) and 0.402 (Experiment) both noticed at $c_{Sn} = 0.5$. The theoretical data of $s_{CC}(0)$ deviate positively from ideal mixing behavior at each concentration of Sn and the magnitude of positive deviation decreases at each concentration in the temperature region, 623-1000 K. This symbolizes that the segregation in SnTl melts lowers when temperature rises from 623 K to 1000 K. The further calculations of $s_{CC}(0)$ at higher temperatures beyond 1000 K signifies that at 1914.5 K, $s_{CC}(0)$ becomes almost equal to $s_{CC}^{id}(0)$. Again, on increasing the temperature from 1914.5 K to 1980 K, $s_{CC}(0)$ becomes less than $s_{CC}^{id}(0)$ which indicates the ordering character of SnTl

melts. Therefore, the segregating character of SnTl melts may transform into ordering character at the temperature about 1914.5 K. The similar trend was earlier observed for segregating alloys like NaK and CdSn melts [11, 14]. However at each temperature, $s_{CC}(0)$ remains maximum at $c_{Sn} = 0.5$ i.e. 0.422 at 623 K, 0.401 at 723 K, 0.377 at 850 K, 0.352 at 1000 K, 0.2497 at 1914.5 K, 0.2469 at 1950 K and 0.2446 at 1980 K. Therefore, the temperature dependence of $s_{CC}(0)$ exhibits the symmetric behavior for SnTl melts in the temperature region 623 -1980 K.

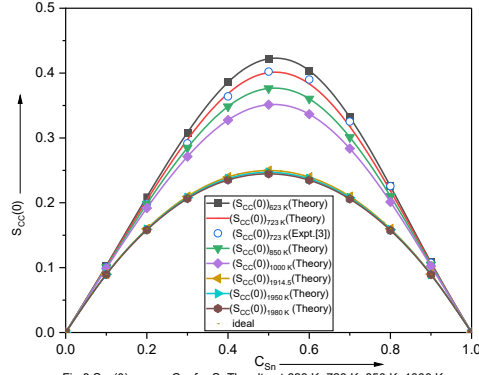


Fig.8 $s_{CC}(0)$ versus C_{Sn} for SnTl melts at 623 K, 723 K, 850 K, 1000 K, 1914.5 K, 1950 K and 1980 K

The theoretical data of α_1 for SnTl melts at 623 K, 723 K, 850 K and 1000 K are displayed in Fig.9 with respect to the bulk concentration of Sn. It is pointed out that the experimental data of α_1 are not provided in the literature. The α_1 - C isotherms implies that at each composition and at each temperature, the α_1 is positive with maximum values at $c_{Sn} = 0.5$ such as 0.0425, 0.0391, 0.0347 and 0.0297 at 623 K, 723 K, 850 K and 1000 K respectively for SnTl melts. This expresses that SnTl melts have symmetric nature and the segregation in SnTl melts gradually decreases when the temperature is raised from 623-1000 K. Further, the magnitude of the α_1 refers to feebly segregating behavior of SnTl melts.

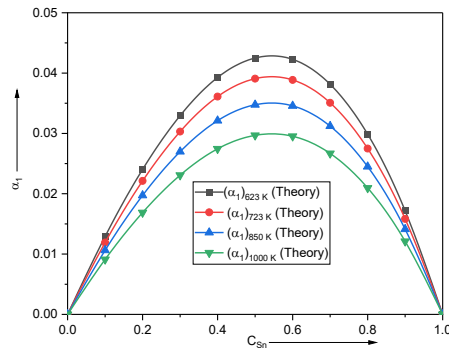


Fig. 9 α_1 versus C_{Sn} for SnTl melts at 623 K, 723 K, 850 K and 1000 K

The theoretical predictions of E^{XS} via equation (3) for SnTl melts relative to the composition of Sn at 623 K, 723 K, 850 K and 1000 K are incorporated in Fig.10. Obviously, $\frac{E^{XS}}{RT}$ has negative value at each composition throughout the concentration of Sn from 0.1 to 0.9 at each temperature for SnTl melts. This intimates that SnTl melts is a segregating

alloy in the temperature ranging from 623 K to 1000 K. Again, the magnitude of negative value of $\frac{E^{XS}}{RT}$ decreases with the elevation of temperature which suggests that the segregation in SnTl melts degrades when the temperature is elevated from 623-1000 K. The further calculations beyond 1000 K, it is observed that at 1914.5 K, $\frac{E^{XS}}{RT}$ becomes almost zero which refers to the ideal behavior of SnTl melts. On further increasing the temperature beyond 1914.5 K i.e. at 1950 K and 1980 K, $\frac{E^{XS}}{RT}$ expresses the positive value which is a sign of ordering nature of the liquid alloy. Thus, the present theoretical analysis suggests that the transition from segregating to ordering behavior of SnTl melts may take places at the temperature about 1914.5 K. This type trend is also noticed for NaK and CdSn melts [13,14].

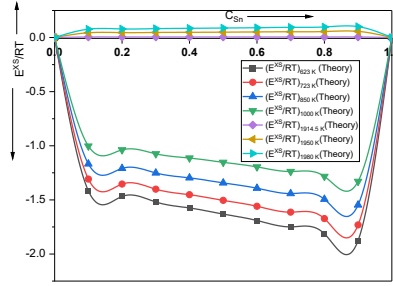


Fig.10 E^{XS}/RT versus C_{Sn} for SnTl melts at 623 K, 723 K, 850 K, 1000 K, 1914.5 K, 1950 K and 1980 K

3.4 Results for surface properties of SnTl at different temperatures

The equations (17a), (17b) and (20) are employed to analyse the σ , C_i^S and $S_{CC}^S(0)$ for SnTl melts at 623 K, 723 K, 850 K and 1000 K using the theoretical data of γ_{Sn} and γ_{Tl} at the undertaken temperatures. The required values of S_i ($i=Sn, Tl$) at the various temperatures, equation (18) is employed for which V_i ($i=Sn, Tl$) are determined at the corresponding temperatures. For the calculations of V_i ($i=Sn, Tl$), the required physical quantity are presented in Table 3.

Table 3: Data for physical properties of SnTl [33]

Metal	M.P. (T_m in K)	Atomic mass (M in Kg)	Density (ρ in Kg m^{-3})	Temp ^r . Coefft. of Density ($\frac{\partial \rho}{\partial T}$ in Kg m^{-3} K $^{-1}$)
Sn	405.99	0.11869	6980	- 0.61
Tl	575.65	0.20437	11350	-1.30

The surface tension of pure i^{th} component at the desired temperature (T) may be calculated from the relation

$$\sigma_i(T) = \sigma(T_m) + \frac{\partial \sigma}{\partial T}(T - T_0) \quad (39)$$

where, T_m = melting temperature

$$\frac{\partial \sigma}{\partial T} = \text{temperature coefficient of surface tension}$$

The needed parameters for pure Sn and Tl are listed in Table 4.

Table 4: Surface tension and coefficient of surface tension for Sn and Tl [33]

Metal	Surface tension (σ in mNm^{-1})	Coefficient of surface tension ($\frac{\partial \sigma}{\partial T}$ in $\text{mNm}^{-1}\text{K}^{-1}$)
Sn	560	- 0.09
Tl	464	- 0.08

The equations (19) and (20) are utilized to determine the partial excess free energy of both the components Sn and Tl in the bulk and at the surface for the required temperatures on using $\lambda = 0.82$.

The equations (17a) and (17b) are solved simultaneously to achieve the values of C_{Sn}^s and σ for SnTl melts

relative to the bulk concentration of Sn i.e. C_{Sn}^b i.e. C_{Sn} . The concentration dependence of C_{Sn}^s at 623 K, 723 K, 850 K and 1000 K for SnTl melts is mentioned in Fig. 11 as a function of C_{Sn} .

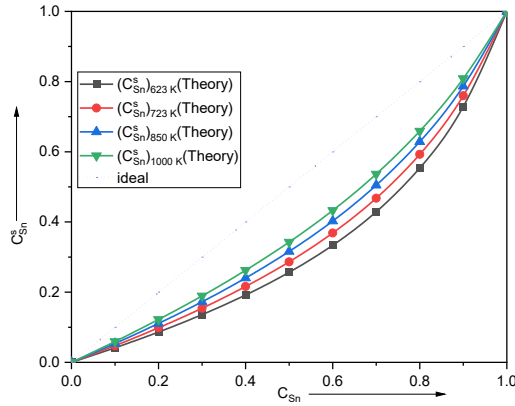


Fig.11 C_{Sn}^s versus C_{Sn} for SnTl melts at 623 K, 723 K, 850 K and 1000 K

It is clear that the surface concentration of Sn (i.e. C_{Sn}^s) exhibits negative deviation from the ideal surface concentration in the region, $C_{Sn} = 0.1$ to 0.9 at each temperature i.e. from 623- 1000 K for SnTl melts. This indicates that at the surface the number of Sn-atoms is less than that of Tl-atoms at each temperature under consideration i.e Tl-atoms segregates the surface with the increase in the bulk concentration of Sn. Again, the negative deviation of C_{Sn}^s decreases with the rise in temperature from 623-1000 K which exhibits similar trend as observed for InZn melts [36].

The theoretical data of surface tension σ relative to the bulk concentration of Sn for SnTl melts at 623 K, 723 K, 850 K and 1000 K are displayed in Fig. 12. Obviously, the surface tension of SnTl melts increases with increase of Sn-atoms at each temperature under consideration. This is due to the fact that Sn has larger value of surface tension than that of Tl. Again, σ - C_{Sn} isotherms indicate that the surface tension of SnTl melts decreases with the elevation of temperature from 623 K to 1000 K in the complete region of the composition of Sn. It is notable that the theoretical data of σ are not compared with the experimental data due to unavailability.

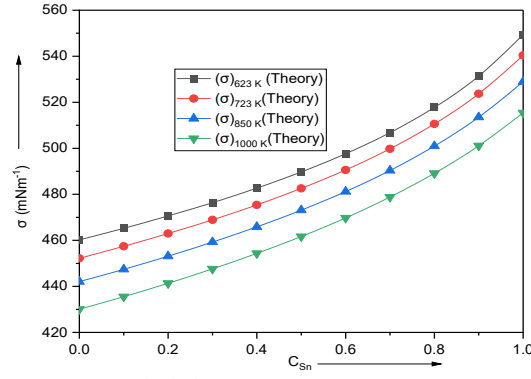


Fig.12 σ versus C_{Sn} for SnTl melts at 623 K, 723 K, 850 K and 1000 K

The theoretical values of $S_{CC}^S(0)$ evaluated from equations (21) and (22) for SnTl melts at 623 K, 723 K, 850 K and 1000 K are mentioned in Fig. 13. It is clear that $S_{CC}^S(0)$ increases with the rise in temperature in the composition range, $0.0 \leq C_{Sn} \leq 0.6$ and then the crossover effect is observed beyond $C_{Sn} = 0.6$. The $S_{CC}^S(0)$ exhibits the peak value i.e. 0.91 at $C_{Sn} = 0.75$ for 623 K while for temperatures 723 K, 850 K and 1000 K, the peak values are 0.38, 0.36 and 0.34 respectively, observed at $C_{Sn} = 0.7$. This shows the similar atoms pairing (Sn-Sn) at the surface [36] and the segregation is strongest for 623 K followed by 723 K, 823 K and 1000 K respectively for SnTl melts in the higher concentration region of Sn. Further, the results suggest the maximum possibility of phase segregation at the surface in the composition range, $C_{Sn} = 0.7$ to 0.8.

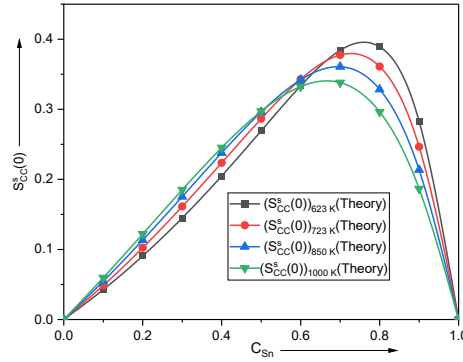


Fig. 13 $S_{CC}^S(0)$ versus C_{Sn} for SnTl melts at 623 K, 723 K, 850 K and 1000 K

3.5 Results for Transport Properties of SnTl at Different Temperatures

The equation (24) is applied for the assessment of $\frac{D_M}{D_{id}}$ for SnTl melts at 623 K, 723 K, 850 K and 1000 K. The theoretical data of $\frac{D_M}{D_{id}}$ depicted in Fig. 14 shows that $\frac{D_M}{D_{id}} < 1$ at each temperature in the complete composition

range of Sn, $C_{Sn}=0.1$ to 0.9 which is an indication of segregating character of SnTl melts. Again, the magnitude of $\frac{D_M}{D_{id}}$ shows the declination with the elevation of temperature from 623-1000 K which clarifies the decrease in the segregating nature of SnTl melts. Further, the value of $\frac{D_M}{D_{id}}$ is close to 1 which advocates that the degree of segregation in SnTl melts is least [6] and hence the system is feebly segregating in nature.

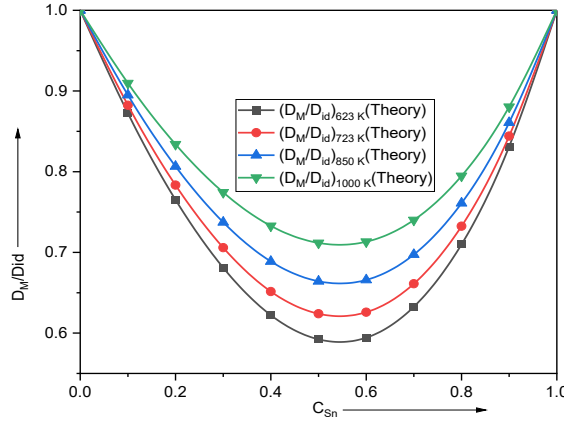


Fig. 14 D_M/D_{id} versus C_{Sn} for SnTl melts at 623 K, 723 K, 850 K and 1000 K

The temperature and concentration reliance of viscosity for SnTl melts has been predicted theoretically on using equation (29). The values of η for pure Sn and Tl are determined [37] at 623 K, 723 K, 850 K and 1000 K. The theoretical data of η for SnTl melts at 623 K, 723 K, 850 K and 1000 K are illustrated in Fig.15. It is pointed out that no experimental data of η for SnTl melts is available for comparison. The η - C isotherms illustrate that η decreases on increasing the concentration of Sn at each temperature due to the smaller value of viscosity for Sn than that of Tl. Again, the viscosity of SnTl melts decreases with the elevation of temperature from 623- 1000 K and the minima are observed in the vicinity of $C_{Sn} = 0.6$ which is close to $C_{Sn} \cong 0.55$ [6].

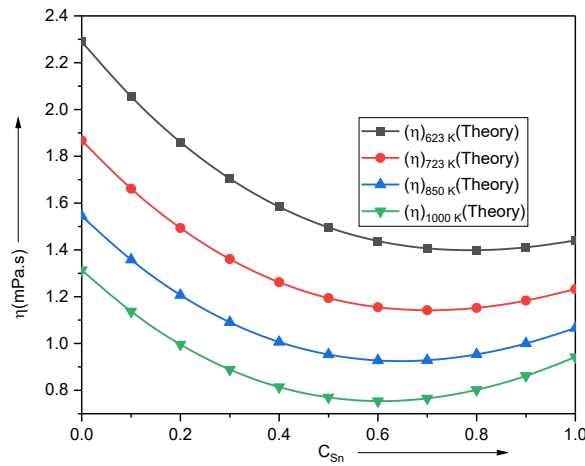


Fig. 15 η versus C_{Sn} for SnTl melts at 623 K, 723 K, 850 K and 1000 K

Conclusions

The thermodynamic, microscopic, surface and transport properties for SnTl melts are effectively explain by QLT model. The experimentally observed symmetries in G_M , G_M^{XS} , S_M and H_M for SnTl melts are described successfully. The concentration dependence of the bulk properties for SnTl melts refers to the segregating nature of SnTl melts at 723 K. The temperature and concentration reliance of G_M , activity, $S_{CC}(0)$, α_1 , E^{XS} , surface properties and transport properties reveal that the segregating behavior of SnTl melts decline when temperature rises from 623– 1000 K and nature of segregation is feeble. Further, the theoretical results predict that the segregating nature of SnTl melts may transform to ordering behavior at temperature about 1914.5 K.

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