



Temperature and Concentration Dependent Electrical Resistivity of Cu_x-Sn_{100-x} Liquid Binary Alloy

Abstract:

In the present paper, temperature and concentration dependent electrical resistivity of liquid Cu-Sn alloys as a function of Sn concentration along with different temperature have been studied. Our well-established model potential has been used to incorporate the ion-electron interaction. To incorporate the exchange and correlation effects, three different forms of local field correction functions viz. Hartree (H), Farid et al. (F), and Sarkar et al. (S) have been used. The electrical resistivity of binary system have been studied using Faber-Ziman formulation combined with Ashcroft-Langreth (AL) partial structure factor. It is observed that out of three local field correction functions, the values of electrical resistivity computed using Hartree screening function is found to be less deviation with experimental values compared to other two screening functions. Overall, the present results of electrical resistivity are found to be good agreement with experimental results.

Keywords: Electrical Resistivity, Pseudopotential, Local field correlation functions

1. Introduction:

The theoretical or experimental study of electrical resistivity (ρ) of transition metals and their alloys have been of considerable interest in the field of physics and material sciences [1-4]. The theoretically most commonly accepted method for studying the resistivity of liquid binary alloy is the electrical conduction theory developed by Ziman [5-6] formulation and this concept has been very useful for liquid binary alloys. In the present paper, Cu-Sn alloys are widely useful in industry fields, material and machine, etc. because of their interesting mechanical, electrical and chemical properties [1]. The Cu-Sn alloy system shows outstanding properties due to its characteristic of the intermetallic compounds [1]. The aim of this study is to determine principal regularities in the variation of the electrical resistivity of copper-tin alloys at various temperature and different concentration with the help of our well known model potential [7] along with three different local field correlation functions due to Hartree[8], Farid et al[9] and Sarkar et al[10] to judge the screening deviation with reference experimental value.

Recently P Jia et al [1] has reported the experimentally electrical resistivity of Cu-Sn alloy. This work has motivated us to investigate theoretically, temperature dependence and concentration dependent electrical resistivity of Cu-Sn alloy with the help of pseudopotential formalism combined with Faber-Ziman (FZ) formulation [3,4].

2. Computational Method:

In the present study, electrical resistivity has been computed with the help of our well recognized model potential. The proposed model potential in q-space used to describe the electron-ion interaction of the complex system is of the form[7],

$$V_b(q) = \frac{-4\pi Ze^2}{\Omega_0 q^2} \left[\cos(qr_c) - \frac{\exp(-1)qr_c}{1+q^2r_c^2} \{ \sin(qr_c) + qr_c \cos(qr_c) \} \right] \quad (1)$$

Here Z , Ω , \mathbf{q} , e and r_c are the valency, atomic volume, wave vector, charge of electron and the parameter of the potential respectively. In the present paper, the parameters of the potential for pure Cu and Sn have been determined following the procedure of Heine and Weaire [2,3]. The approach of FZ [5] is used to study the concentration and temperature dependence of the electrical resistivity of

liquid binary mixture [2,3]. The electrical resistivity for binary alloys in Faber and Ziman formulations is given by[2-4] ,

$$\rho = \frac{3 \pi \Omega m^2}{4 e^2 \hbar k_F^6} \int_0^{2k_F} S(q) |V(q)|^2 q^3 \theta(2k_F - q) dq \quad (2)$$

Where, n is the electron density related to the Fermi wave number, θ is the unit step function that cuts off the q integration at $2k_F$ corresponding to a Fermi surface, $S(q)$ the structure factor and $V(q)$ the screened ion pseudopotential form factor. From the rearrangements of the various constants, one can write the formula for the electrical resistivity of the binary alloys in the following form [2-4]:

$$\rho = \frac{12.81\Omega}{K_F^6} \int_0^{2k_F} q^3 \lambda(q) dq \quad (3)$$

With

$$\lambda(q) = (1-x) S_{11}(q) V_1^2(q) + 2[x(1-x)]^{1/2} S_{12}(q) V_1(q) V_2(q) + x S_{22}(q) V_2^2(q) \quad (4)$$

Here, $V_1(q)$ and $V_2(q)$ denote the screened form factors for elements A and B, $S_{ij}(q)$ are the Ashcroft-Langreth partial structure factors of the binary metallic complexes[2-4], x is the concentration of second metallic component of $A_{1-x}B_x$ mixture[2-4].

3. Results and Discussion

The input parameters used in the present computations are presented in Table 1. The concentration dependence of the electrical resistivity at eight different temperatures are examined by varying the Sn concentration from $x = 0$ to $x = 100$ ($x = 0, 10, 20, 33, 40, 50, 60, 75, 80, 100$) and temperature dependent of resistivity for seven different alloys are $Cu_{10}Sn_{90}$, $Cu_{20}Sn_{80}$, $Cu_{33}Sn_{67}$, $Cu_{40}Sn_{60}$ and $Cu_{50}Sn_{50}$, $Cu_{75}Sn_{25}$ and $Cu_{80}Sn_{20}$ alloy

Table-I: Input parameters and constants

Input		1000K	1050K	1100K	1150K	1200K	1250K	1300K	1350K
Cu	$\sigma(\text{au})$	4.324	4.318	4.312	4.306	4.298	4.292	4.285	4.283
Sn		5.240	5.224	5.208	5.193	5.177	5.162	5.119	5.122
Cu	$\Omega(\text{au}^3)$	85.43	85.90	86.36	86.83	87.29	87.76	88.22	88.69
Sn		199.6	200.3	201.2	201.9	202.7	203.5	204.3	205.0
Cu	η	0.496	0.491	0.486	0.481	0.476	0.472	0.467	0.463
Sn		0.377	0.372	0.368	0.363	0.358	0.354	0.349	0.345

3.1 Temperature dependence resistivity

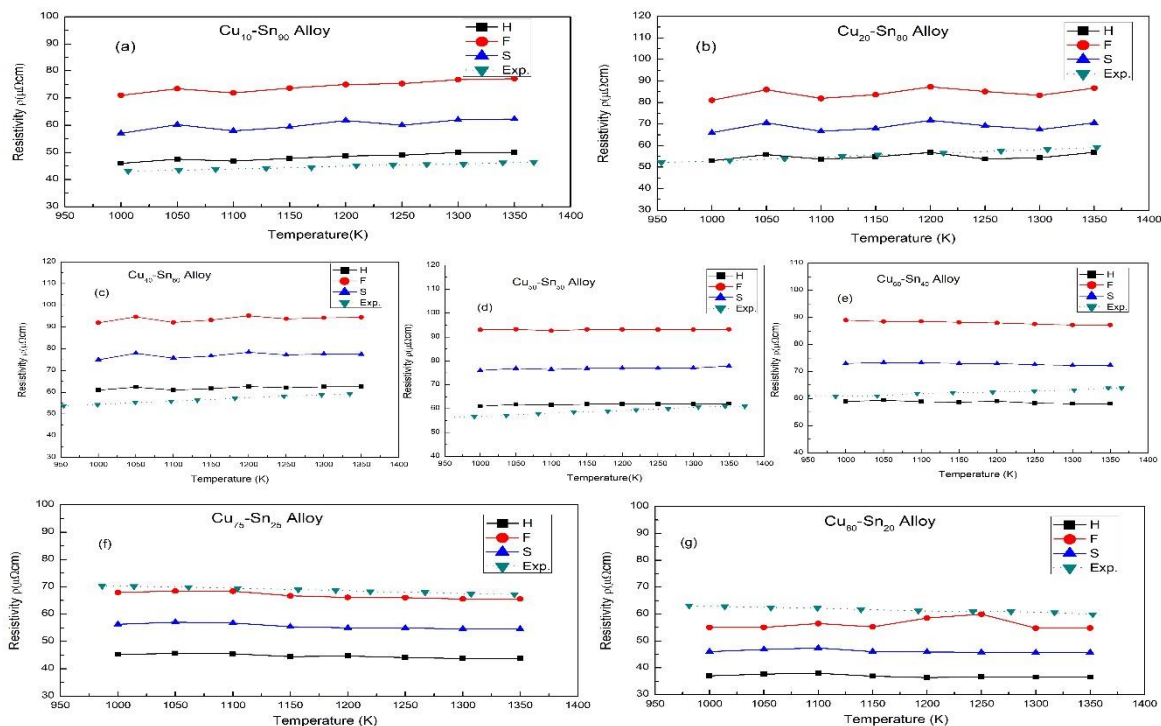


Figure-I (a to g) Temperature dependent electrical resistivity of Cu_x-Sn_{100-x} alloy at seven different combination.

Fig.I (a to g) represent the computed values of electrical resistivity for temperature dependent at seven different combination of Cu-Sn alloy. From Fig. I(a to e), it is seen that, temperature dependent electrical resistivity computed using H function shows the good agreement for $Cu_{10}Sn_{90}$, $Cu_{20}Sn_{80}$, $Cu_{33}Sn_{67}$, $Cu_{40}Sn_{60}$ and $Cu_{50}Sn_{50}$ alloys[1] compare to other screening function but for $Cu_{75}Sn_{25}$ (fig.I(f))and $Cu_{80}Sn_{20}$ alloys (fig.I (g)) are calculated electrical resistivity using F[9] local field functions is found to be good compared with experimental data. From fig. I(f) and Fig.I(g) it is observed that, the resistivity of $Cu_{75}Sn_{25}$ and $Cu_{80}Sn_{20}$ alloys linearly decreases with increases of temperature. Present results show symmetrical behaviour with respect to experimental data.

3.2 Concentration dependence of resistivity

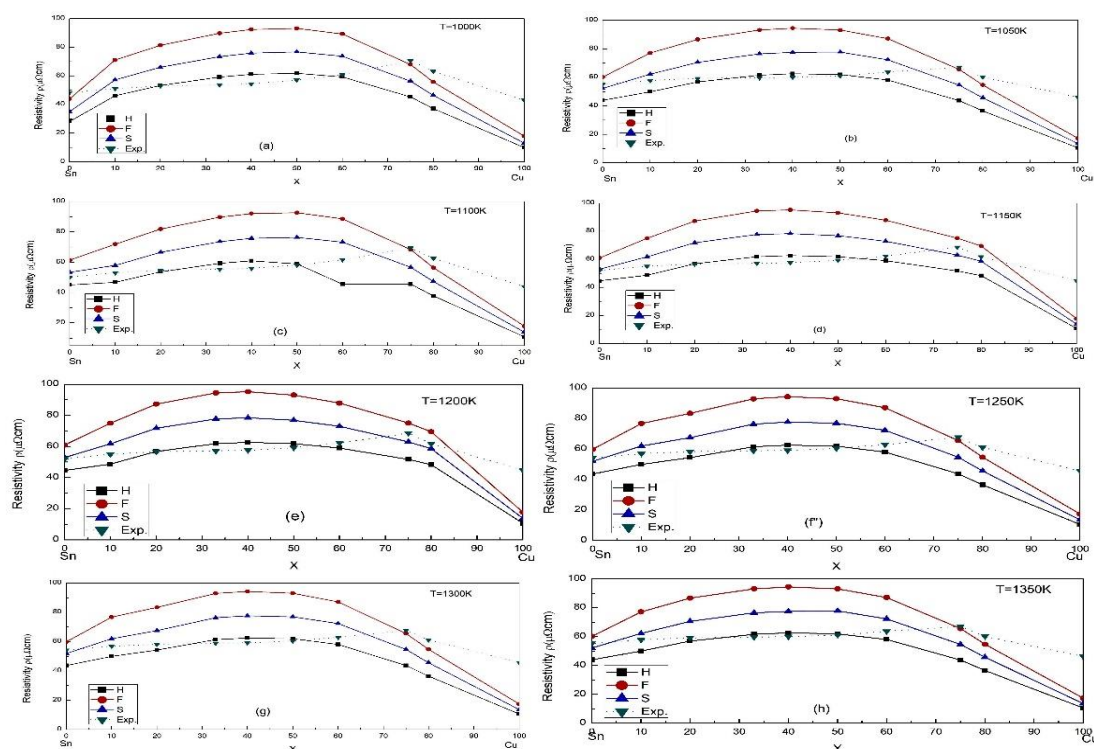


Figure. II (a to h) Concentration dependence electrical resistivity of $\text{Cu}_x\text{-Sn}_{100-x}$ alloy at different temperatures

Fig. II (a to h) shows calculated electrical resistivity using concentration dependence for $\text{Cu}_x\text{-Sn}_{100-x}$ alloy at eight different temperatures (1000K to 1350K in step size 50K). From the Fig. I & II it is seen that, among three employed local field correction functions, H [8] gives the minimum numerical value of the electrical resistivity, while the local field correction functions due to F [9] gives the maximum value. In the present findings of the resistivity of Cu-Sn binary alloy due to S local field correction function is laying between H and F functions for temperature dependent resistivity and concentration dependent resistivity. The results due to H function show better agreement with experimental results among the other local field correction functions.

From Figure II it is found that, the present results for Cu-Sn liquid binary alloy at eight different temperatures computed using H screening function is found to be good agreement with the available experimental results compared to other screening functions but at Sn-75% & 80% concentration F [9] and S [10] screening functions are shown in good agreement with experimental data compared to H screening function. The relative percentile deviation is described in Table-II. It is observed that H function less deviation with respected to experimental data. The experimental electrical resistivity value shows its maxima at $\text{Cu}_{75}\text{Sn}_{25}$ alloy and present results due to three local field correction functions show the maximum at $\text{Cu}_{50}\text{Sn}_{50}$ alloy.

Table-II: Percentile deviation with respect to experimental values

Temperature	H	F	S
1000K	10.08%-6.83%	62.87%-5.15%	20.22%-11.41%
1050K	10.68%-8.92%	35.19%-13.05%	11.09%-6.79%
1100K	12.15%-1.22%	33.31%-6.87%	10.06%-6.89%
1150K	11.51%-1.63%	33.22%-10.89%	9.98%-3.48%
1200K	8.58%-3.46%	38.20%-26.33%	13.68%-6.48%
1250K	9.19%-3.72%	36.2-18.11	12.77%-7.57%
1300K	10.52%-7.70%	5.18%-3.24%	14.64%-3.62%
1350K	6.63%-5.61%	5.27%-3.13%	14.75%-5.25%

The present study clearly indicate that proper description of exchange and correlation function is required for the study of electrical resistivity of liquid binary alloy.

4. Conclusion:

Finally we can conclude that the electrical resistivity of Cu-Sn alloy due to H local field correlation function is found to be good agreement with experimental data. Computed electrical resistivity of temperature dependent resistivity and concentration dependent resistivity show the symmetrical behavior with respect to available experimental data. In temperature dependent, the resistivity of $\text{Cu}_{75}\text{Sn}_{25}$ and $\text{Cu}_{80}\text{Sn}_{20}$ alloys decrease linearly with increases temperature. Hence, our well recognize model potential is found suitable for studying the resistivity of liquid binary alloys. Also, the present investigation predicts that the present study of the electrical transport properties is sensitive to the selection of the proper local field correction function.

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