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Electrical Resistivity of Liquid Alkali Na-based Binary Alloys

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Abstract

The study of the electrical resistivity ρ_L of alkali Na-based binary alloys $Na_{1-x}Li_x$, $Na_{1-x}K_x$, $Na_{1-x}Rb_x$ and $Na_{1-x}Cs_x$ have been made by well-recognized model potential of Gajjar et al. The most recent exchange and correlation functions due to Farid et al (F) and Sarkar et al (S) are used for the first time in the study of electrical resistivity of liquid binary mixtures and found suitable for such study. The results, due to the inclusion of Sarkar et al's local field correction function, are found superior to those obtained due to Farid et al's local field correction function. Electrical resistivity of Na-based binary alloys compare well with the experimental data available in the literature.

Key Words: Pseudopotential; Electrical Resistivity; Alkali Na-based liquid binaries.

1. Introduction

Ziman's nearly free electron (NFE) [1] theory has been fairly successful in describing the quantitative behavior of electrical resistivity in simple liquid metals. The resistivity of liquid binary alloys has been studied by application of the nearly free electron theory by Faber and Ziman [2]. This theory has found many successful applications but it is recognized that calculations are extremely sensitive to details of the pseudopotentials and structure factors, which are inputs to the theory. The electrical resistivity of liquid metals and alkali alloys have been studied experimentally by using a rotating magnetic field, four probe methods for temperatures up to 1200 K, diffraction model formula [3, 4] and theoretically by several authors [5–17] using Ziman's formula [1].

In the present study, the electrical resistivity ρ_L of $Na_{1-x}Li_x$, $Na_{1-x}K_x$,$Na_{1-x}Rb_x$ and $Na_{1-x}Cs_x$ alkali binary alloys are computed with the help of pseudopotential formalism. The well recognized model potential (in r-space) of Gajjar et al [18–20] used to describe the electron-ion interaction in these systems is of the form

$$\begin{aligned} V(r) &= \frac{-Z e^2}{r_c^3}\left[2-\exp\left(1-\frac{r}{r_c}\right)\right] r^2 \;;\; r < r_c \\ &= \frac{-Z e^2}{r} \qquad\qquad\qquad\qquad ;\; r \geq r_c, \end{aligned} \tag{1}$$

where r_C is the parameter of the potential and Z is the valency. This form has the feature of a Coulombic term outside the core and varying cancellation due to a repulsive and attractive contributions to the potential within the core. The detailed information of this potential is given in the literature [18–20]. The model

potential parameter r_C is adjusted in such a way that the present yielding shows excellent agreement with the experimental data.

The approach of Faber-Ziman [2] is used to study the concentration dependence of the electrical resistivity of K-based alkali binary mixture. In the present computation of electrical resistivity of binary mixture, the most recent local field correction functions due to Farid et al (F) [21] and Sarkar et al (S) [22] are employed for the first time to investigate the influence of exchange and correlation effects with reference to the static Hartree (H) [8] screening function. The mathematical expressions of these three exchange and correlation functions used in the present computations are as follows :

$$f_F(q) = A_F Y^4 + B_F Y^2 + C_F + \left[\left(A_F Y^4 + B_F Y^2 + C_F \right) \left(\frac{4 - Y^2}{4Y} \right) \ln \left| \frac{2+Y}{2-Y} \right| \right] , \tag{2}$$

$$f_S(q) = A_S \left(1 - \left\{ 1 + B_S Y^4 \right\} \exp \left\{ -C_S Y^2 \right\} \right) \quad , \tag{3}$$

and

$$f_H = 0, \tag{4}$$

where A_F, B_F, C_F, A_S, B_S and C_S are the constants of Farid et al's (F) [21] and Sarkar et al's (S) [22] exchange and correlation functions and $Y = q \ / \ k_F$ with k_F be the Fermi wave vector of the alloys, respectively.

2. Computational Methodology

The Faber-Ziman formula for electrical resistivity of binary alloys is given by [2]

$$\rho_L = \frac{3\,\pi\,m^2}{4\,e^2\,\hbar^3\,k_F^6\,n} \int_0^\infty S(q)\ |\,V(q)\,|^2\ q^3\,\theta\,(2k_F - q)\,dq. \tag{5}$$

Here n is the electron density related to the Fermi wave number, θ the unit step function that cuts off the q-integration at $2k_F$ corresponding to a perfectly sharp Fermi surface, S(q) is the structure factor and V(q) the screened ion pseudopotential form factor.

From rearrangements of the various constants, one can write the formula for the electrical resistivity of the binary alloys in the form [2]

$$\rho_L = \frac{12\ \Omega}{k_F^2} \int_0^{2k_F} \lambda(q)\ q^3\ dq, \tag{6}$$

with

$$\lambda\ (q) = (1-x)\,S_{11}\,V_1^2\,(q) + 2\,\sqrt{x\ (1-x)}\,S_{11}\,S_{22}\ V_1\,(q)\ \ V_2\,(q) + x\,S_{22}\,V_2^2\,(q)\,. \tag{7}$$

Here $V_1(q)$ and $V_2(q)$ denote the model potentials for elements A and B, S_{ij} are the partial structure factors, x is the concentration of the second metallic component of $A_{1-x}B_x$ mixture. We have used Ashcroft-Lengreth's [23] formulations to generate the partial structure factor of the binary metallic complexes.

3. Results and Discussion

The input parameters and constants used in the present computations are written in Table 1, which are taken from the literature [13, 15, 16]. The computed results of electrical resistivity are presented in Tables 2–5.

Table 1. The input parameters and constants.

Metals	Z	k_F (a.u.)	Ω (a.u.)	r_c (a. u.)
Li	1	0.5768	154.29	1.4543
Na	1	0.4742	277.76	2.0232
K	1	0.3826	528.67	2.6369
Rb	1	0.3616	626.13	2.7883
Cs	1	0.3233	876.12	3.5910

Table 2. Electrical Resistivity (in $\mu\Omega$·cm) of $Na_{1-x}Li_x$ binary alloy.

x	H	F	S	Exp. [13]
0.0	8.41	18.03	12.96	9.6
0.1	13.72	29.55	20.96	-
0.2	17.80	38.05	26.98	35.0
0.3	20.70	43.77	31.14	-
0.4	22.46	46.93	33.55	34.0
0.5	23.16	47.78	34.34	33.0
0.6	22.83	46.52	33.63	32.0
0.7	21.54	43.39	31.52	-
0.8	19.33	38.54	28.11	30.0
0.9	16.19	32.09	23.42	-
1.0	12.06	24.02	17.39	26.0

Table 3. Electrical Resistivity (in $\mu\Omega$·cm) of $Na_{1-x}K_x$ binary alloy.

x	H	F	S	Exp. [16]
0.0	8.41	18.03	12.96	9.60
0.1	14.93	32.13	22.95	20.0
0.2	20.03	43.78	30.97	28.9
0.3	23.80	52.96	37.08	35.0
0.4	26.23	59.43	41.21	39.0
0.5	27.26	62.86	43.22	42.5
0.6	26.82	62.87	42.90	42.0
0.7	24.84	59.06	40.08	39.5
0.8	21.26	51.11	34.60	34.5
0.9	16.06	38.70	26.33	26.0
1.0	9.20	21.46	15.10	15.0

Table 4. Electrical Resistivity (in $\mu\Omega$·cm) of $Na_{1-x}Rb_x$ binary alloy.

x	H	F	S	Exp. [16]
0.0	8.41	18.03	12.96	9.60
0.1	18.27	39.12	28.00	26.0
0.2	25.89	56.67	40.04	40.0
0.3	31.60	70.94	49.42	57.0
0.4	35.44	81.59	56.08	66.8
0.5	37.27	87.89	59.67	72.5
0.6	36.86	88.91	59.71	72.8
0.7	34.01	83.75	55.76	71.0
0.8	28.64	71.71	47.49	60.0
0.9	20.71	52.27	34.70	46.0
1.0	10.16	24.68	17.06	27.5

Table 5. Electrical Resistivity (in $\mu\Omega$·cm) of $Na_{1-x}Cs_x$ binary alloy.

x	H	F	S	Exp. [15]
0.0	8.41	18.03	12.96	9.60
0.1	38.02	82.82	58.53	42.5
0.2	62.11	141.63	97.37	80.0
0.3	83.16	198.36	132.78	112.5
0.4	101.39	252.32	164.73	140.0
0.5	115.13	297.99	190.18	162.5
0.6	120.89	324.45	202.96	165.0
0.7	114.36	317.40	195.14	154.0
0.8	93.15	266.77	161.58	130.0
0.9	58.94	173.11	103.76	95.0
1.0	14.89	41.08	25.64	44.6

The concentration dependence of the electrical resistivity ρ_L is examined by varying concentration $x = 0$ to $x = 1$ in the step size of 0.1 of the second metallic component. Most fascinating exchange and correlation screening functions due to Farid et al (F) and Sarkar et al (S) have used for the first time in such study. In Figures 1–4, the present outcomes of the electrical resistivity ρ_L for $Na_{1-x}B_x$ (B: Li, K, Rb, Cs) of alkali-alkali elements viz. $Na_{1-x}Li_x$, $Na_{1-x}K_x$, $Na_{1-x}Rb_x$ and $Na_{1-x}Cs_x$ alloys are shown with the experimental results [13, 15, 16]. As concentration x of the B element increase, the resistivity ρ_L increases and reaches the maximum value, after that the further increase in x decreases the ρ_L of the binary system. From the Figures 1–4 it is seen that, the present results due to Sarkar et al's (S) exchange and correlation function is found to be in fair agreement with the experimental results [15, 16] for $Na_{1-x}Rb_x$ and $Na_{1-x}Cs_x$ alloys, while for $Na_{1-x}K_x$, alloy show excellent agreement both in magnitude and gradient with experimental data [13]. The good agreement may be indicative of the free electron behaviour of these alloys in the whole concentration range. The relative influence of Farid at al (F) and Sarkar et al (S) exchange and correlation functions with respect to static Hartree (H) dielectric function is 98.23%-193.72% and 44.26%-76.40%, respectively. These two observations suggest that the proper choice of exchange and correlation function is essential for the study of the electrical transport properties of binary system.

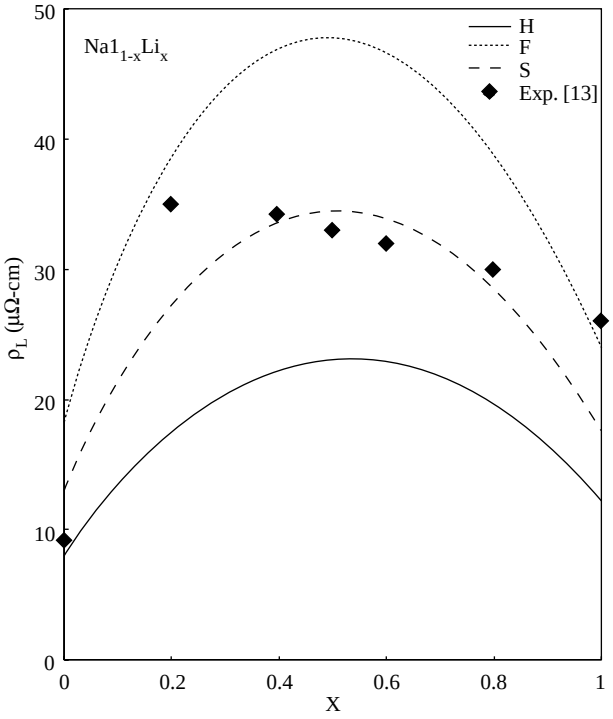

Figure 1. Electrical Resistivity of $Na_{1-x}Li_x$ binary alloy.

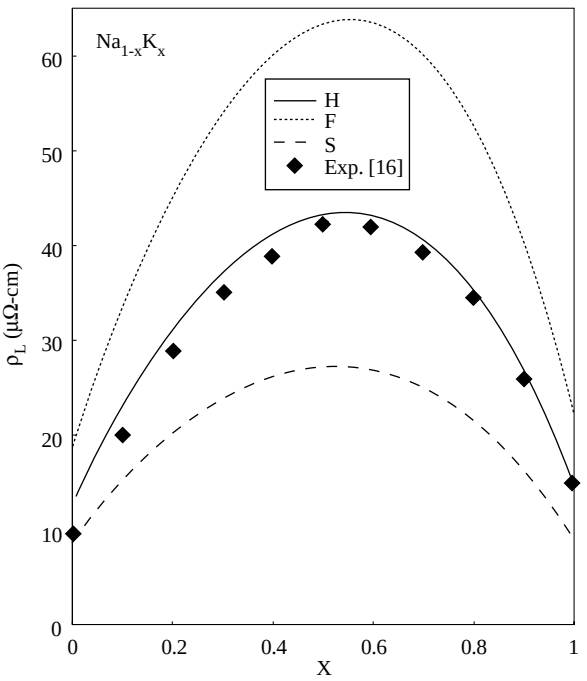

Figure 2. Electrical Resistivity of $Na_{1-x}K_x$ binary alloy.

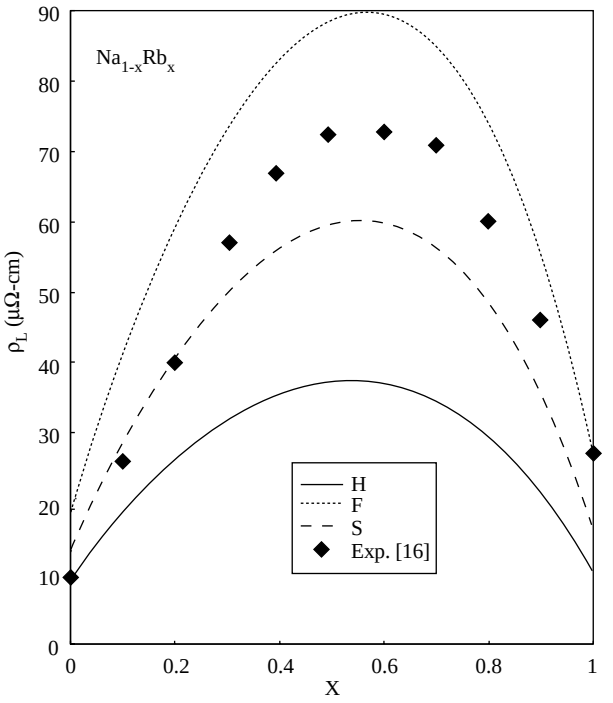

Figure 3. Electrical Resistivity of $Na_{1-x}Rb_x$ binary alloy.

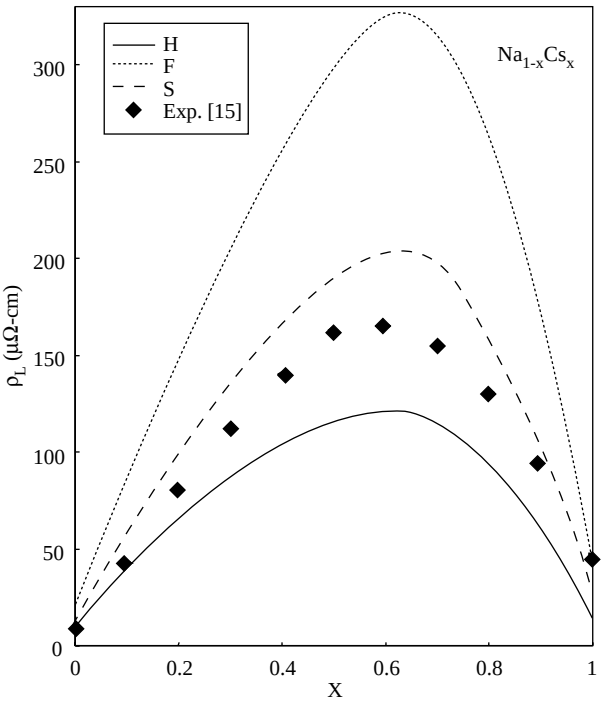

Figure 4. Electrical Resistivity of $Na_{1-x}Cs_x$ binary alloy.

4. Conclusion

The overall picture of the present computations not only confirm the applicability of the model potential for such study of alkali-alkali binary alloys but it also establishes the use of more prominent dielectric functions in the study of electrical transport properties of binary mixtures. Such study on electrical transport properties of other binary liquid alloys and metallic glasses are in progress.

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