OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 1, No. 5, May 2007, p. 227 - 230

Electrical resistivity of Li-based liquid binary mixtures

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The electrical resistivity (ρ_L) of Li-based liquid binary mixtures viz. $Li_{1-X}Na_X$, $Li_{1-X}Mg_X$, $Li_{1-X}In_X$ and $Li_{1-X}Tl_X$ has been studied by model potential formation. The most recent local field correction functions due to Farid et al. and Sarkar et al. are used in the present computations. The values of the electrical resistivity (ρ_L) obtained by Farid et al. local field correction function are higher than those obtained by Hartree and Sarkar et al. local field correction functions. The computed values describe reasonably the experimental data.

(Received after revision March 20, 2007; accepted April 5, 2007)

Keywords: Model potential, Electrical resistivity, Li-based binary mixtures

1. Introduction

During the last several years there has been an increasing interest in the properties of liquid metals and liquid metallic mixtures. Such type of liquids exhibits metallic as well as fluid-like behaviour and hence can help to make a link between the theory of the liquid states and the theory of the electronic states in metals. Therefore, the study of electrical transport properties of liquid metals and their mixtures is of interest either experimentally or theoretically. There exist a large number of calculations for the electrical resistivity of liquid binary mixtures using the model potential formalism. In most of these calculations, well known pseudopotentials have been employed with the conventional dielectric screening functions [1-11]. Recently Vora et al. [10, 11] have reported the electrical resistivities of liquid binaries using model potential formalism. Hence, in the present study, the electrical resistivity of (ρ_L) of $Li_{1-X}Na_X$, $Li_{1-X}Mg_X$, $Li_{1-X}In_X$ and $Li_{1-X}Tl_X$ binary mixtures is investigated with the help of model potential formalism.

The approach of Faber-Ziman [12] is used to study the concentration dependence of the electrical resistivity of Li-based binary mixture. The most recent local field correction functions due to Farid et al. [13] and Sarkar et al. [14] are used to investigate the influence of exchange and correlation effects with reference to the static Hartree [15] screening function.

2. Computational methodology

The Faber-Ziman formula for electrical resistivity of binary mixtures is given by [12]

$$\rho = \frac{3\pi m^2}{4e^2 \hbar^3 n k_F^6} \int_0^\infty S(q) |V(q)|^2 q^3 \, dq \, \theta(2k_F - q) . \qquad (1)$$

where n, the electron density, is related to Fermi wave number b_F and θ is the unit step function that cuts of 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.

This equation (1) is initially applied to the liquid metals only, but, later, was restructured to investigate the resistivity of $A_{1=X} B_X$ liquid binary alloys [1-12]. Hence equation (1) is written as

$$\rho = \frac{3\pi m^2}{4e^2 \hbar^3 n k_F^6} \int_0^\infty \lambda(q) q^3 \, dq \, \theta(2k_F - q) , \qquad (2)$$

with

$$\lambda(q) = (1-X) S_{11} V_1^2(q) + 2\sqrt{X(1-X)} S_{11} S_{22} \, V_1(q) \, V_2(q) + X S_{22} V_2^2(q) . \qquad (3)$$

Here $V_1(q)$ and $V_2(q)$ denote the model potentials for metallic elements A and B. S_{ij}, X are the partial structure factors and concentration of the second metallic component of $A_{1=X} B_X$ mixtures, respectively. Here we have used Ashcroft-Lengreth's [3] formulations to generate the partial structure factor of the binary metallic complexes.

From the rearrangements of the various constants in equation (2), one can write the formula for the electrical resistivity of the binary mixtures in the form

$$\rho_L = \frac{12 \, \Omega_O}{k_F^2} \int_0^{2k_F} \lambda(q) \, q^3 \, dq , \qquad (4)$$

Here Ω_O and k_F are the atomic volume and Fermi wave vector of binary alloys, respectively.

The model potential of Gajjar et al. [10,11,16-18] used to describe the electron-ion interaction in a binary system is given by,

$$W(r) = \frac{-Ze^2}{r_c^3}\left[2-\exp\left(1-\frac{r}{r_c}\right)\right]r^2 \ ; \ r \le r_c$$
$$= \frac{-Ze^2}{r} \ ; \ r \ge r_c \quad . \qquad (5)$$

We denoted by r_C the parameter of the potential and Z the valence of binary mixtures. This form has 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 [10,11,16-18].

The mathematical expressions of three local field correction functions proposed by Farid et al. [13], Sarkar et al. [14] and Hartree [15] used in the present computations to see the effect of exchange and correlation are as follows:

$$f_F(q) = A_F Y^4 + B_F Y^2 + C_F + \left[\left(A_F Y^4 + B_F Y^2 + C_F\right)\left(\frac{4-Y^2}{4Y}\right)\ln\left|\frac{2+Y}{2-Y}\right|\right], \qquad (6)$$

$$f_S(q) = A_S\left(1-\left\{1+B_S Y^4\right\}\exp\left\{-C_S Y^2\right\}\right), \qquad (7)$$

and

$$f_H = 0. \qquad (8)$$

We denoted by $Y = q/k_F$ and q is the wave vector. A_F, B_F, C_F, D_F, A_S, B_S and C_S are the atomic volume dependent parameters of F and S-local field correction functions. The mathematical expressions of these parameters are given in [13, 14].

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 [19-22]. The computed results of electrical resistivity are displayed in Figs. 1-4.

Table 1. The input parameters and constants.

T (K)	Metal	Ω (a. u.)	η	σ (a. u.)	r_c (a. u.)
500	Li	161.54	0.3730	4.864	2.5435
	Na	312.99	0.3492	5.932	2.1679
651	Li	166.31	0.3432	4.777	2.5679
	Mg	173.22	0.4869	5.441	1.6679
651	Li	166.31	0.3432	4.777	2.5679
	In	193.82	0.4724	5.592	1.4266
800	Li	170.21	0.3200	4.703	2.5881
	Tl	223.31	0.2801	4.925	1.4625

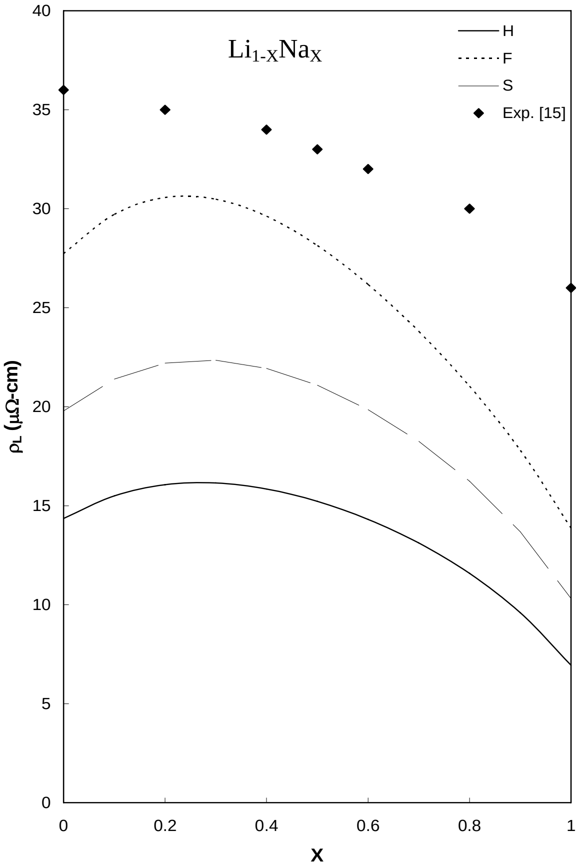

Fig. 1. Electrical resistivity of $Li_{1-X}Na_X$ binary mixture.

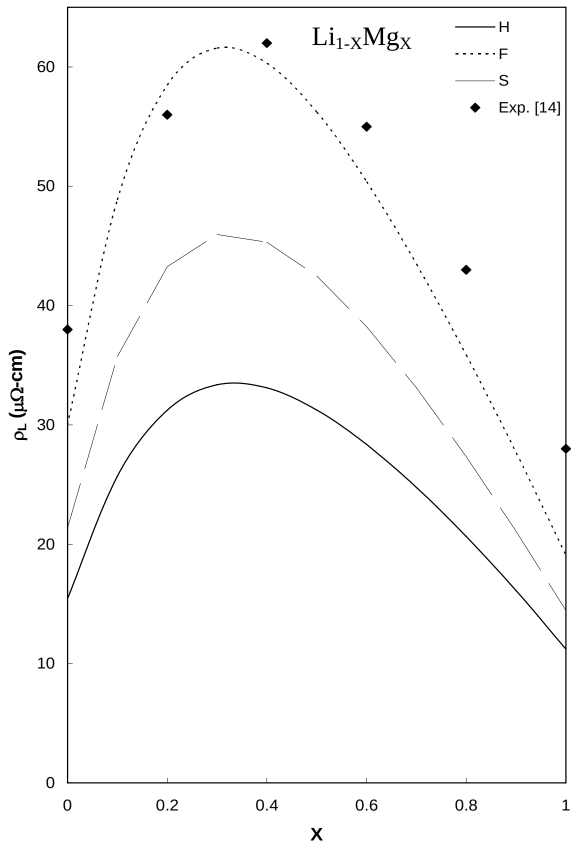

Fig. 2. Electrical resistivity of $Li_{1-X}Mg_X$ binary mixture.

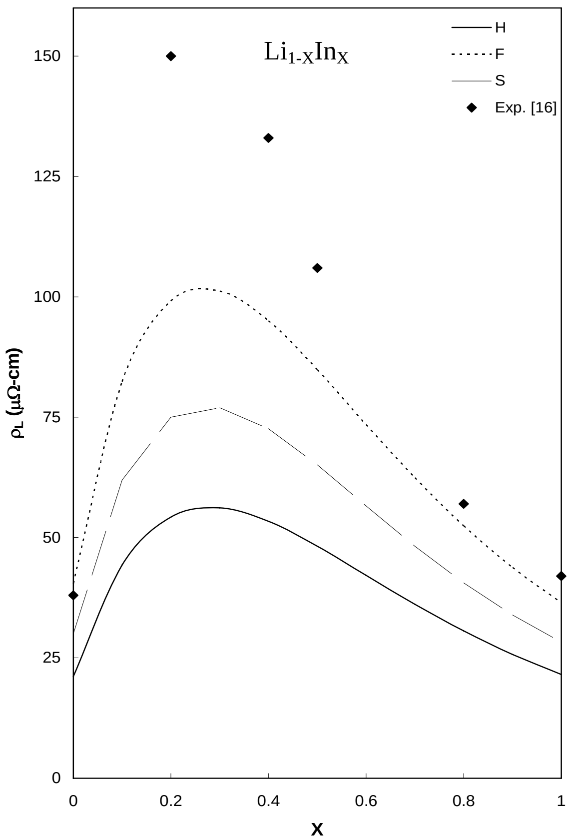

Fig. 3. Electrical resistivity of $Li_{1-X}In_X$ binary mixture.

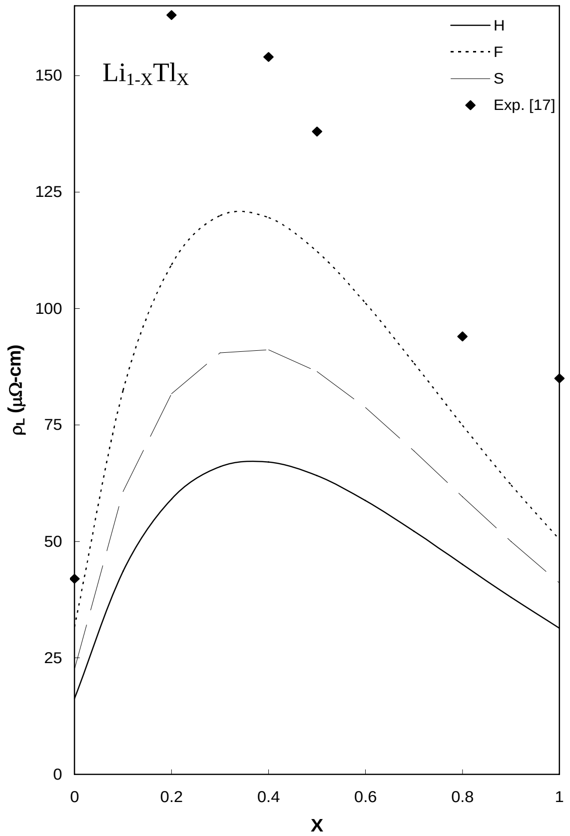

Fig. 4. Electrical resistivity of $Li_{1-X}Tl_X$ binary mixture.

The concentration dependence of the electrical resistivity (ρ_L) is examined by varying x = 0 to x = 1 in the step size of 0.1. Most fascinating screening functions of Farid et al. [13] and Sarkar et al. [14] are used in the present study to study the screening influence with respect to static Hartree [15] local field correction function. The present values of the electrical resistivity (ρ_L) for $Li_{1-x}B_x$ (B: Na, Mg, In, Tl) of binary mixtures viz. $Li_{1-x}Na_x$, $Li_{1-x}Mg_x$, $Li_{1-x}In_x$ and $Li_{1-x}Tl_x$ mixtures are shown together with the experimental results [19-22] in Figs. 1-4. As concentration x of the 'B' element increases the electrical resistivity (ρ_L) increase and reaches the maximum value, after that the further increases in x decrease the electrical resistivity (ρ_L) of the system. From the Figs. 1-4 it can be seen that, the present yielding generated from F-local field correction function for $Li_{1-x}Na_x$, $Li_{1-x}In_x$ and $Li_{1-x}Tl_x$ binary mixtures show lower values while those for $Li_{1-x}Mg_x$ mixture shows fair agreement both in magnitude and gradient in comparison with experimental data [19-22]. There is a reasonable agreement found in the values of the electrical resistivity (ρ_L) of $Li_{1-x}Tl_x$ and $Li_{1-x}In_x$ liquid binaries with experimental data [19-22]. The presently electrical resistivity (ρ_L) computed from H-local field correction function show lower values, those determinated by form F-function have higher values for all binary mixtures, while the outcomes due to S- local field correction function lie between these two local field correction function.

The good agreement may be indicative of the free electron behaviour of these mixtures in the whole concentration range. Here also, the calculated electrical resistivities of the lithium systems increase like alkali-alkali systems. The peak of the curve increases with the increase of their electronegativity differences. The present study indicates the free electron behaviour of the mixtures in the whole composition range and all the constituent atoms are randomly distributed in the system.

The relative influence of F and S-local field correction function with respect to H-dielectric function on the computed electrical resistivity of binary mixtures is 60.61% - 94.09% and 28.96%-48.57%, respectively. These two observations suggest that the proper choice of local field correction function is essential for the study of the electrical transport properties of binary system.

The is a fitting formula of Farid et al. [13] for the dielectric screening function of the degenerate electron liquids at metallic and lower densities, accurately reproduces the Monte-Carlo results as well as it also satisfies the self consistency condition in the compressibility sum rule and short range correlations. In the formula of Farid et al. [13], many parameters are included; Sarkar et al. [14] have proposed a simple form of local field correction function with less numbers of parameters. Hence the obtained values with Farid et al. [13] local field correction function are in closer agreement with experimental data than with Sarkar et al. [14] one.

4. Conclusion

The overall picture of the present computations confirms not only the applicability of the model potential for the present study of the aforesaid properties of Li-based binary mixtures but it also establishes the use of more prominent local field correction function in the study of electrical transport properties of binary mixtures.

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