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Electrical Transport Properties of Liquid $Li_{1-x}Cs_x$ Alloy

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ABSTRACT

The current article represents the electrical transport properties namely electrical resistivity (ρ), thermal conductivity (σ) and thermoelectric power (Γ) of liquid alkali $Li_{1-x}Cs_x$ alloy using pseudopotential theory. The electron-ion interaction is estimated through the model potential given by Fiolhais*et al.*. A very famous PercusYevick(PY) hard sphere reference system[2]is used for the structure factor calculation of the liquid alloy under the study. For the very first time, the current study represents the effect of total eight local field correction functions (due to Hartree (H), Hubbard and Sham (HS), Nagy (N), Vashishta-Singwi (VS), Taylor (T), Sarkar *et al.* (S), Ichimaru-Utsumi (IU)and Farid*et al.* (F)[3-10]) with this universal potential in the PY hard sphere reference system. The numerical value and the trend for all three transport properties obtained through this study are in a good agreement with that of the other theoretical calculated values[3] and experimental available data.

KEYWORDS: Pseudopotential theory, Electrical properties, Liquid alkali alloy.

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INTRODUCTION

The $Li_{1-x}Cs_x$ alloy differs structurally than the other alkali alloys, as it is having large difference in the ion radius. This makes the alloy very difficult to predict theoretically via model potential.Nearly free electron theory given by Ziman[13, 14] is found successful for the resistivity (ρ)calculation of the liquid metal[3-8]. The extension of the theory for the liquid alloys has been given in the form of Faber-Ziman theory[15]. To represent the electron-ion interaction the very transferable model pseudopotentialgiven by Fiolhais*et al.*[1]has been used. To estimate the exchange and correlation effect with different functions, total eight local field correction functions due to Hartree (H) , Hubbard-Sham (HS), Nagy (N), Ichimaru-Utsumi (IU),Vashishta-Singwi (VS), Sarkar *et al.* (S), Taylor (T) and Farid*et al.* (F) are employed[3-8]. The whole study of the electrical transport properties has been carried out under the PY hard sphere reference system[2]which is already proven successful for calculation of the said properties of alloys[3-5].The main goal of the present research is to find an ideal potential which can be employed for the thorough electrical study of liquid alloy without any kind of parameter fitting. This aim is achieved with the help of potential of Fiolhais*et al.*and their co-workers[1]. The form of the potential used is as given in reference[1]. Out of the two available choices of the parameters (Universal parameters and individual parameters) the set of first one is used in this study. To provide a detailed platform to the researchers, apart from electrical resistivity(ρ), thermal conductivity(σ) and thermo electric power(Γ) are also included in the article.

COMPUTATIONAL METHODOLOGY

The expression for the electrical resistivity of an alloy according to the Faber-Ziman theory can be given by[3, 15],

$$\rho = \frac{3\pi m^2}{4Ze^2h^3nk_f{}^6}\int_0^\infty q^3dq(x_1V_1{}^2S_{11} + 2(x_1x_2)^{1/2}V_1V_2S_{12} + x_2V_2{}^2S_{22})\theta(2k_f - q), \quad (1)$$

Where V_i and S_{ij} stand for screened potential for element 1 and 2 and partial structure factors respectively. $\theta$is unit step function and it is used to cut off the integration at $2k_f$ at sharp Fermi surface.

The thermo electric power can be written as[3-4, 6-10],

$$\Gamma = -\left(\frac{\pi^2k_B^2T}{3|e|E}\chi\right)\Bigg|_{E=E_F} \quad (2)$$

Where,

$$\chi = 3 - \frac{2S(2k_f)V^2}{\left\langle S(q)\left|V(q)^2\right|\right\rangle}. \qquad . \qquad (3)$$

The temperature gradient can cause the heat transfer in the liquid. This thermal conductivity can be obtained from the following equation[3-4, 6-10],

$$\sigma = \frac{\pi^2 k_B^2 T}{3e^2\rho}. \qquad (4)$$

RESULTS AND DISCUSSION

Table 1 shows the input parameters and constants used in the computation of the electrical transport properties, in which Z, **Ω,** K_f are respectively valance, volume and Fermi wave vector.

Table No. 1: "Input parameters and constants"

Metal	Ω (a.u.)	K_f(a.u.)	α(a.u.) [1]	R(a.u.)[1]
Li	146.46	0.5768	3.549	0.361
Cs	757.73	0.3233	2.692	0.920

Table No. 2: "Electrical resistivity (μΩ-cm) of $Li_{1-x}Cs_x$"

x	H	HS	N	IU	VS	SS	T	F	Others [3]	Expt. [3, 11,12]
0.0	6.49	8.16	12.34	12.07	9.87	9.10	11.14	12.24	21.87,33.09,27.09	24.70
0.1	8.82	11.64	18.89	19.16	14.94	13.55	17.39	19.50	-	-
0.2	16.22	20.99	34.67	33.52	26.59	24.23	30.60	34.10	-	-
0.3	28.13	35.83	61.15	55.06	44.64	40.86	50.58	55.95	-	-
0.4	42.34	53.78	95.36	82.37	67.04	61.31	75.74	83.73	-	-
0.5	48.61	63.02	115.12	103.57	81.70	73.85	94.47	105.67	-	-
0.6	59.56	77.85	147.51	131.50	102.66	92.21	119.63	134.38	-	-
0.7	67.94	89.66	175.78	156.58	120.64	107.55	142.06	160.34	-	-
0.8	70.04	93.34	189.05	168.47	128.12	113.34	152.62	172.90	-	-
0.9	57.00	76.74	160.83	142.01	107.03	93.98	128.69	146.02	-	-
1.0	12.79	17.35	44.54	24.49	21.62	19.24	22.67	24.56	37.05,50.65,72.83	36.00

The electrical resistivity(ρ) of the $Li_{1-x}Csx$ alloy calculated with various correction functions is as shown in the Table 2. The resistivity(ρ) of the alloy $Li_{1-x}Cs_x$ is compared with the theoretical available other result[3] for two extreme nodes of the concentration (x) related to metal and with experimental data[3, 11,12]. It can be observed from the Table 2 that a qualitative agreement between the presently calculated results and the above compared both results for lower value of concentration (x).

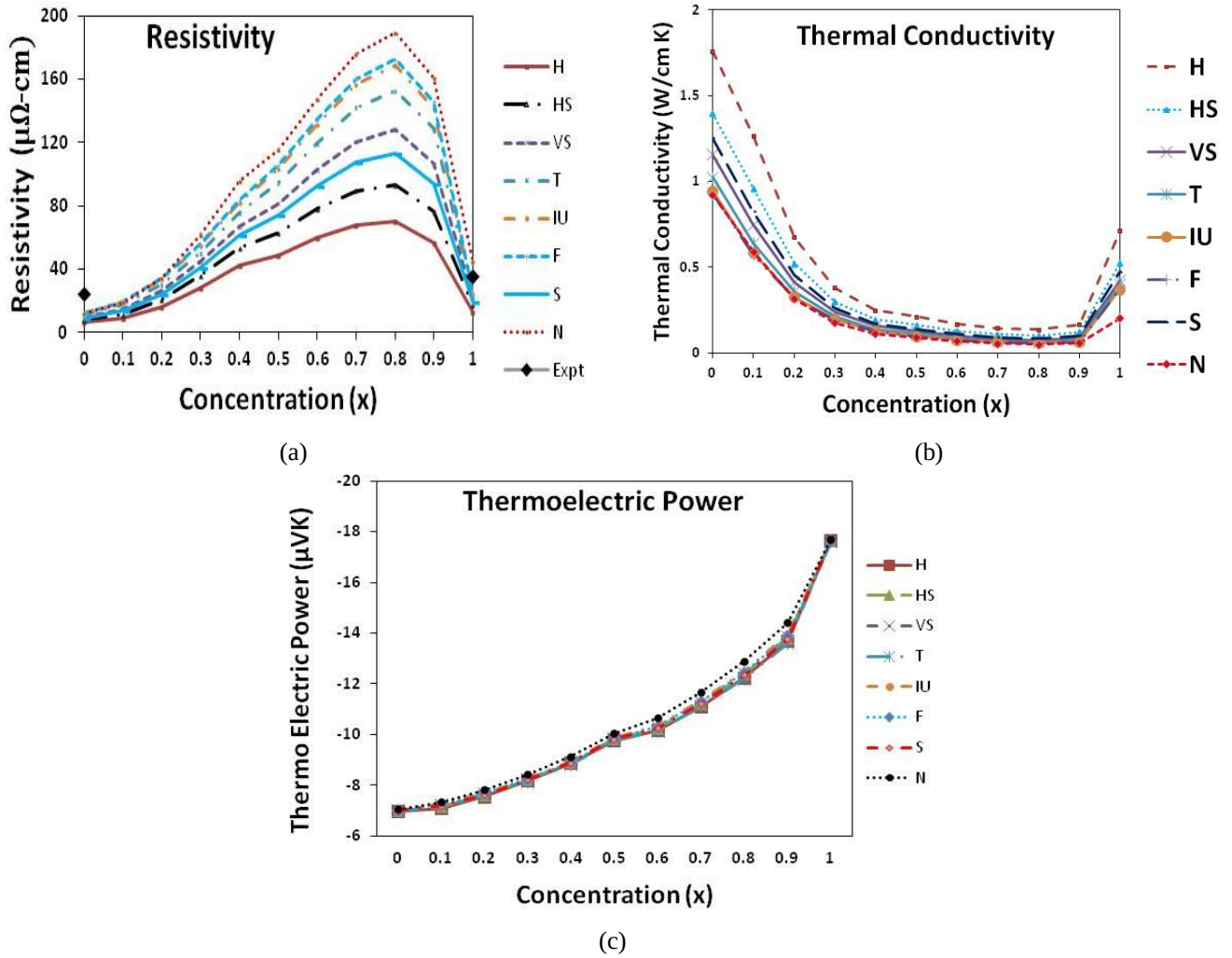

Figure 1. Variation in (a) Resistivity (ρ), (b) Thermal Conductivity(σ)and (c) Thermoelectric power $(\Gamma)$with respect to concentration (x)

Fig. 1(a) depicts the trend of the variation in resistivity (ρ) with respect to concentration (x). The resistivity (ρ) is found minimum for lowest and highest concentration values (x) and increase for the intermediate concentration (x). The Large influence of local field correction function with respect to static Hartree dielectric function (H) is observed for resistivity values. Fig. 1(b) shows the thermal conductivity variation at various concentrations (x) for all of eight local field corrections. The maximum

values of the thermal conductivity (σ) are obtained for the correction function due to H, whereas the minimum is obtained for the correction functions due to N for all the concentration values (x). The thermoelectric power(Γ) for the alloy under the study is presented in Fig. 1(c). The continuity in Fig. 1(a) and Fig. 1(b) follows the same type of trend as obtained for the other alkali based binary alloys proves the sound efficiency of the adopted method for the study, particularly, of $Li_{1-x}Cs_x$ alloy.

CONCLUSIONS

The electrical transport properties of very rarely predicted liquid alkali binary alloy $Li_{1-x}Cs_x$ has been studied using pseudopotential theory. Total eight different local field correction function are employed to get the exchange and correlation effect. The results for electrical resistivity(ρ) obtained in the current calculation agreed with the results of others[3] and experimental available data[3,8, 9]for many of the correction functions. The trends of variation of thermal conductivity (σ)as well as thermoelectric power (Γ) are found same for all the correction functions. Through this work, the Fiolhais*et al.*[1]potential is proven applicable for investigation of the electrical transport properties the alloy liquid alloy under research.

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