CONCENTRATION DEPENDENT ELECTRICAL TRANSPORT PROPERTIES OF Co-Cr BINARY ALLOYS AT VARIOUS TEMPERATURES

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Abstract: The concentration dependent electrical transport properties viz., electrical resistivity, thermo electrical power and thermal conductivity of Co-Cr binary alloys at various temperatures (800, 1000, 1200 K) are studied. In the present work, electrical resistivity is calculated according to Faber-Ziman model, combined with the Ashcroft-Langreth partial structure factors and within our potential formalism. Five different forms of exchange-correlation functions due to Hartree (H), Taylor (T), Ichimaru and Utsumi (IU), Farid et al (F) and Sarkar et al (S) are used to the local field correction. The present results of electrical resistivity due to S function are in good agreement with experimental data as compared to results obtained using other functions. The S function, which satisfies the compressibility sum rule in long wave length limit more accurately as compared to T, IU and F functions which may be responsible for the better agreement of results, obtained using S function. In the absence of experimental data of thermal conductivity of Co-Cr alloys, we are not putting any concrete argument, but our predicted results may be useful for further research in this direction. Present results confirms that the present model potential along with the S function is able to determine correctly the electrical transport properties of Co-Cr alloys at various temperatures.

Keywords: liquid alloys, electrical resistivity, pseudopotential, exchange and correlation function.

Introduction: The theoretical study of electronic transport properties of transition metals and their alloys has been of considerable interest [1] for many years within pseudopotential formalism. So that a large amount accepted method for studying the electronic transport properties of transition metals alloys is the electrical conduction theory developed by Ziman formulation[1-2]. This concept has been very useful over the last few decades for transition metals alloys [1-4].

As is known, Co-Cr transition metal (TM-alloy) alloys based on the iron –subgroup metal take up a special interest in modern technology [5-6], since they are important starting material for many industrial applications. The aim of this study is to determine principal regularities in the variation of the electrical resistivity and thermal conductivity of cobalt–chromium alloys at various temperatures [5]. So, that in the present study, we have investigated theoretically, concentration dependent electrical resistivity and thermal conductivity of Co-Cr alloy with the help of pseudopotential formalism combined with FZ formulation.

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

$$V_b(q) = \frac{-4\pi Z e^2}{\Omega q^2}\left[\cos(q r_c) - \frac{q^2 r_c^2}{1+q^2 r_c^2}\right] \quad (1)$$

Here Z, Ω, 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 Co and Cr have been determined following the procedure of Heine and Weaire [8,9]. The approach of Faber and Ziman [2-4] is used to study the concentration dependence of the electrical resistivity of liquid binary mixture [8-11]. In the present computation of electrical transport properties of liquid binary alloys, the local field correction functions due to Hartree (H) [12], Taylor (T) [13], Ichimaru and Utsumi (IU) [14], Farid et al (F) [15] and Sarkar et al. (S) [16] are employed for the investigation of exchange and correction effects.

The electrical resistivity for binary alloys in Faber and Ziman [3] formulation is given by,

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

Where, n is the electron density related to the Fermi wave number, θ the unit step function that cuts off the q integration at $2k_F$ corresponding to a perfectly sharp 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:

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

With

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

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[5], x is the concentration of second metallic component of $A_{1-x}B_x$ mixture.

It is well known that, if temperature gradient applied to metal then the conduction electron will carry a heat. Even though an electric current is prevented from flowing and that indeed they are responsible for the major part of the thermal conductivity, the expression can be written as [8-9]

$$\sigma_L = \frac{\pi^2 k_B^2 T}{3 e^2 \rho_L} \quad (5)$$

Here, e, E_F, T, and k_B are the electronic charge, Fermi energy, temperature in Kelvin and the Boltzmann's constants.

Results and Discussion: The constants and parameters used in the computations are tabulated in the table 1. The computed electrical resistivity along with experimental data and five different local field correlation functions due to Ichimaru-Utsumi [9], Farid et al [10] and Sarkar et al [11] are used to judge screening influence with reference to the more commonly employed dielectric functions of Taylor [13] and Hartree [12] are shown in figure 1, 2 and 3 for Co-Cr at different temperatures. In addition packing fraction of binary alloys kept at 0.45. From the figures 1-3 it is seen that, the present results for Co-Cr at different temperature due to Sarkar et al [16] and Hartree [12] local field correction function is found to be good agreement with the experimental results and The computed results of electrical resistivity using the local field correction functions namely T, IU and F functions are very high compared to experimental data. The relative percentile deviation of Hartree and Sarkar et al local field correlation function with respect to experimental data is at 800K temperature, they are 17.073%-7.493% and 37.45%-17.56% respectively, at 1000 K, 6.54%-9.42% and 24.701%-19.391% respectively and for 1200K temperature 23.07%-8.342% and 0.74%-24.247% respectively. The calculated values of the electrical resistivity yield the desired nature both in magnitude and gradient. The experimental value of resistivity dependence shows asymmetry with respect to Co -50% at Cr concentration. The experimental resistivity curve shows its maxima at Co- 65% at Cr alloys and present results due to five different local field correction function shows the maximum at Co-50% at Cr alloy and also ρ_L dependence the symmetry behaviours with respect to Co-50% at Cr concentration.

Table 1. Input parameters and constant used in the calculation.

Input	T=800K		T=1000K		T=1200K	
	Co	Cr	Co	Cr	Co	Cr
σ (au)	4.075	4.160	4.1074	4.185	4.1414	4.2056
Ω (au^3)	78.7057	84.054	80.6282	85.2880	82.6469	86.5350
r_c (au)	1.35584	1.3858	1.36679	1.3743	1.37811	1.39947

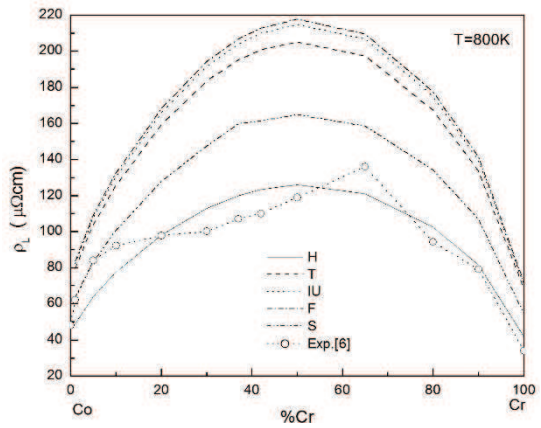

Fig 1. Electrical resistivity of $Co_{(1-x)}Cr_{(x)}$ alloy at T= 800

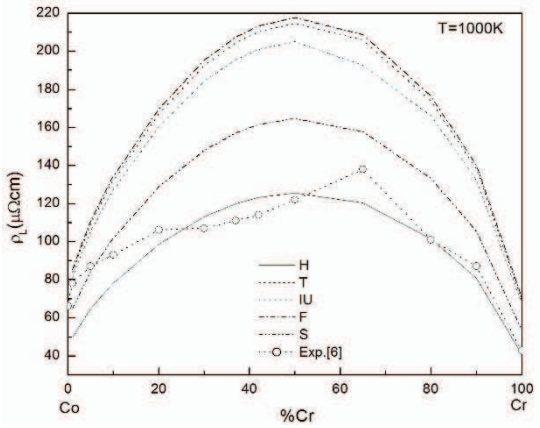

Fig 2. Electrical resistivity of $Co_{(1-x)}Cr_{(x)}$ at T= 1000 K

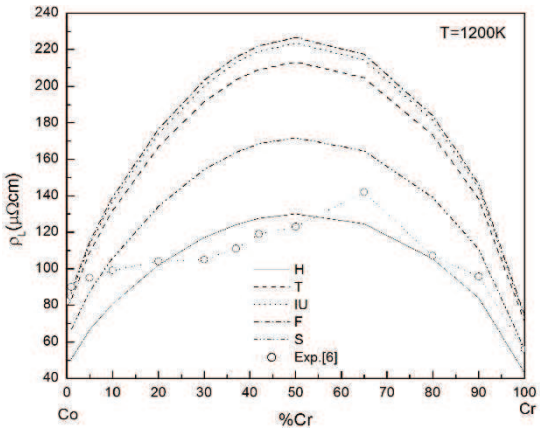

Fig 3. Electrical resistivity of $Co_{(1-x)}Cr_{(x)}$ alloy at T= 1200 K

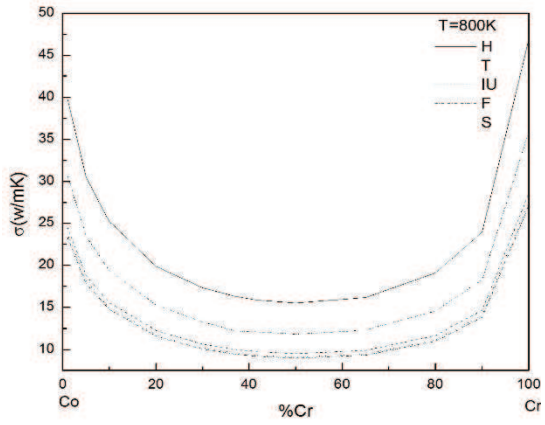

Fig 4. Thermal conductivity of $Co_{(1-x)}Cr_{(x)}$ alloy at T= 800 K

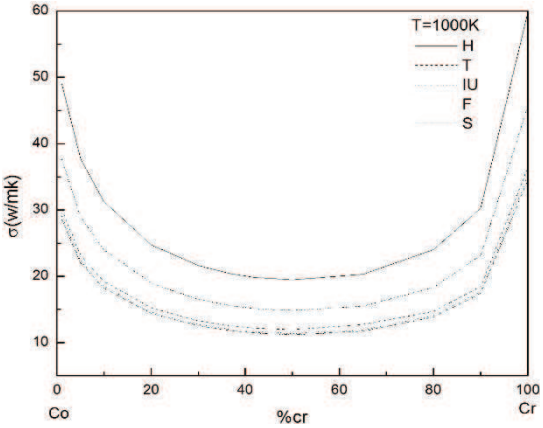

Fig 5. Thermal conductivity of $Co_{(1-x)}Cr_{(x)}$ alloy at T= 1000 K

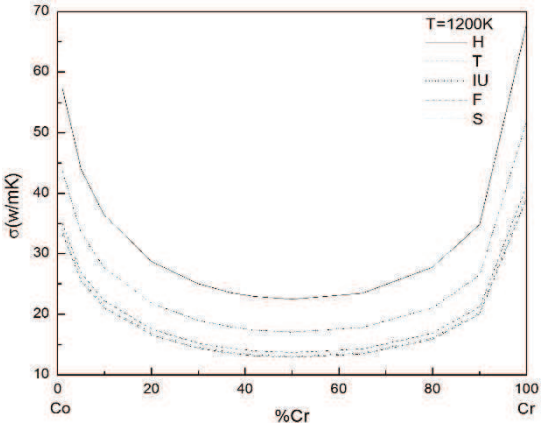

Fig 6. Thermal conductivity of $Co_{(1-x)}Cr_{(x)}$ alloy at T= 1200 K

In comparison with the presently computed result of the Thermal conductivity (σ) from static H-function, the percentile influence at different temperature for Co_x-Cr_{1-x} alloys of T, IU, F and S functions are the order of the respectively at 800K, respectively at 1000K and respectively at 1200K. The results of electrical resistivity computed with H and S achieve the good agreement with the experimental result. The results of electrical resistivity computed with other three functions namely T, IU and F functions are very high compared to experimental data. Accordingly, results of thermal conductivity using these three functions are very low compared to experimental data. These observations suggest that the proper choice of exchange and correlation function is essential for the study of the electrical transport properties of binary system.

Conclusion: The calculated electrical resistivity shows symmetrical behaviour with respect to Cr concentration. The presently computed isotherm of electrical resistivity is in accordance with the experimental results. The results of electrical resistivity and thermal conductivity obtained using S function show good agreement with experimental results at low and high Cr concentration. Near equi-atomic composition, presently obtained results using H function are in good agreement with experimental data. So, it can be concluded that the exchange-correlation effects play important role in determining transport properties of the alloys and the overall picture of the present computation thus, confirms not only applicability of our model potential for study of the electric resistivity and thermal conductivity of binary alloys but it also establishes the use of more prominent dielectric functions in the study of electric transport properties of such liquid binary mixtures.

Acknowledgments: The authors BYT is thankful to UGC for providing financial support under major research project.

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