

ELECTRICAL TRANSPORT PROPERTIES OF Ni-Cr BINARY ALLOYS

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Abstract. *Electrical transport properties viz. electrical resistivity and thermal conductivity of Ni-Cr binary alloys are determined by our recognized single parametric potential model in a wide range of Cr concentration. In this work, screening functions of Ichimaru and Utsumi, Farid et al. and Sarkar et al. are employed along with the Hartree and Taylor functions to study the relative influence of the exchange and correlation effect. The Ni-Cr liquid alloys are studied as a function of their composition at three different temperatures ($T=800\text{K}$, 1000K , 1200K). The present finding of electrical resistivity agrees within 2-12% with experimental findings when the H dielectric function is employed.*

Keywords: Liquid alloys, Electrical resistivity, Pseudopotential, Exchange and correlation effects.

I. INTRODUCTION

The electrical transport properties of liquid metals and their alloys are of immense important theoretically as well as experimentally because of increasingly manifold interests of not only physicists but also chemists. During last three decades numbers of efforts are made to study electrical transport properties of liquid metals and their alloys. The Faber-Ziman [1-4] model remain successful in predictive the electrical transport properties of binary. Thakore et al. [3-4] have successfully reported that the structures and electrical transport properties using Ashcroft and our well established local model potential for different binary alloys Al-Cu and Sn-Sb, respectively. Very recently, we carefully computed the electrical resistivity and thermal conductivity of liquid Ni-Cr at 1400K [5]. We have also reported that electrical transport properties using the nearly free electron theory developed by Faber and Ziman formalism, along with a well established potential model [3-5].

As, it is known that Ni-Cr transition metal (TM-alloy) alloys based on iron –subgroup metal take up a special interest in modern technology [6]. Since, they are important starting material for many industrial applications and manufacture of surgical implant. Glagoleva et al [6] have measured experimentally electrical resistivity and thermal conductivity at various temperatures. They have found that the electrical transport properties more sensitive at high temperature. In the present work, we report the results of our theoretical study of electrical transport properties of liquid alloy Ni-Cr. The objective of the paper is of two fold: one is to study the influence of the screening functions and the second is to study the temperature effect. For these, five different form of the local field correction functions are used and three different temperatures T=800K, 1000K, 1200K are considered.

II. COMPUTATIONAL METHOD

The electrical resistivity for binary alloys in Faber and Ziman [1, 2] formulation is given as,

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

where, n is the electron density related to the Fermi wave number, θ the unit step function that cuts off the \mathbf{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. To incorporate the electron-ion interaction we have used Gajjar's recognized model potential [5, 7]. In momentum space the unscreened bare-ion form factor is given by [5, 7],

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

Here Z , Ω , q , e and r_c are the valency, atomic volume, wave vector, charge of the electron and the parameter of the potential, respectively. The approach of Faber and Ziman [1-2] is used to study the concentration dependence of the electrical resistivity of liquid binary mixture [6]. In the present computation of electrical transport properties of liquid binary alloys, the local field correction functions due to Hartree (H) [8], Taylor (T) [9], Ichimaru and Utsumi (IU) [10], Farid *et al.* (F) [11] and Sarkar *et al.* (S) [12] are employed for the investigation of exchange and correction effects. Hartree function does not involve any kind of exchange and correlation effects. While, other four functions are satisfied compressibility sum rule and they have been used earlier by many researchers to analyse various physical, electrical and magnetic properties of liquid metals and their alloys [3-6]. The parameters of the model potential for pure Ni and Cr have been determined using $q = q_0$ condition. Hence, the present study does not include any kind of fitting process. On the rearrangements of the various constants, one can write the formula (1) for the electrical resistivity of the binary alloys in the following form:

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

with

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

Here, $V_1(q)$ and $V_2(q)$ are denoted as the screened form factors for elements A and B , $S_{ij}(q)$ are the Ashcroft-Langreth partial structure factors of the binary metal complexes [6], x is the concentration of a second metallic component of the $A_{1-x}B_x$ mixture.

When the temperature gradient applied to metal, 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 for conductivity is written as [3, 4]

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

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

III. RESULTS AND DISCUSSIONS

The input parameters used in the present computations are presented in Table 1. Moreover, packing fraction of liquid binary alloys is kept at 0.45. The concentration dependence of the electrical resistivity at three different temperatures are examined by varying the Cr concentration from $x = 0$ to $x = 1.0$ ($x = 0, 0.05, 0.1, 0.2, 0.3, 0.5, 0.65, 0.9, 0.95, 1.0$).

Table 1. Input parameters used in the calculation

Input	T=800 K		T=1000 K		T=1200 K	
	Ni	Cr	Ni	Cr	Ni	Cr
$\sigma(\text{au})$	4.05139	4.16	4.07713	4.185	4.1035	4.2056
$\Omega(\text{au}^3)$	77.3345	84.054	78.8589	85.288	80.4014	86.55
$r_c(\text{au})$	1.348	1.3858	1.3570	1.3930	1.3655	1.3990

Figs. 1-3 represent the computed values of electrical resistivity for Ni-Cr alloy at 800 K, 1000 K and 1200 K, respectively. From the Figs. 1-3 it is seen that, among five employed local field correction functions, H gives the minimum numerical value of the electrical resistivity, while the local field correction functions due to F gives the maximum value. In the present findings of the electrical resistivity of Ni-Cr binary alloy due to T , IU and S local field correction functions are laying between H and F functions. The results due to H and S functions show comparable agreement with experimental results among all five local field correction functions. At 800K temperature, the deviation in the electrical resistivity with experimental values is 10.58-3.77%, 76.86-56.17%, 83.60-63.76%, 85.83-66.0% and 41.27-21.92% of H , T , IU , F and S functions, respectively. At 1000 K, such deviation is found as 5.24-2.31%, 59.23-54.04, 66.69-59.28%, 69.0-62.0% and 25.0-28.15% of H , T , IU , F and S functions, respectively. For 1200K temperature, such deviations are 12.98-2.5%, 59.39-41.72%, 66.89-46.88%, 69.24-49.03% and 12.90-24.015% from experimental data is observed for H , T , IU , F and S functions, respectively. From Fig. 1-3, it is also seen that as the temperature of binary liquid increases, the electrical resistivity also increases favorite metallic behavior of binary mixture Ni-Cr over the full range of concentration.

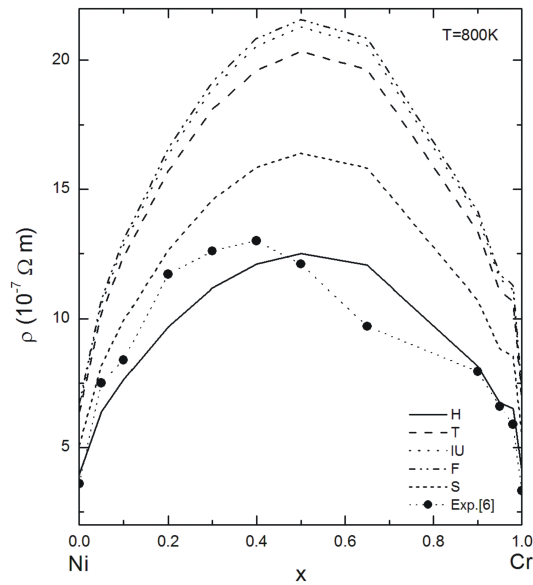


Fig. 1. Electrical resistivity of $\text{Ni}_{1-x}\text{Cr}_x$ alloy at $T = 800 \text{ K}$

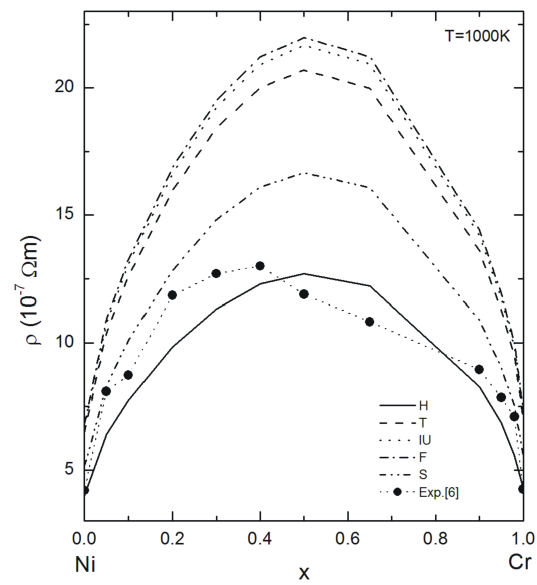


Fig. 2. Electrical resistivity of $\text{Ni}_{1-x}\text{Cr}_x$ alloy at $T = 1000 \text{ K}$

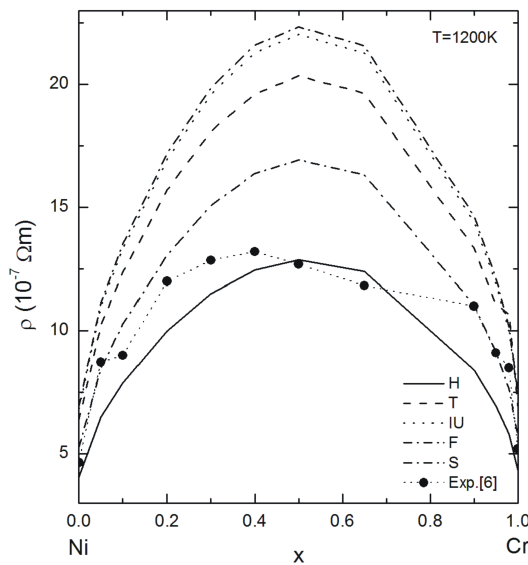


Fig. 3. Electrical resistivity of $\text{Ni}_{1-x}\text{Cr}_x$ alloy at $T = 1200 \text{ K}$

In Figs. 4-6, thermal conductivity of binary Ni-Cr alloy is shown along with the experimental results [6]. For $0 < x < 1$, the thermal conductivity of binary mixture $\text{Ni}_{1-x}\text{Cr}_x$ is found to be lower than the thermal conductivity of pure components Ni, Cr. Moreover, H gives the maximum value of the thermal conductivity; while the screening functions F gives the minimum value the conductivity of the Ni-Cr alloy in comparison to other screening functions.

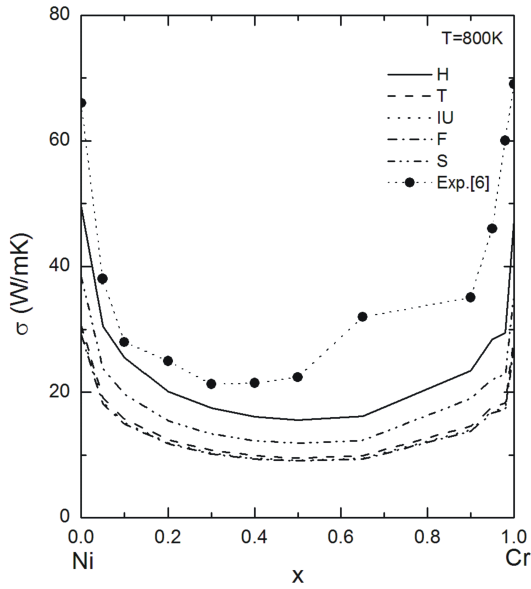


Fig. 4. Thermal conductivity of $Ni_{1-x}Cr_x$ alloy at $T = 800$ K

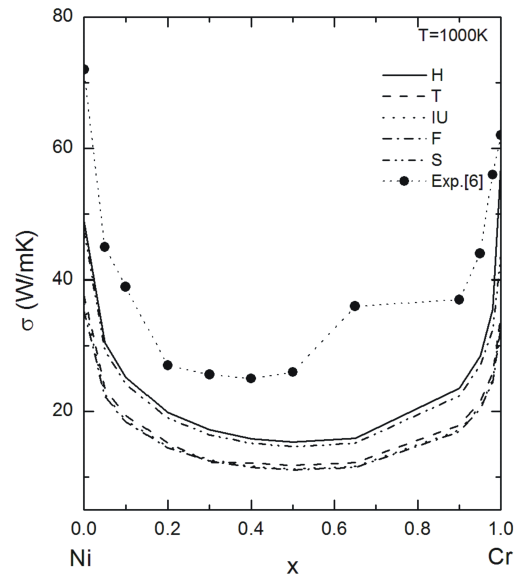


Fig. 5. Thermal conductivity of $Ni_{1-x}Cr_x$ alloy at $T = 1000$ K

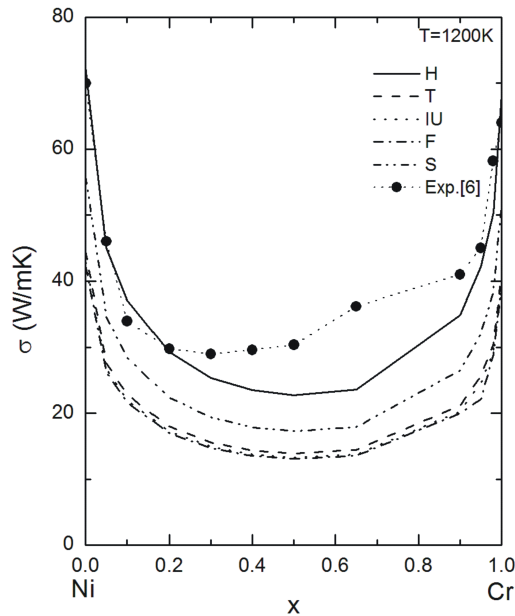


Fig. 6. Thermal conductivity of $Ni_{1-x}Cr_x$ alloy at $T = 1200$ K

In the case of thermal conductivity, deviation with respect to experimental data is found in the H, T, IU, F and S screening functions and the values are 24.71-22.02%, for H screening function, 55.30-53.50% for T screening function, 56.99-55.10% for IU screening function, 57.32-55.80% for F screening function and 44.13-41.84% for S screening function for $Ni-Cr$ alloy at

$T = 800$ K. Similarly, at 1000K, such deviations found are 38.52%-20.37%, 52.88-47.62%, 55-49.33%, 55.6-50.89% and 41.44-34.20% for H , T , IU , F and S functions, respectively. At 1200K temperature, such deviations are 23.69-3.37%, 52.03-36.33%, 54.17-38.77%, 54.82-39.64% and 40.38-20.32% for H , T , IU , F and S functions, respectively.

The computed values of the electrical transport properties viz. the electrical resistivity and thermal conductivity is found to be quite sensitive to the selection of the appropriate screening functions.

The screening function due to IU and F shows the peak around the $q \approx 2k_f$, so that the present results of electrical resistivity give higher value than the other screening function. The S function is obtained very mild peak around the $q \approx 2k_f$. Hence, it can be said that the S function gives very good results compared with the IU and F functions. Overall, the results of electrical transport properties computed here for Ni-Cr binary mixture suggests that the proper choice of exchange and correlation function is essential for the study of the electrical transport properties of binary system.

IV. CONCLUSION

At last we conclude that electrical transport properties of $Ni_{1-x}Cr_x$ alloys due to H and S local field correction functions are found to be in good agreement with experimental results. The S function, which satisfies the compressibility sum rule in the long wavelength limit more accurately as compared to T , IU and F functions and hence gives better results. Thus, the present computation confirms not only applicability of our model potential for the 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 electrical transport properties of such liquid binary mixtures.

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