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Electrical Transport Properties of Amorphous $Ni_{13}Pd_{67}P_{20}$ Alloy

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Abstract *– The theoretical study of electrical transport properties viz. electrical resistivity, thermo -electrical power (TEP) and thermal conductivity is performed in the present work using newly proposed potential. Five different forms of screening functions have been employed to incorporate the exchange and correlation effects. The structure factors due to hard core fluid theory are used for the computation of transport properties. The present results of transport properties are compared with the experimental results are discussed.*

Keywords*: Liquid alloys, Electrical resistivity, Pseduopotential*

I. Introduction

The electrical transport properties of the liquid ternary alloys have found great interest during the last several years. The study of electrical transport properties of liquid alloys remains one of the favorite quantities experimentally as well as theoretically [1-3].Liquid alloys of noble metals with polyvalent metals show non-linear concentration dependence of physical properties. They show maximum electrical resistivity at particular concentration [4]. Recently Philippe Maitrepierre et al [5] successfully reported the temperature dependent electrical resistivity liquid Ni13Pd67P20 ternary alloy. In the present work, we have reported the partial structure factor at equi-atomic concentration and electrical resistivity of liquid Ni13Pd67P20 ternary alloy at room temperature.

II. Theory and Method of Computation

The total structure factor for quaternary liquid alloys have been calculated through [6]

$$\begin{aligned} S(q) &= x1\ S_{11}(q) + x2\ S_{22}(q) \\ &+ S3\ S_{33}(q) + 2\sqrt{x1x2}\ S_{12}(q) \\ &+ 2\sqrt{x1x2}\ S_{13}(q) + 2\sqrt{x2x3}\ S_{23}(q) \end{aligned} \qquad (A)$$

The electrical resistivity of liquid $Ni_{13}Pd_{67}P_{20}$ ternary alloy in Faber-Ziman formulation is given by [7]

$$\rho_L = \frac{6\pi^2 m^2}{4e^2 h^3 n k_F^6} \int_0^{2k_f} \lambda(q) q^3 dq^{-}(2k_f - q) \qquad (B)$$

Where $^{-}(2k_f - q)$ is the step function that cuts off the integration corresponding to perfectly sharp Fermi surface [7].

$$\begin{aligned} \lambda(q) &= x_1 S_{11}(q) V_{s1}^{\ 2}(q) + x_2 S_{22}(q) V_{s2}^{\ 2}(q) \\ &+ x_3 S_{33}(q) V_{s3}^{\ 2}(q) + 2\sqrt{x_1 x2} S_{12}(q) V_{s1}(q) V_{s2}(q) \\ &+ 2\sqrt{x_2 x_3} S_{23}(q) V_{s2}(q) V_{s3}(q) \\ &+ 2\sqrt{x_1 x_3} S_{13}(q) V_{s1}(q) V_{s3}(q) \end{aligned} \qquad (C)$$

V_{ij} are the screened model potential, $S_{ij}(q)$ are the Faber-Ziman partial structure. x_i is concentration. q is the q-space wave vector, n is the density and k_f is the Fermi vector ,e and h are the charge of electron and Planck's constant, respectively. m is the mass of electron. Our well defined newly proposed model potential is to describe bare ion interaction [8].

$$W(r) = \frac{-2ze^2 e^*}{r} - e^1 e^{\frac{-r}{rc}} \frac{ze^2}{r} \qquad ; \quad r \le r_c$$

$$= \frac{-ze^2}{r} \qquad ; \quad r \geq rc \quad \text{(D)}$$

For the exchange and correction effects, we have used five different forms of local field correction functions. There are due to Hartree (H) [9], Taylor (T) [10], Ichimaru and Utsumi (IU) [11], Farid et al (F) [12] and Sarkar et al (S) [13]. Hartree function does not involve any kind of exchange correlation effects. On rearrangement of various terms, eq (1) can be written as,

$$\rho_L = \frac{6\pi^2 m^2}{4e^2 h^3 n k_F^6} \int_0^{2k_f} \lambda(q) q^3 dq \theta q \theta(_f - 1) \qquad \text{(E)}$$

Where Ω is effective atomic volume. The expression of thermoelectric power TEP is given by [8]

$$Q_L = \frac{-\pi^2 k_B^2 T}{3eE_f} E_f \left(\frac{\partial}{\partial E} \ln \rho_L \right)_{E=E_F} \qquad \text{(F)}$$

The thermal conductivity TC can be computed from the relation given by [11],

$$\sigma_L = \frac{\pi^2 k_B^2 T}{3|e|^2 \rho_L} \qquad \text{(G)}$$

III. Result and Discussions

Table 1 Input parameter and constant (in atomic unit a.u.)

Metal	Z[14]	M[15]	Ω[15]
Ni	8	58.71	83..192
Pd	10	106.4	114.893
P	2	30.97	157.785

The input parameters are taken from the literature [14, 15]. Fig. 1 shows the presently calculated total structure factor of Ni-Pd-P system along with the experimental results [5]. A good agreement between the presently calculated values and experimental results is found. In particular, in long wavelength limit, a good agreement is observed, which suggest that atomic arrangement is well described by PY theory. The peak height and corresponding q value are almost same, suggesting that packing and coordination are also well reproduced.

Shown in the Table 2 are the presently calculated electrical transport properties of Ni-Pd-P system at equi-atomic concentration. It is observed that presently calculated value of electrical resistivity is in good agreement with the experimental results. The results due to three screening functions namely IU, F and S are near to each other, showing precision in the present calculations. On the other hand, the H and T functions generate values, which are near to each other as well as to that of experimental results. H function, which does not involve any screening effect, gives a measure of relative effects of exchange-correlation. For the complete description of model potential and screening function, first principles based pseudo potentials are required. However, in the absence of same, present combination generates good results, which can be used for further research in this field. The results of thermoelectric power and thermal conductivity are also reported, which can be an additional set of data.

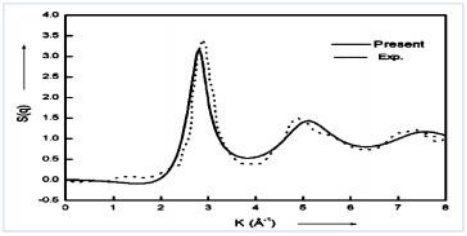

Fig.1. Theoretical and experiment results of structure factor [5].

Table 2 Electric transpor tproperties ρL in μΩcm.,Q_L in μvolt k^{-1} and σ_L (10^{-3}) of $Ni_{13}Pd_{67}P_{20}$ ternary alloy.

	H[9]	T[10]	IU[11]	F[12]	S[13]	Exp.[5]
ρ_L	134.01	135.87	147.17	148.14	143.93	130±14
Q_L	1.8170	1.817	1.274	1.275	1.265	-
$\boldsymbol{\sigma_L}$	6.183	6.191	4.227	4.292	4.66	-

IV. Conclusion

We conclude here that our newly proposed model potential produced satisfactorily good agreement for electrical transport properties like resistivity, thermoelectric power and thermal conductivity of Ni13Pd67P20 ternary system at room temperature. It is obvious that the present results are generated without any fitting procedure. This also confirms the applicability of the model potential in the aforesaid properties and supports the present approach in the absence of first principles calculations.

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