

# The Transport Properties and Superconducting Transition Temperature $T_c$ of Transition Metals

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**Abstract—** The electrical resistivity and the thermo -electric power of the molten transition metals have been investigated using the pseudo- potential approach. The formalism includes the effect of d- bands explicitly. A good agreement for molten transition metals Ni and Pd is observed. Superconducting transition temperature of transition metal Selenium also calculated.

**Keywords-** Electrical Resistivity, Transition Metals, Superconductivity, Model-Potential.

## I. INTRODUCTION

The electrical transport properties of molten metals have been a favourable subject with the theoretical workers using model potential approach. A good success has been obtained in the case of simple and polyvalent molten metals by Ziman [1] and his co-workers [2]. The same formalism has been extended [3] to the case of liquid noble metals also with mixed success. The molten transition metals could not be investigated in the same approach of their complex structure due to the d-bands. The t-matrix formalism [4] for the liquid transition metals have been only qualitative. Therefore, in the present paper the author has formulated the expressions for the electrical resistivity and the thermo electric power of liquid transition metals taking into account the effect of d-bands explicitly in the model potential approach.

The formulation is carried out in terms of Dirac time dependent perturbation theory. Suppose a single ionic centre scatters an electron from state  $\vec{k}$  to  $\vec{p}$ . The time dependent Schrodinger equation is given by

$$i\hbar \frac{\partial \psi}{\partial t} = H_0 \psi + V \psi \quad (1)$$

Where  $H_0$  is the Hamiltonian in the absence of the scattering centre. Let the stationary states of  $H_0$  be  $\psi_p(\vec{r})$  with corresponding eigen values  $E_p$ . The effect of d-bands will be to modify the wave function  $\psi_p(\vec{r})$ . The wave function at time t will then be written as

$$\psi = \left[ \sum_p a_p(t) \psi_p(\vec{r}) + \sum_d a_d \psi_d(\vec{r}) \right] e^{-iE_p t / \hbar} \quad (2)$$

Where the states  $\psi_d(\vec{r})$  are the atomic d - states. According to Harrison [5], these d-states satisfy.

$$H_0\psi_d(\vec{r}) = E_d\psi_d(\vec{r}) - \Delta\psi_d(\vec{r}) \quad (3)$$

Where  $\Delta$  is given by

$$\Delta\psi_d(\vec{r}) = \delta v\psi_d(\vec{r}) - \langle\psi_d|\delta v|\psi_d\rangle\psi_d(\vec{r}) \quad (4)$$

And  $\delta v$  is the difference between the atomic potential and the true potential in the neighbourhood of single ion. The probability of the electron being found in state  $\vec{p}$  at time  $t$  is  $|a_p(t)|^2$ . If the electron is in state  $k$  at time  $t = 0$  then,

$$\begin{aligned} a_k(0) &= 1 \\ a_p(0) &= 0 \quad \vec{p} \neq \vec{k} \end{aligned} \quad (5)$$

Substituting this into the wave equation (1) and integrating over the volume  $\Omega$  of the metal after multiplying by  $\psi_p^*e^{iE_p t/\hbar}$ , I find

$$\begin{aligned} i\hbar \frac{\partial a_p}{\partial t} &= \left[ \int a_d \psi_p^*(\Delta)\psi_d dr + \int \psi_p^* v \psi_k dr \right] e^{i(E_p - E_k)t/\hbar} \\ &= [V_{dp} + V_{kp}] e^{i(E_p - E_k)t/\hbar} \end{aligned} \quad (6)$$

The electrical resistivity is then calculated following Ziman's [1] analysis and is given by

$$\rho = \frac{3m^2\Omega}{4e^2\hbar^3K_F^2} \int |V_{dp} + V_{kp}|^2 (1 - \cos\theta) dw \quad (7)$$

Where  $m$  and  $e$  are electronic mass and charge respectively.  $K_F$  is the Fermi wave vector and  $\theta$  is the angle between states  $\vec{k}$  and  $\vec{p}$ . Further,

$$|V_{kp}|^2 = N^{-1}s(k)|U(k)|^2$$

And the analysis of Harrison [5] provides to the second order in  $\Delta$ ,

$$|V_{dp}|^2 = N^{-1}s(k)(E_d - E_k)^2 \quad (8)$$

Substituting these values and changing the variable of integration, one evaluates.

$$\rho = \frac{3\pi\Omega\Omega m^2}{\hbar^3 e^2 K_F^2} \int_0^1 s(k)[|U(k)| + (E_d - E_k)]^2 4 \left(\frac{k}{2k_F}\right)^3 d\left(\frac{k}{2k_F}\right) \quad (9)$$

The same expression can be obtained in another way also. Moriarty [3] has considered the effective model potential for transition metals as the sum of the model potential and the by hybridization term. In the present case, the pseudo-potential can be taken as the model potential  $U(k)$  and the hybridization term is given by approximately  $(E_d - E_k)$  for the resistivity of molten transition metals. The integral in equation (9) is dominated by the value at  $k = 2k_F$  Evans [6] and, therefore, to a good approximation, the electrical resistivity can be expressed as

$$\rho = \frac{3\pi m^2 \Omega \Omega}{\hbar^3 e^2 K_F^2} s(2k_F)[|U(2k_F)|^2 + (E_d - E_F)^2] \quad (10)$$

Using this equation, the thermo-electric power will be given by

$$Q = -\frac{\pi^2 k_B^2 T}{3|e|E_F} \left[ 1 + \frac{2E_F(E_d - E_F)}{|U(2k_F)|^2 + (E_d - E_F)^2} \right] \quad (11)$$

where I have assumed that structure factor  $s(2k_F)$  and the model potential  $U(2k_F)$  are independent of energy. The equations (10) and (11) were used to calculate the electrical resistivity and the thermo-electric power of liquid nickel and palladium. The input data used in the calculations are given in table (1) with the references

therein. The result are shown in table (2) along with the experimental values. It can be seen that the electrical resistivity agree very well with the experimental values. The deviation in the case of the thermo-electric power can be due to the assumptions made in deriving equation (11).

## RESULTS AND DISCUSSIONS

Table I

Input data (all quantities are in atomic units)

Metal	Z[7]	$E_d$	$E_F$	$r_a$	$s(2k_F)$ [8]
Nickel Palladium	0.83	0.5081	0.4635	0.44	0.70
	0.59	0.3324	0.3139	0.57	1.50

Where  $E_F = 2k_F^2$ ;  $k_F^3 = 3\pi^2 z / \Omega_0$

Table II

Electrical resistivity and thermo-electric power of liquid transition metals

Metal	Temp.(K)	$\rho_{cal}$	$\rho_{exp}$	$Q_{cal}$	$Q_{exp}$
Ni	1725	82.82	85.00	-20.60	-36.00
Pd	1825	79.01	83.00	-46.89	-41.00

The calculated results are in good agreement with the experiment data.

Theory and Calculation of superconducting temperature  $T_c$  for bcc Se:

The superconducting transition temperature  $T_c$  is calculated by using Allen Dynes [9] and McMillan [10] formula in given as.

$$T_c = \frac{\omega_{log}}{1.2} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right) \quad (a)$$

$$\text{Where } \lambda = 2 \int_0^\infty d\omega \frac{\alpha^2 F(\omega)}{\omega} \quad (b)$$

$$\omega_{log} = \frac{\exp 1}{\lambda} \int_0^\infty \frac{d\omega}{\omega} \alpha^2 F(\omega) \log \omega \quad (c)$$

Usually  $\lambda$  is called the dimensionless electron phonon coupling constant  $\omega_{log}$  the logarithmic averaged phonon frequency and  $\mu^*$  the effective screened coulomb repulsion constant whose value is usually taken to be between 0.1 to 0.15. In the case of monatomic metals  $\lambda$  can be expressed in the following form.

$$\lambda = \frac{N(\epsilon_F) \langle I^2 \rangle}{M \langle \omega^2 \rangle} = \frac{\eta}{M \langle \omega^2 \rangle} \quad (d)$$

Where  $M$  is the mass of the atoms and  $\langle \omega^2 \rangle$  denotes the average of squared phonon frequencies. Further  $\langle I^2 \rangle$  represents the Fermi surface average of squared electron phonon coupling interaction and  $\eta = N(\epsilon_F) \langle I^2 \rangle$  is called the Hopfield parameter.

The electron phonon coupling constant  $\lambda$  and the superconducting transition temperature  $T_c$  calculated as a function of pressure for body centered cubic Selenium. The two values for  $T_c$  correspond to two different values of  $\mu^*$  (0.10 to 0.12). The units of  $N(\epsilon_F)$  and  $\eta$  are state/Ryd/atom/spin and Ryd/A<sup>2</sup>, respectively.

Table III

<b>P(GPa)</b>	<b>N(<math>\epsilon_F</math>)</b>	<b><math>\eta</math></b>	<b><math>\omega_{log}(\mathbf{k})</math></b>	<b><math>\langle \omega^2 \rangle \langle \mathbf{k}^2 \rangle</math></b>	<b><math>\lambda</math></b>	<b><math>T_c(\mathbf{k})</math></b>
128.6	2.73	0.73	224.73	291.92 <sup>2</sup>	0.83	11.29, 9.90
149.6	2.62	0.75	248.03	-316.41 <sup>2</sup>	0.73	9.53, 8.11
165.6	2.55	0.77	264.62	335.11 <sup>2</sup>	0.66	8.03, 6.64

The value of  $\lambda$  increases, but the rate of change exceeds that of  $\omega_{log}$ . As a result the value of  $T_c$  increases considerably with decreasing pressure. The results agree well with the experimental data.

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