Bulletin of Pure and Applied Science
Physics, Vol.42D No.2S (Special Issue)
NCAEST-2023 P.44-49
Original Research Article

Print version ISSN 0970 6569
Online version ISSN 2320 3218
DOI: 10.62427/bpas.2023.42D.2S.6
Available online at www.bpasjournals.com

Electronic- Transport Properties of Solid Liquid Metals by Modified Pseudo Potential Theory

[1]Versha Joshi*, [2]Vimal Sagar, [3]JN Thakur and [4]Supriya Kumari

Author's Affiliations:
[1]Research Scholar, University Department of Physics, B.N.M.U. Madhepura, Bihar 852113, India
[2]Associate Professor, University Department of Physics, B.N.M.U. Madhepura, Bihar 852113, India
[3]Professor, University Department of Physics, B.N.M.U. Madhepura, Bihar 852113, India
[4]Assistant Professor & Head, Department of Physics, SBN College Garhirampur, Munger University, Bihar 811211 , India

***Corresponding author:**
Versha Joshi
Research Scholar, University Department of Physics, B.N.M.U. Madhepura, Bihar 852113, India
E-mail: versha.joshi19@gmail.com

ABSTRACT The Pseudo potential method is based on some fundamental assumptions for the calculations of physical and chemical properties of metals. In the present paper, the form factors are used to calculate different physical and chemical properties using the structure factors of metals and alloys. Our calculated results are found excellent and good agreement with standard experimental values.

KEYWORDS Crystal Potential, Conduction Band, Screening Potential, Pseudo Potential.

How to cite this article: Joshi V., Sagar V., Thakur J.N. and Kumari S. (2023). Electronic- Transport Properties of Solid Liquid Metals by Modified Pseudo Potential Theory. *Bulletin of Pure and Applied Sciences- Physics,* 42D (2 Special Issue), 44-49.

1. INTRODUCTION

Our understanding of metals begin in 1900, when Drude suggested that the electrons were free to run through the entire metal rather than simply associated with individual atoms and Somerfield applied quantum statistic to explain this phenomenon(John, 2001; Ashcroft and Mermin, 1976; Yu and Cardona, 1996; Charles, 1996; Burns, 1995). Theoretical understanding of a wide variety of properties developed rapidly using the nearly free electrons approximation of Ziman and Bradley have given expressions for the computation of electrical resistivity, conductivity thermoelectric power etc of solid and liquid metals by using modified pseudo potential theory (Ziman, 1967). At the same time known, Fermi, Surface could rule out many models which have been proposed to study some property of particular metal. Out of this work comes one fact which is fundamental of the "pseudo potential theory". It is interesting to note that the nuclear and solid state physics has been concurrently using analogous method. In view of this we look for a method which starts from the atomic structure and provides a method to construct the different types of crystal potentials (Thakur, 1980). In this approach the input required other than fundamental constants are the core eigen values, core wave

function and Lattice constants. This Pseudo potential method is based on three fundamental assumptions for the calculations of physical/chemical properties of metals. Viz, (i) The self consistent field approximation (ii) The small core approximation and (iii) The perturbation theory. The base ionic potentials calculated from the core eigen functions and core eigen values include within itself the following components for the study of electronic transport properties of metals and alloys: (a) Valence charge potential (b) Core potential (c) Conduction Band core exchange potential. (d) Conduction electron potential (e) screening potential and (f) Repulsive potential **(**Harrison, 1970). Vora reported the electrical transport properties of some mono valent, divalent and poly valent liquid metals using made potential formalism and concluded that the comparative study of his work and standard theoretical/experimental findings(Vora, 2008). Thakur et al. used different local field correction function and found good agreement with the standard experimental results (Thakor et al., 2011). The generalized mean spherical approximation technique is embraced for the processing the structure factor of liquid metals (Jani and Vora, 2018). Bhatai et al. confirmed that the t-matrix approach is mere approximate and physically sound for particular case of transition metals **(**Bhatai, Bhatt and Vyas, 2019).

In the present paper, the form factors are used to calculate different physical and chemical properties using the structure factors of metals and alloys. The results obtained from our work are found in excellent and good agreement with experimental values of Cusack.

2. THEORETICAL TREATMENT

In self consistent field approximations, the Schrodinger equation for the conduction band state k is given by the following equation (Harrison, 1970).

$$H\,\Psi_k = (T+V(r))\,\Psi_k = E_k\Psi_k \qquad (1)$$

Where H is the Hamiltonian, T is the kinetic energy, V(r) is the self consistent potential assumed spherically symmetric. Ψ_k & E_k are the eigen functions and eigen value of the k^{th} state respectively.

We expand Ψ_k as a linear combination of orthogonal plane wave (OPW) and hence we have

$$\Psi_k = \Sigma\, a_q OPW_k(q) \qquad (2)$$

Substitution of Ψ_k in Equ (1) gives

$$(T+W(r))\varphi_k = E_k\varphi_k \qquad (3)$$

whereφ_k is the pseudo-wave functiondefined by the following equation.

$$\varphi_k = \Sigma a_q k+q \qquad (4)$$

and$$W(r) = V(r) + \Sigma(E_k-H)\ |\ \alpha >< \alpha\ | \qquad (5)$$

W(r) is known as the pseudopotential.

Linearization of the optimum pseudo potential leads to (Harrison, 1970).

$$W(r) = V(r) + \Sigma\,(\nabla^2 + \langle k\ W\ k\rangle - E_\alpha)\,|\alpha >< \alpha| \qquad (6)$$

where E_α is the eigen values of the core state.

The pseudo potential V (r) consists of the following (Harrison, 1970).

(a) The valence charge potential V^a_q (r).
(b) Core potential V^b_q (r).
(c) Conduction band core exchange potential V^c_q (r). This potential is modified by Slater's Xα - exchange α is called electronic exchange parameter.
(d) Conduction electron potential V^d_q (r). This arises on account of use of a single un-normalized OPW. In calculation of above mentioned potentials the contribution of the valence electron has been left over. These electrons are responsible for the screening variations of the ionic potential. The modified potentials are called screening potential and Repulsive potential.
(e) The screening potential.
(f) The repulsive potential.

All these potentials discussed above are calculated by the formula given by the following equation (Thakur, 1980).

(i) The valence charge and core potential are given by

$$qV^{ab} = \left(\frac{4\pi}{\Omega_0}\right)\frac{2}{q^2}[n(q) - n(0) - z] \quad (7)$$

WhereΩ_0 is atomic sphere volume and $n(q)$ is core electron density and is equal to

$$n(q) = \int \frac{sinqr}{qr} U(r)dr \quad (8)$$

Where $U(r) = \sum_{nl}(2l+1)\psi_{nl}^2(r)$ and $\psi_{nl}$are the wave functions of 1s, 2s & 2p states of core electrons moving in the orbit.

(ii) The conduction Band core Exchange potential is given by

$$qV^c = -\left(\frac{1.2707}{q}\right)\frac{4\pi}{\Omega_0}\int sinqr[rU(r)]^{\frac{1}{3}}dr \quad (9)$$

as this potential arises due to exchange interaction between conduction and core electrons.

(iii) The conduction- Electron potential

$$qV^d = -\frac{8\pi z}{q^2\Omega_0}\left[\frac{z^*}{z} - 1\right]\frac{n(q)}{n(0)} \quad (10)$$

(iv) The screening potential is given by

$$qV^f = \frac{4}{\pi^2 q^2}\int_{k<k_F}^{q} \frac{<k+q/\omega^R/k>}{k^2-|k+q|^2} d^3k \quad (11)$$

Where $< k+q/\omega^R/k >$ is the repulsive potential.

(v) Repulsive potential is given by

$$< k+q/\omega^R/k >= \sum_{nl}(k^2 + f_{nl})(2l+1)$$

$$< k+q/nlo >< k|nlo > Pl(cos\theta)$$

$$+\frac{\sum_{nl}(k^2+f_{nl})(2l+1) < k/nlo >^2}{1-\sum(nl+1) < k/nlo >^2}$$

$$\times \sum (2l+1) < k+q/nlo >< k/nlo > Pl(cos\theta) \quad (12)$$

wheref_{nl} = core shift and

$$< k/nlo >= \left(\frac{4\pi}{\Omega_0}\right)^{\frac{1}{2}} \int r\psi_{nl}(r) j_l(kr)dr \quad (13)$$

where$j_l(kr)$ is Bessel's function and$k, q \& k_F$ are electron wave vector, phonon wave vector and Fermi wave factor respectively. These values are tabulated in Table 1.

The modified screened form factor is expressed as

$$< k+\frac{\frac{q}{\omega}}{k} >= \frac{V_q^{ab}+V_q^c+V_q^d}{\epsilon^*(q)} + < k+\frac{\frac{q}{\omega^R}}{k} > - \frac{GV_q^f}{\epsilon^*(q)} \quad (14)$$

where$GV_q^f/\epsilon^*(q)$ is correction term.

The correction term is screening potential given by

$$G(q) = A\left(1 - e^{-B\eta^2}\right) \quad (15)$$

$$\text{And}(q) = (1-G(q))(\epsilon(q)-1)+1 \quad (16)$$

where$\epsilon(q)$ is the Hartree Dielectric function

Using the nearly free-electron approximation for the computation of the electrical resistivity, which is given as (Ziman, 1967).

$$\rho = \frac{3\pi\Omega_0}{e^2\hbar U_F^2}\int_0^1 4|\langle k+q|w|k\rangle|^2 a(a)\left(\frac{q}{2k_F}\right)^3 d\left(\frac{q}{2k_F}\right) \quad (17)$$

Where Ω_0 is the atomic volume, Z is the valence U_F^2 the Fermi velocity and $a(q)$ the liquid structure factor, Thermo electric power Q at temperature T is obtained from

$$Q = -\frac{\pi^2 k_B^2 T}{3|e|E_F}\chi \quad (18)$$

Where k_B is the Boltzmann constant and

$$\chi = -E_F\left|\frac{\partial ln\rho(E)}{\partial E}\right|_{E=E_F} \quad (19)$$

The different components of the screened potentials are plotted in Fig –I and contributions of core states (1s, 2s & 2p) are plotted in Figure 2.

3. RESULT AND DISCUSSION

The screened components of valence charge core potential $V_{ab}^{*}\left(=V_q^{ab}/\in^{*}(q)\right)$, conduction band core exchange potential $V_c^{*}\left(=V_q^{c}/\in^{*}(q)\right)$, conduction exchange potential $V_d^{*}\left(=V_q^{d}/\in^{*}(q)\right)$ and screening potential $V_f^{*}\left(=V_q^{f}/\in^{*}(q)\right)$ and repulsive potential $<k+q/\omega/k>$ core are plotted in Fig. I using table 1.

The calculated value of Electrical Resistivity and Thermoelectric power of sodium are Tabulated in Table 2 and are compared with experimental values. Electrical Resistivity, ρ (μΩ cm) and Thermo electric power Q (μv/k) of sodium at the melting point, 100^0C are tabulated in Table 2. The calculated values of electrical resistivity and thermo electrical power are compared with standard experimental values and found excellent and good agreement with standard experimental values.

The conduction band core exchange potential is modified by statistical $\chi\alpha-$ change i.e. $\alpha=0.73115$ &$\alpha=1$ and repulsive potential by $\beta=1$ &$\beta=5/8$, where β is correction factor. The orthogonality coefficients $<k/nlo>$ for core states, $<k/100>,<k/200>$ and $<k/210>$ are plotted in Figure 2.

Number of core electrons n(q), the valence charge and core potentials V_q^{ab}, the conduction-band-core exchange potential V_q^{c}, the conduction electron potential V_q^{d}, screening potential V_q^{f} and repulsive potential $<k+q/\omega^{R}/k>$ of sodium.

The screening potential and repulsive potential are computed by using the orthogonality coefficient which depends on the wave function of 1s, 2s & 2p core states in case of sodium. It is found that 2s- State contributes predominantly in comparison to core states 1s and 2p. The 2p state contributes very little at lower k/k_f (k= Electron wave vector; k_f = Fermi wave vector). 1s core state got relatively small effect is comparison to other states. The contributions of 1s and 2s states are practically constant within the range k/k_f =0 to 1.0. The contribution due to 2p state increased rapidly and reaches maximum at k/k_f =1.0. The only positive component of the ionic potential of sodium is repulsive potential where as the valence charge potential core potential , conduction band core exchange potential, conduction electron potential and screening potential are negative in magnitude. The resultant potential is called pseudo potential and this potential is weak in magnitude. The pseudo potential form factors are calculated by using the Hartee dielectric functions and pseudo potential.

Table 1: Different types of Potentials

q/K_F	$n(q)$	V_q^{ab}	V_q^{c}	V_q^{d}	V_q^{f}	$<k+q/\omega^{R}/k>$
0.0	9.99998		-0.21126			+0.35836
0.2	9.98980	-10.16118	-0.20954	-0.74270	-23.00025	+0.35770
0.4	9.96295	-2.60780	-0.20448	-0.18517	-5.49294	+0.35555
0.6	9.91849	-1.20871	-0.19635	-0.08193	-2.30269	+0.34715
0.8	9.85680	-0.71868	-0.18559	-0.08193	-1.21595	+0.34715
1.0	9.77846	-0.49148	-0.17274	-0.02908	-0.69712	+0.34715
1.2	9.68414	-0.36765	-0.15844	-0.01999	-0.45676	+0.33313
1.4	9.57467	-0.29258	-0.14334	-0.01453	-0.30753	+0.32402
1.6	9.45097	-0.24345	-0.12807	-0.01098	-0.20608	+0.31351
1.8	9.31406	-0.20936	-0.11318	-0.00855	-0.14302	+0.30161
2.0	9.16502	-0.18457	-0.09916	-0.00681	-0.7361	+0.2882

Table 2:

ρcalc	Q calc	ρ expt. (Cusack 1963)	Q expt (Cusack 1963)
9.22	-8.18	9.65	-9.9

The calculated values are in excellent agreement with experimental values.

This shows the variation of different types of potentials (figure 1).

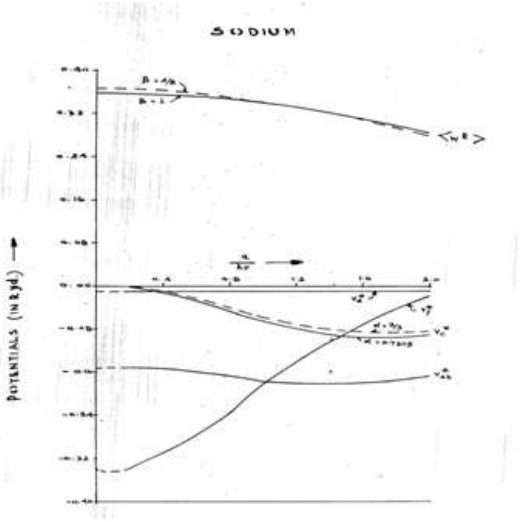

Figure 1: Different component of screened crystal potentials

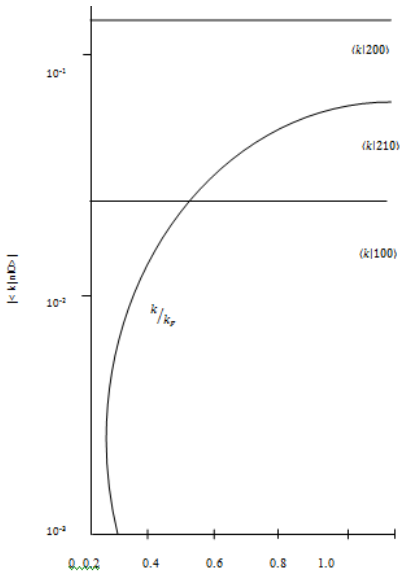

Figure 2: Orthogonality coefficients $< k/nlo >$ for 1s, 2s & 2p states of Sodium

4. CONCLUSIONS

(i) Valence charge and core potential decreases with the increase of q/k_f

(ii) Conduction B and core exchange potential decreases with the increase of q/k_f.

(iii) Conduction electron potential increased very slowly with the increase of q/k_f.

(iv) Screening potential increases rapidly as q/k_f. Increases

All the above components are "NEGATIVE"

(v) Repulsive potential decreases with the increase of q/k_f and this component is Positive.

(vi) It is found (Fig- 2) that 2s state contributes predominantly is comparison to 1s & 2p states. The 2p state contributes very little at lower $/k_F$. It crosses 1s state at $k/k_F = 0.37$ and reaches the intermediate value between 1s & 2s states at $k/k_F = 1$.

(vii) The 1s – state has got relatively small effect in comparison to other states.

(viii) The contributions of 1s & 2s states are practically constant within the range $k/k_F = 0$ to 1.0 and contribution due to 2p – state increases rapidly and reaches maximum at $k/k_F = 1.0$.

REFERENCES

1. Ashcroft N.W and Mermin N.D. (1976). Solid State Physics, Holt, Rinehart and Winston, New York.

2. Burns G. (1995), Solid State Physics, Academic Press, Boston.

3. Bhatai K. G., Bhatt N.K. and Vyas P.R and Gohel V.B. (2019). Comparative study of transport properties using transition metal model potential (TMMP) for 16 liquid metals Pramana Journal of Physics, 92(28), 1-8.

4. Charles K. (1996). Introduction to Solid State Physics, Wiley, 7th Edition, New York.

5. Harrison W.A (1970). Solid State Theory, McGrow Hill, New York.

6. Jani M.H. and Vora A.M. (2018). Theoretical Study of Electrical Transport Properties of Some Simple Liquid Metals by Pseudo potential, International Journal of Scientific Research and Reviews, 7(1), 321-328.

7. John S. (2001). Band Theory and Electronic Properties of Solids, Oxford University Press.

8. Thakur J. (1980). Fermi Energy, Density of States, and Electronic Properties. Phys. stat. sol(b) 100, 103.

9. Thakor P.B. et al. (2011). Electronic transport properties of liquid lanthanides, Advanced Materials Letters, 2(4), 303-308.

10. Vora A.M. (2008). Electrical Transport Properties of Some Liquid Metals, High Temperature, 46(6), 800-810,

11. Yu P. and Cardona M. (1996). Fundamentals of Semiconductors, Springer, Berlin.

12. Ziman J.M. (1967). The electron transport properties of pure liquid metals. Advances in Physics, 16, 551.

****