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CALCULATION OF ELECTRICAL RESISTIVITY OF LIQUID METALS USING THE PERCUS YEVICK STRUCTURE FACTOR AND MODEL POTENTIAL

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ABSTRACT

In this work, the Model potential with the Percus Yevick structure factor was used to calculate electrical resistivity of liquid metals. The results obtained are in very good agreement with the experimentally determined values. From the results it showed the Model potential with the Percus Yevick structure factor can be used effectively to predict theoretically experimental values of electrical resistivity of any liquid metal.

Keywords:* *Electrical resistivity, Model potential, Structure factor, Form factor, Percus Yevick, Liquid metals.

1.0 INTRODUCTION

Resistivity is the material property that pertains to how difficult it is for electrical current to flow through said materials. Materials with high resistivity are known as insulators while materials with low resistivity are known as conductors. Resistivity posses the largest range of values for any physical property and it is essential in many materials applications including resistors in electrical circuits, dielectrics, resistive heating and superconducting.

The Ziman's nearly free electron (NFE) theory has been fairly successful in describing the quantitative behavior of the electrical resistivity in simple liquid metals. This is because in these metals the mean free path is about one hundred times the interatomic distance and the weak scattering picture should be valid. Even for the heavy polyvalent metals (e.g. mercury, thallium and lead) where the mean free path is only about two interatomic distances, the NFE model can yield results, which are in reasonable agreement with experiments. Calculations of electrical resistivity using structure factor from various experiments or different versions of bare ion potential and dielectric function, gives correct order of magnitude but differ among themselves [1].

2.0 LITERATURE REVIEW

Baria [1] calculated the electrical resistivity of liquid metals using the structure factor derived via the charge hard sphere model with the model potential; results obtained are in agreement with experimental values of electrical resistivity.

Amah *et al.*, [2] calculated the electrical resistivity of liquid metals using the structure factor that depends on the ionic positions with Agumented Plane Wave method (APW) results obtained are in good agreement with experimental values of electrical resistivity.

Aditya [3] calculated the electrical resistivity of liquid metals using Ashcroft empty core (EMC)[4] model pseudopotential results obtained are in agreement with experimental values of electrical resistivity.

Thakore *et al.*[5] calculated the electrical resistivity of liquid Lanthanides using a Model potential constructed by them results obtained are in agreement with experimental values.

In this present paper, the electrical resistivity of liquid metals will be calculated differently using the Model potential proposed by Pandya *et al.*[6] with the Percus-Yevick (PY) [7] structure factor to calculate electrical resistivity of liquid metals.

3.0 AIM AND RESEARCH PROBLEMS

The aim of this work is to calculate the electrical resistivity of liquid metals using Model pseudopotential method with the Percus-Yevick structure factor.

Research problems: to calculate the electrical resistivity of liquid metals without dependence on temperature; to use an approach that will improve on previously calculated values of electrical resistivity of liquid metals by other researchers.

4.0 MATERIALS AND METHOD

The material that was used in this work is CodeBlocks C++ program package. The model pseudo potential [6] in this work is given as:

$$W_{ion}(r) = \sum_{n=1}^{2} B_n e^{-(r/na)} \qquad r < R_c \qquad (1)$$

the Pseudopotential of the electron has this form when it is inside the core radius R_c and r is the electron distance from the nucleus.

$$W_{ion}(r) = -\frac{Z_s}{r} \qquad r > R_c \qquad (2)$$

the Pseudo potential of the electron has this form when it is outside the core radius R_c and r is the electron distance from the nucleus.

The Fourier transform of the model pseudo potential in q-space is given as:

$$W_{ion}(q) = 4\pi a^3 \rho \left[\frac{B_1 H_1}{\left(1 + a^2 q^2\right)^2} + \frac{8 B_2 H_2}{\left(1 + 4a^2 q^2\right)^2} \right] - \frac{4\pi Z_s \rho}{q^2} . \cos q R_c \qquad (3)$$

where Z_s, a, q, ρ are the effective number of valence electrons per atom, measure of the softness of the repulsive potential, wave vector and number density. B_1,B_2 are coefficients of the Dirichlet series and H_1,H_2 are represented as the sum of the repulsive and the oscillatory contributions.

$\rho = \frac{1}{\Omega_o}$, where Ω_o is the atomic volume

$$B_1 = \frac{Z_s}{R_c}\left[1 - \frac{2a}{R_c}\right] e^{\frac{R_c}{a}}, \quad B_2 = \frac{2Z_s}{R_c}\left[\frac{a}{R_c} - 1\right] e^{\frac{R_c}{2a}}$$

$$H_1 = 2 - e^{(Y_1)[Y_1(1+X_1)-(1-X_1)]} \times \frac{\sin qR_c}{aq} + \left[2 + Y_1(1+X_1)\right] \times \cos qR_c$$

$$H_2 = 2 - e^{(Y_2)[Y_2(1+X_2)-(1-X_2)]} \times \frac{\sin qR_c}{2aq} + \left[2 + Y_2(1+X_2)\right] \times \cos qR_c$$

where $X_1 = a^2 q^2$, $X_2 = 2^2 a^2 q^2$, $Y_1 = \frac{R_c}{a}$, $Y_2 = \frac{R_c}{2a}$

The Thomas Fermi dielectric constant [8] is used to screen the form factor in this work and given as:

$$\varepsilon(q) = 1 + \frac{k_o^2}{q^2}, \quad k_o = 0.815 k_F \left(\frac{r_s}{a_o}\right)^{\frac{1}{2}}$$

where k_F is Thomas-Fermi wave vector

The structure derived via the Percus Yevick Hard sphere (PHYS) model is one of the most straightforward and extensively used model and is obtained from the exact solution of the Percus-Yevick equation for Hard-Sphere (PY) diameter (σ), which is obtained, to get best fit of S(q) with the experimental data. The PY integral equation to yield the structure factor using the expression as:

$$S(q\sigma) = \frac{1}{(1 - nc(q\sigma))} \qquad (5)$$

where σ is Hard-sphere diameter and the direct-correlation function $c(q\sigma)$ in momentum space is yield as follows:

$$c(q\sigma) = -4\pi\sigma^3 \int_0^1 dss^2 \frac{\sin(sq\sigma)}{sq}\left(\alpha + \beta s + \gamma s^2\right) \qquad (6)$$

The parameter α, β and γ are the functions of packing density parameter η, the function of total fluid volume occupied by the sphere defined as:

$$\eta = \left(\frac{\pi}{6}\right) n\sigma^3, \quad \alpha = \left(\frac{(1+2\eta)^2}{(1-\eta)^4}\right), \quad \beta = \left(\frac{-6\eta\left(1+\frac{\eta}{2}\right)}{(1-\eta)^4}\right)$$

and $\gamma = \left(\frac{\frac{1}{2}\eta(1+2\eta)^2}{(1-\eta)^4}\right)$

On integrating the equation (6) over the volume of the sphere, the expression for the structure factor turns out to be:

$$S(q) = \left[1 + \left\{\frac{24\eta}{(1-\eta)^4 y^6}\right\} \left\{ \begin{array}{l} (1+2\eta)^2 y^3 (\text{siny} - \text{ycosy}) \\ -6\eta\left(1+\frac{\eta}{2}\right)^2 y^2 \left\{2y\sin y - \left(y^2 - 2\right)\cos y - 2\right\} \\ +\frac{\eta}{2}(1+2\eta)^2 \left\{\left(4y^3 - 24y\right)\sin y - \left(y^2 - 12y^2 + 24\right)\cos y + 24\right\} \end{array} \right\}\right]^{-1}$$

In which $y = q\sigma$

The liquid metal resistivity (ρ) [9] is given as:

$$\rho=\left(\frac{4\pi^{3}\hbar}{e^{2}}\right)\left(\frac{Z}{k_F}\right)\int_{o}^{1} S(q)\,|\,W(q)\,|^{2}\, q^{3}dq \qquad (7)$$

where S(q), $\hbar$, e, W(q) are the structure factor, reduced Planck's constant, electronic charge and screened form factor.

Let $G(q)=S(q)\left|W(q)\right|^{2} q^{3}$

Equation (7) reduces to

$$\rho=\left(\frac{4\pi^{3}\hbar}{e^{2}}\right)\left(\frac{Z}{K_F}\right)\int_{0}^{1} G(q)dq \quad (8)$$

The integral in equation (7) was evaluated using the trapezoidal scheme in the limit of 0 to 1.

5.0 RESULT AND DISCUSSION

The input parameters used in the calculation are given in Table 1 and the comparison between the calculated values of electrical resistivity of liquid metals in this work and others previously calculated with the experimental values of electrical resistivity of liquid metals are given in Table 2. The experimental values of electrical resistivity gotten from Faber [10].

From table 2 calculated values of electrical resistivity are in good agreement with experimental values and have a higher accuracy when compared with Bari and Aditya values of electrical resistivity. Sodium (Na) and potassium (K) have the lowest resistivity values; meaning that they are very good conductors of heat and electric current while lead (Pb) and caesium (Cs) have the highest resistivity values indicating that they are very good insulators; heat and electric current do not pass through them easily.

6.0 CONCLUSION

From the results obtained it showed that the Model potential with the Percus Yervick structure factor can be used effectively to predict theoretically experimental values of electrical resistivity of any liquid metal since it gives values which are in close agreement with experimental values of electrical resistivity and has improved previous values calculated by other researchers.

Table 1. Input Parameters Used in the Calculation of Electrical Resistivity

Metals	Z	G(q)(a.u)	$K_f(a.u^{-1})$
Li	1	0.2301	0.58
Na	1	0.0742	0.48
K	1	0.0821	0.39
Rb	1	0.1332	0.36
Cs	1	0.2016	0.34
Ag	1.5	0.1216	0.66
Cd	2	0.2014	0.74
Au	2	0.1582	0.64
Mg	2	0.1565	0.72
Al	3	0.1223	0.91
Pb	4	0.3177	0.83

Table 2: Comparing calculated values with Bari, Aditya and experimental values of Electrical Resistivity (in μΩcm)

Metals	Present work	Experimental value	Bari	Aditya
Li	24.61	24.70	21.15	38.76
Na	9.59	9.60	8.44	15.51
K	13.06	13.00	11.48	20.58
Rb	22.95	22.50	23.62	50.05
Cs	36.79	36.00	31.29	89.23
Ag	17.15	17.00	---	108.15
Cd	33.77	34.00	34.65	49.06
Au	30.66	31.00	---	439.93
Mg	26.97	26.00	29.13	37.93
Al	25.02	24.00	25.58	30.23
Pb	94.97	95.00	94.57	129.16

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