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Temperature dependence of electrical resistivity of liquid alkali metals (Li, Na and K)

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ABSTRACT

In the present paper we have studied the temperature dependence of electrical resistivity of simple liquid metals through the Harrison's first principle (HFP) pseudopotential technique. The structure factor needed for liquid metals has been taken from experimental measurements [X-ray and neutron diffraction]. The results have been compared with experimental data and theoretical values of other authors. Reasonable agreement has been obtained. © 2010 Trade Science Inc. - INDIA

KEYWORDS

Electrical resistivity;
Pseudopotential;
Liquid alkali metals.

INTRODUCTION

The present theoretical investigation is concerned with the study of the temperature dependence of the electrical resistivity of liquid alkali metals near and above their respective melting points. For the purpose the Harrison's first principle (HFP) pseudopotential technique has been used. This is basically an orthogonized plane wave (OPW) technique first proposed by Herring^[15] and later developed by Phillips & Kleinman^[17], Harrison^[11-13], Cohen and others^[5-8] and Antoncick^[1]. Hence we have been encouraged to use this technique for the present investigation. In the following sections we present the formalism for the computation of electrical resistivity followed by result, discussion and conclusion.

FORMALISM

The theory of electrical resistivity of simple metals was developed through the pioneering work of Bardeen (1937), Faber^[9], Bhatia and Krishnan^[3], Gerstenkron^[10],

Bailyn^[2] and others. It was Ziman^[20] who re-discovered this basic formula at the time when the concept of pseudopotential was being introduced. Ziman's formula based on nearly free electron approximation could successfully describe the behavior of conduction electrons in simple liquid metals e.g. alkali metals. In this approach the conduction electrons are supposed to form a degenerate electron gas having spherical Fermi surface. They are scattered by the irregular arrangement of metallic ions. Their scattering can be treated within the framework of perturbation theory which gives rise to a finite relaxation time τ , which is substituted in the Boltzman equation to derive the transport properties.

The electrical conductivity is given by

$$R = \frac{1}{3} e^2 v_F^2 N(E_F) \tau \quad (1)$$

where, e is the electronic charge, v_F is the velocity of electron on the Fermi sphere, $N(E_F)$ is the electronic density of states on the Fermi surface and τ is the relaxation time.

The relaxation time τ is given by

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$$\frac{1}{\tau} = \int (1 - \cos \theta) Q(\theta) d\omega \quad (2)$$

where, $Q(\theta)$ is the scattering probability through an angle θ into the solid angle $d\omega$. There are various form of equation (1) but Ziman^[21] has shown that this expression is based on minimum number of approximations.

The transition rate per unit solid angle between states $|k\rangle$ and $|k'\rangle$ on the Fermi surface is given by

$$Q(\theta) = \frac{2\pi}{\hbar} \left| \langle k | W | k' \rangle \right|^2 \frac{1}{2} N(E_F) / 4\pi \quad (3)$$

Since the spin of the electron does not change on scattering only half of density of states will be available for transition. Hence a factor of half has been introduced in equation (3). Here W is the crystal potential which may be expressed as

$$W(\mathbf{r}) = \sum_j w(\mathbf{r} - \mathbf{r}_j) \quad (4)$$

where, \mathbf{r}_j is the center of the j^{th} ion carrying the potential $w(\mathbf{r} - \mathbf{r}_j)$, by an argument exactly equivalent to the standard calculation of x-ray or neutron diffraction by liquid ions.

We get the matrix elements for the crystal potential

$$\langle k | W | k' \rangle = w(\mathbf{k}, \mathbf{q}) \frac{1}{N} \sum_j \exp(i\mathbf{q} \cdot \mathbf{r}_j) \quad (5)$$

where, $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ and $w(\mathbf{k}, \mathbf{q})$ is the Fourier transform of the potential of an ion normalized to atomic volume. The rest part on r.h.s. gives the structure factor $a(\mathbf{q})$. Squaring the expression and taking the statistical average over the arrangement of ion in the liquid gives us

$$|\langle k | W | k' \rangle|^2 = N^{-1} |w(\mathbf{k}, \mathbf{q})|^2 a(\mathbf{q}) \quad (6)$$

where, $a(\mathbf{q})$ is the structure factor and $w(\mathbf{k}, \mathbf{q})$ is the form factor, putting together the above equation and using

$$\mathbf{q} = 2\mathbf{k}_F \sin \theta/2 \quad (7)$$

we get the basic formula for electrical resistivity,

$$R = \frac{3\pi Z \Omega_0}{\hbar e^2} \frac{1}{v_F^2} \int_0^2 |w(\mathbf{k}, \mathbf{q})|^2 a(\mathbf{q}) \frac{1}{4} \left(\frac{q}{k_F} \right)^3 d \left(\frac{q}{k_F} \right) \quad (8)$$

COMPUTATION AND RESULT

The form factor has been computed through various combinations of input parameters viz, core energy eigenvalues ϵ_{nl} , Xa-exchange parameter α and

orthogonalization hole parameter β . To compute the temperature co-efficient of the electrical resistivity the form factors have been computed at two different temperatures one above the melting point of respective metals. For Li these temperatures are 170°C and 250°C for Na 105°C and 200°C for K, these are 70°C and 105°C. The above temperatures have been chosen because the experimental structure factors are available at these temperatures which are required for electrical resistivity calculations.

Lithium

It is observed that with both the eigenvalues Herman-Skillman^[14] and Clementi^[4] to be referred to as H and C eigenvalues. The form factors using $\alpha = \alpha_{vt}$ and $\beta = 1$ give the closest agreement with the experimental data that is 23.7 and 23.4 against 24.8 $\mu\Omega\text{cm}$ at 170°C and 29.0 and 27.8 against 29.1 $\mu\Omega\text{cm}$ at 250°C. However, with both the eigenvalues $\alpha = 2/3$ and $\beta = 5/8$ also gives reasonable agreement at 250°C.

Sodium

None of the form factors give close agreement with the experimental data the H-eigenvalues, with $\alpha = 2/3$ and $\beta = 5/8$ gives the resistivity 12.6 $\mu\Omega\text{cm}$ and the Clementi eigenvalues with $\alpha = 2/3$ and $\beta = 5/8$, gives the resistivity 13.3 against 9.43 $\mu\Omega\text{cm}$ at 105°C. At 200°C the H-eigenvalues with $\alpha = 2/3$ and $\beta = 5/8$ gives the resistivity 13.7 against 12.38 $\mu\Omega\text{cm}$ and Clementi eigenvalues with $\alpha = 2/3$ and $\beta = 1$ gives the resistivity 17.8 against $R_{\text{expt.}} = 12.38 \mu\Omega\text{cm}$. It is to be mentioned that using Harrison first principle pseudopotential technique and experimental structure factor Singh^[19] has obtained $R = 14.2$ to 19.55, Khan^[16] has obtained $R = 12.0$ -26.8 and Prasad^[18] has obtained $R = 27.8$ -18.4 using HFP technique. Hence our results are in reasonable agreement with experiment.

Potassium

For Potassium the C-eigenvalues with $\alpha = 2/3$ and $\beta = 5/8$ gives $R = 13.7$ and the H-eigenvalues with $\alpha = 2/3$ and $\beta = 5/8$ gives $R = 12.0$ against $R_{\text{expt.}} = 13.95 \mu\Omega\text{cm}$ at 70°C. At 105°C the H-eigenvalues with $\alpha = 2/3$ and $\beta = 5/8$ gives $R = 15.8$ and C-eigenvalues with the same combination gives $R = 13.3$ against $R_{\text{expt.}} = 14.64 \mu\Omega\text{cm}$.

The temperature dependence of electrical resistivity of Li, Na and K has been shown in Figure 1, 2 and 3 respectively. For Li it is observed that the variation of

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CONCLUSION

From the above mentioned facts it may be concluded that the HFP technique can be successfully used for the computation of the electrical resistivity of liquid metals provided suitable input parameters are used. However, as various approximations are involved within the framework exact reproduction of the experimental data is neither expected nor desired.

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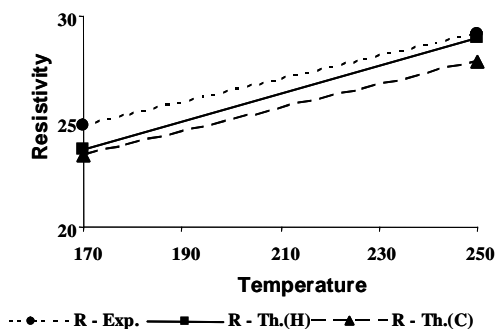


Figure 1 : Temperature dependence of electrical resistivity of Li

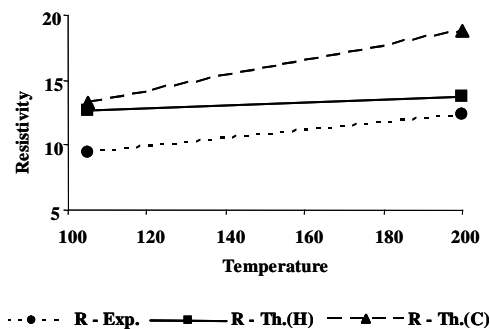


Figure 2 : Temperature dependence of electrical resistivity of Na

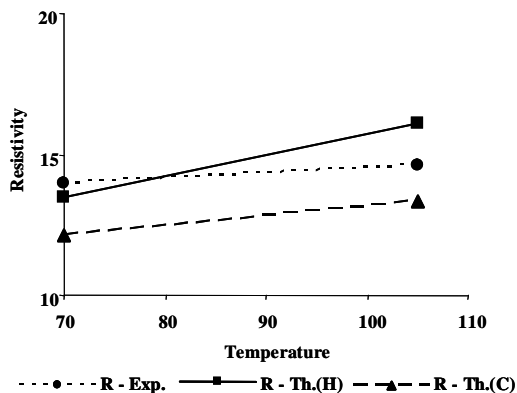


Figure 3 : Temperature dependence of electrical resistivity of K

resistivity agrees well with experimental data. For Na the result computed through C-eigenvalues agrees qualitatively with experiment. The same is the case for K.