International Journal of advancement in electronics and computer engineering (IJAECE)
Volume 3, Issue 2, May 2014, pp.302-305, ***ISSN 2278 -1412***

The Self-Consistent Resistivity of Liquid Metals with Finite Mean Free path Using Local Pseudopotential

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Abstract *– Using local Heine-Abrenkov model potential self-consistent resistivity and mean free path are computed and compared with the results obtained using other models. The pseudopotential parameters are determined from zero pressure condition and experimental bulk modulus. The present study helps to understand uncertainty in the electron position, momentum and blurring of the Fermi surface.*

Keywords*: Resistivity, Mean Free path, Pseudopotential,*

I. Introduction

The data on the Hall coefficient, the Lorentz number, the electrical and thermal resistivity, the thermo-power and magnetic susceptibility of liquid metals and their alloys can be interpreted in terms of the nearly-free electron model. The most used expression in the nearly-free electron model is the well known Ziman formula for the resistivity. Two key ingredients are appear in it, namely the structure factor S(q) and screened pseudopotential. These two quantities are not independent, since the pseudopotential determines the forces between ions, which ultimately determine the structure of the liquid. In any case, the theoretical values of the electrical resistivity are very sensitive to the accuracy of the structure factor.

Interest in the study of the transport properties of liquid metals continues unabatedly. The hope is that the information so obtained will throw some light on the interactions in the corresponding solid metals [1]-[6]. Ziman's theory successfully takes into account all multi-phonon process, Debye-Waller factors, Umklapp process, coupling to transverse phonons and anharmonic phonon effect without going through an intermediate description of the lattice, oscillations in terms of phonons. Ziman's theory is based on the long mean free path (MFP) approximation [7]-[9] founded on single site scattering. But, in practice, the MFP of conduction electron in liquid metals has a finite range. The finiteness of the MFP, following the Heisenberg uncertainty principle, results in a blurred Fermi surface instead of a sharp one which is assumed in the Ziman's theory. According to Mc Caskill and March [6] the finite MFP, l and blurring width, Δq say, are related by $l\Delta q \sim 1$. Hence it is interesting to examine the effect of Δq on the resistivity if l is roughly known or assumed to have a value that is given by other theoretical or experimental works. A truly self-consistent theory incorporating Fermi surface blurring has not been developed [4].

Our motivation arose out from the above aspects and prospects of electronic and transport properties. We have used Heine-Abrankov model potential to investigate the electronic transport properties of simple metals. For this reason, in the present work, we determined potential from zero pressure condition and Bulk Modulus B (experimental) to study equation of state, Gruneisian parameter and pressure derivative of bulk modulii..

II. Theory

The well known Ziman formula for resistivity is given by

$$\rho_{\text{Ziman}} = \frac{3\pi m^2}{4Ze^2\hbar^3 n k_F^6} \int_0^\infty dq\, q^3 S(q) \left|V(q)\right|^2 \theta(2k_F - q) \quad (1)$$

Where, S, V, Z, e, m and n denote the static structure factor, screened electron-ion interaction in q-space, effective s-electron occupancy number, electron charge,

mass and conduction electron density respectively. The unistep function which cuts off the integration at $2k_F$ corresponding to the sharp Fermi surface. It is defined as, for $q \leq 2k_F$. In the present work, we have used hard-sphere solution of Percus-Yevick equation with static factor 0.45. The resistivity (ρ) and finite mean free path (*l*) are related by equation $\rho = \frac{\hbar k_F}{ne^2 l}$.

Taking blurring into account the formulation of resistivity is reviewed by [5] is given by

$$\rho_{sc} = \frac{3\pi^2 m^2}{4Ze^2\hbar^3 n k_F^6} \int_0^\infty dq\, q^4 S(q) |V_{ion}(q)|^2 \, \Gamma(q, k_F, l) \quad (2)$$

The expression for $\Gamma(q, k_F, l)$ is taken from ref. [7] Eq.1 and Eq.2 must be solved iteratively to get self-consistent value of the electrical resistivity ρ. In the present study the Percus-Yevick equation for structure factor S(q) with packing fraction 0.45 is used.

In real space Heine-Abrenkov model potentialis given by,

$$V_{ion}(q) = -\frac{UZe^2}{r} \qquad when\ r \leq R_m$$
$$= -\frac{Ze^2}{r} \qquad when\ r > R_m \quad (3)$$

III. Results and Discussion

The pseudopotential used in the present calculation has two parameters R_m and U are given in Table 1 with Vashistha-Singhwi parameters. We compare our pseudopotential form-factors with non-local [8] and local pseudopotential form factors [3] in Fig.1, Fig.2, Fig.3 and Fig.4 for Na, k, Rb and Cs.

TABLE I
Pseudopotential parameter and Washistha-Singhwi parameters

Metal	Pseudopotential Parameter		Vashistha-Singwi Parameter	
	A	B	R_m	U
Na	1.0778	0.2855	2.08	-0.3025
K	1.1673	0.2705	3.0	-0.5328
Rb	1.1975	0.2657	4.20	-0.9659
Cs	1.2346	0.2601	4.90	-1.019

We have plotted the form factors up to $q=2k_F$, which is a reasonable cut off limit for the present calculation to check its validity. To confirm our form-factors, primarily as test cases, we have compared our results with other most promising theoretical results [3-8]. This is the usual guidelines to explore more of any pseudopotential for further investigation, because in the absence of identical experimental results of form factors, it is difficult to make a quantitative comparison of observed data. Examining critical Fig.1 to Fig.4, it may be inferred that their behavior is almost identical and they are free from any abnormal behavior in this region.

The computed values of the resistivity using Eq.1 and Eq.2 are compared with other theoretical findings in Table 2. Our computed results are well comparable with results due to Baria [3] that have used their single parameter pseudopotential. They found that their results of self-consistent formulation are excellent. In our case it is interesting to note that self-consistent treatment yields smaller resistivity values then original Ziman formula. Our results are better than recently reported results of Geertsma et al [2]. who have used Linear Response theory (LRT) to calculate the screened pseudopotential and structure factor was obtained from the pair potential using Modified Hyper Neted Chain (MHNC) theory of liquid. We conclude that for the real test of the pseudopotential;l, we must examine static, dynamic and electrical properties with potential determines from zero pressure condition.

TABLE II
The mean free path l, ρ_{Ziman}, ρ_{sc} and values in the brackets are experimental

Metal	Mean Free Path, *l* (cm)	ρ_{Ziman} (μΩ-cm)	ρ_{sc} (μΩ-cm)	ρ_{Ziman} (μΩ-cm) other	ρ_{sc} (μΩ-cm) other
Na	360.05	8.18	7.88 (9.6)	15.8[2], 8.44[3], 5.3[9]	9.82[3]
K	400.67	11.57	11.02 (13.0)	18.5[2], 11.48[3], 11.1[9]	4.08[3]
Rb	281.22	18.17	17.9 (22.0)	20.8[2], 23.62[3], 19.8[9]	23.09[3]
Cs	332.40	17.8	17.60 (36)	13.8[2], 31.29[3], 32.7[9]	35.25[3]

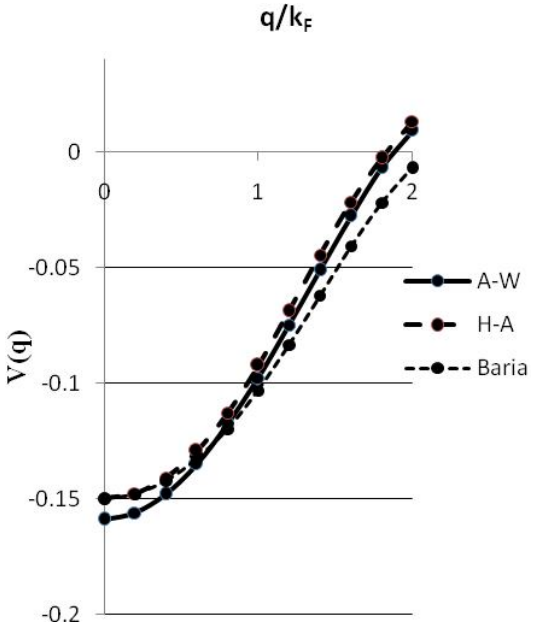

Fig.1. the comparison of the present pseudopotential formfactor (H-A) with local (3) and Non-local (8) for Na

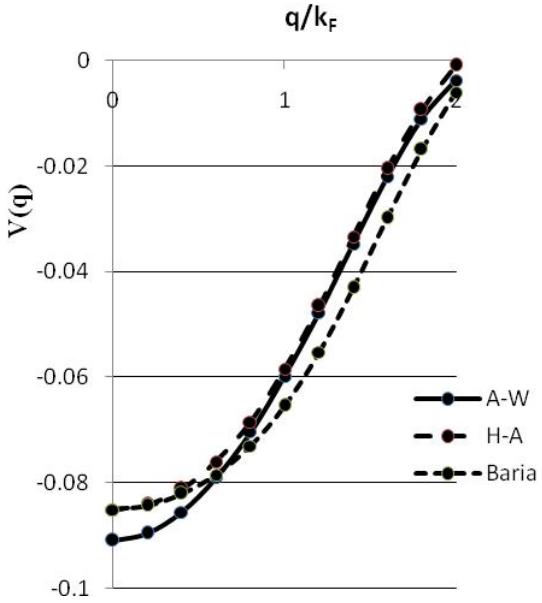

Fig.3. the comparison of the present pseudopotential formfactor (H-A) with local (3) and Non-local (8) for Rb

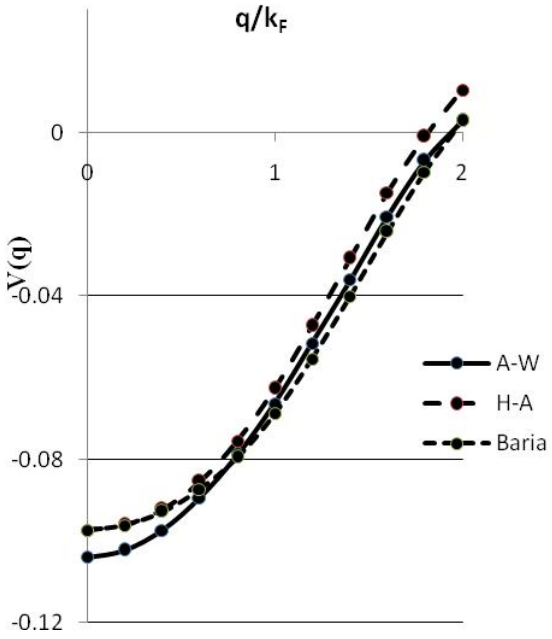

Fig.2. the comparison of the present pseudopotential formfactor (H-A) with local (3) and Non-local (8) for K

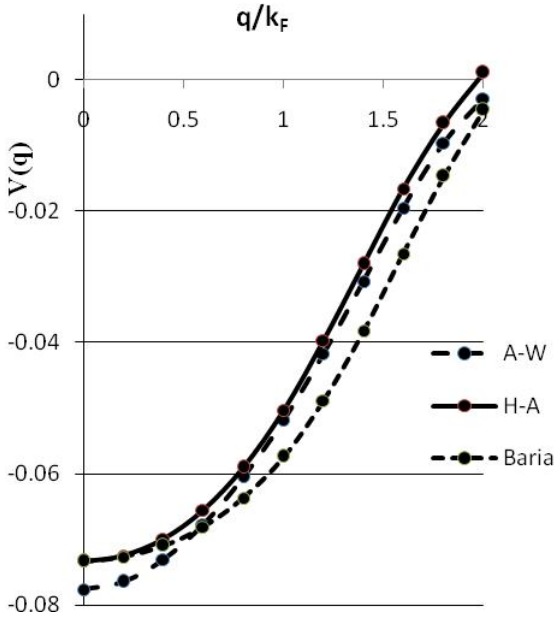

Fig.4. the comparison of the present pseudopotential formfactor (H-A) with local (3) and Non-local (8) for Cs

Acknowledgements

Computational facilities developed using financial assistance provided by Department of Science and Technology (DST), New Delhi through the DST-FIST (Level-1) project (SR/FST/PSI-001/2006), have been utilized to carry out this work.

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