Journal of the Nigerian Association of Mathematical Physics
Volume **19 (November, 2011), pp 519 – 526**

Effects of Screening on the Thermal Resistivity And Compressibility Ratio of Metals

Osiele O. M.[1]* and Adesakin G. E.[2] and Otobo S. I.[3]

[1]Department of Physics,
Federal University of Technology, Akure, Nigeria.
[2]Department of Physics
University of Ado-Ekiti, Ado-Ekiti, Nigeria.
[3]School of General Studies
Auchi Polythenics, Auchi.

Abstract

Models for computing thermal resistivity, compressibility ratio, and screening parameter of metals was developed and used to study the effects of screening on the thermal resistivity and compressibility ratio of metals. The results obtained revealed that the thermal resistivity of metals increases with an increase in the electron gas parameter. It also increases with an increase in the screening parameter showing that the screening in metals affects the thermal resistivity of metals. The results obtained further revealed that thermal resistivity of metals increases with increase in temperature. On the compressibility ratio, the results obtained shows that the compressibility ratio decreases with an increase in the electron gas parameter. Also, the compressibility ratio decreases with an increase in the screening parameter.

Keywords: Thermal resistivity, compressibility ratio, screening, screening parameter and metals.

1. Introduction

Transport processes in solids leads to electrical conductivity, thermal conductivity, thermal resistivity etc. These are affected by electron-electron, electron-impurity and electron-phonon scattering. These scattering processes are temperature dependent. Carriers in conductors move in a definite direction under applied fields and temperature gradients. At the same time they will also be scattered by impurities, defects, and lattice vibrations. The circumstances in which electrons are scattered in a material determines its conductivity or resistivity [1]. Over the years, the thermal resistivity of solids has been studied both theoretically and experimentally. Pecheur and Toussaint [2] applied the Mannori-Ziman-Bayn theory to calculate the thermal resistivity anisotropy of zinc and cadmium in two symmetry directions. The results obtained revealed that thermal resistivity is temperature dependent, and it increases with increase in temperature. The calculation introduced an inelastic contribution peculiar to anisotropic metals. Numerical calculations using inelastic contribution, empirical form factors and experimental phonon spectra revealed that the inelastic contribution could explain the low-temperature behaviour of zinc.

Prakash and Hemkar [3] studied the electrical and thermal resistivities of alkali metals and their temperature dependence in the free electron approximation using the model of Behari and Tripathi [3] for the phonon spectrum. The results they obtained were compared with experimental values and it was found that the results followed the same trend as the experimental values but the agreement with experimental values was poor. Kus [4] studied the electronic thermal resistivity of potassium and lithium and their dilute alloys using two new functional which gives the energy dependence of the trial function. He found that the effect of anitropy was negligible for lithium. He also studied the deviation of dilute potassium alloy from Mathiessen's law. MacDonald and Geldart [5] developed a simple approximation that gave the values of electron-electron contribution to the thermal resistivity of simple metals that are in good agreement with experimental values. The metals were modelled using electron gas with electronic mass and electron-electron interaction to account for crystalline effects. They compared their values of electron-electron scattering contribution to thermal resistivity with the ones published by Kukkonen and Wilkin [6] and found that apart from Al, their results were generally lower for the metals investigated.

[1]*Corresponding authors: ***Osiele O. M.*** E-mail: osiele2001@yahoo.co.uk -, Tel. +2348034437202

Iwamoto [7] studied the effect of screening on the thermal resistivity of alkaline metals by using the screened Coulomb interaction with effective potential composed of the bare Coulomb potential divided by the dielectric function using the static long wavelength limit of the dielectric function. He compared the results obtained with experimental values and the results obtained using other models. The results he got were closed to experimental values and he found that the thermal resistivity of metals is affected by ionic core polarization and band mass. Lundmark [8] studied the exchange and correlation contribution to electron-electron scattering part of the thermal resistivity in Na and K using a Fermi liquid model. He found that at high pressures, the local density approximation (LDA) dielectric function gave results for thermal resistivity of metals that are twenty times higher than results from other dielectric functions or experimental results.

Lundmark [9] calculated the electron-electron scattering contribution to the thermal resistivity of sodium (Na) and potassium (K) for various pressures using isotropic Fermi –liquid model. The fractional Umklapp scattering function calculated in the work were hundred times higher than the most commonly accepted values. This caused the electron-electron scattering part of the thermal resistivity to be five percent higher when compared with earlier calculations where the Umklapp scattering function was omitted.

In this work, we develop models for computing the thermal resistivity, compressibility ratio, and screening parameters of metals. Based on the results obtained from the computing, the effects of screening on the thermal resistivity and compressibility ratio of metals will be studied in order to get an insight into how thermal resistivity and compressibility of metals is affected by screening in the metals.

2. 0 Theoretical Consideration

2.1 Thermal Resistivity of Metals

The thermal resistivity of metals is given [10] as

$$W = \left(\frac{3}{c_v v_f^2}\right)\left(\frac{2\pi^2}{3k\tau_0}\right) \tag{1}$$

where c_v is specific heat capacity, v_f is the Fermi velocity, τ_0 and k are related to the angular averages of the scattering rate.

For a quasiparticle at the Fermi surface, the relaxation time is $2\tau_{0/\pi}{}^2$, where $1/\tau_0$ is proportional to an angular average of the scattering rate i.e

$$\frac{1}{\tau_0} = \left(\frac{m^3(k_B T)^2}{8\pi^4\hbar^6}\right)\frac{1}{2\pi}\int_0^{\pi} d\phi \int_0^{\pi} \frac{\sin\theta' d\theta' w(\theta',\phi)}{\cos\frac{1}{2}\theta'} \tag{2}$$

where $w(\theta',\phi)$ is the collision probability, θ' is the angle between the two incoming particles, ϕ is the angle between the planes of the incoming particles and that of out going particles. For scattering of electrons at the Fermi surface, ϕ is identical with the centre of mass scattering angle θ between the incoming and outgoing relative momenta:

$$\phi = \theta \tag{3}$$

The incident energy in terms of the two incoming momenta leads to

$$\cos\theta' = 1 - \frac{E}{E_F} \tag{4}$$

The transition rate for the collision $\vec{k}_1\sigma_1 + \vec{k}_2\sigma_2 \rightarrow \vec{k}_1'\sigma_1' + \vec{k}_2'\sigma_2'$ is obtained through the Thomas-Fermi golden rule [11] as

$$w(k_1\sigma_1, k_2\sigma_2, k_1'\sigma_1', k_2'\sigma_2') = \frac{2\pi}{\hbar}\left|v(|k_1 - k_1'|)\delta\sigma_1\sigma_1'\delta\sigma_2\sigma_2' - v(|k_1 - k_2'|)\delta\sigma_1\sigma_2\delta\sigma_2\sigma_1\right|^2 \tag{5}$$

where the delta functions of momentum and energy have been left out and σ is the scattering cross section and the potential v(k) is

$$v(k) = \int \exp i(k.r)v(r)dr = -\left(\frac{2\pi\hbar^2}{\mu}\right)f(\theta) \tag{6}$$

where f(θ) is the scattering amplitude in the centre of mass system on the Born approximation, μ is the reduced mass and $\hbar$ is the normalized Planck's constant. For the potential under consideration,

$$f(\theta) = \frac{1}{k_s^2 + k} \tag{7}$$

where k is the wave vector and k_s is the screening wave vector . The transition rate w(θ,ϕ) in equation (2) is obtained by

multiplying equation (5) by ¼ because equation (1) implicitly include the sum over final spins. Hence

$$w(\theta^{'},\phi)=\left(\frac{2\pi}{\hbar}\right)\left(\frac{2\pi\hbar^2}{\mu}\right)^2\frac{\sigma(\theta)}{2} \tag{8}$$

where

$$\sigma(\theta)=\left[|\ f(\theta)|^2\ \right]+|\ f(\pi-\theta)|^2\ -\mathrm{Re}\ ff(\theta)f^*(\pi-\theta) \tag{9}$$

Hence equation (1) becomes

$$\frac{1}{\tau_0}=\frac{2(k_BT)^2}{\pi\hbar\left(\frac{e^2}{a_0}\right)}\frac{1}{a_0^2}\left\langle\frac{\sigma(\theta^{'},\phi)}{\cos\frac{1}{2}\theta^{'}}\right\rangle \tag{10}$$

In the Born approximation,

$$\left\langle\frac{\sigma(\theta^{'},\phi)}{\cos\frac{1}{2}\theta^{'}}\right\rangle=\frac{2\sqrt{\beta}a_0^2}{(k_sa_0)^4}\left(\frac{\sqrt{\beta}}{1+\beta}+\sin^{-1}(1+\beta)^{-1/2}-\frac{\beta\cos^{-1}\left[\frac{\beta}{1+\beta}\right]}{\beta(1+2\beta)^{1/2}}\right) \tag{11}$$

and

$$\beta=\left(\frac{k_s}{2k_f}\right)^2 \tag{12}$$

where k_f is the Thomas-Fermi wave vector . The exact result is

$$\left\langle\frac{\sigma(\theta^{'},\phi)}{\cos\frac{1}{2}\theta^{'}}\right\rangle_{exact}=\frac{a_0^2}{4\pi}\int_0^1\frac{du}{(1-u)^{1/2}}\sum(u) \tag{13}$$

where

$$u=\frac{\varepsilon}{2\varepsilon_f} \tag{14}$$

$$\sum(u)=\sigma_0+\frac{a\sigma_1}{2}+\frac{55}{32}\sigma_2+\left(\frac{10\pi}{2\varepsilon_f\mu}\right)\sin\delta_0\sin\delta_2\cos(\delta_0-\delta_2) \tag{15}$$

and

$$\sigma_1(\varepsilon)=\left(\frac{4\pi}{2\mu\varepsilon}\right)(2l+1)\sin^2\delta_1(\varepsilon) \tag{16}$$

It is assumed that phase shifts beyond δ_2 are negligible. Hence

$$w=\frac{16}{3}\frac{m^2a_0^3r_s^3}{\hbar^3}\left(\frac{a_0^2}{4\pi k}\int_0^1\frac{du}{(1-u)^{1/2}}\sum(u)\right)T \tag{17}$$

The integration in equation (17) is carried out numerically. Kukkonen and Smith [11] by setting $k_s=Ar_s^{1/2}k_f$, obtained the Thomas-Fermi value for A as $\left(\frac{4}{9\pi}\right)^{1/6}\left(\frac{4}{\pi}\right)^{1/2}$. They also found that k and the integrand are weakly dependent on r_s and A. They estimated this dependence and obtained the interpolation formula

$$w=1.10x10^{-8}\left(r_s^{5.04}\ /\ A^{3.06}\right)T\quad cmk/W \tag{18}$$

2.2 Screening parameter and Compressibility

The interaction potential between two electrons in a potential is

$$V(q) = \frac{4\pi e^2}{q} \tag{19}$$

As a result of screening, the electrons avoid each other in accordance with Pauli exclusion principle as the mutual Coulomb repulsion between them. This interaction can be written as

$$U_{\text{int}} = \frac{V(q)}{\varepsilon(q)} \tag{20}$$

where ε(q) is the dielectric constant expressed as

$$\varepsilon(q) = 1 + \frac{\lambda_s^2}{q^2} \tag{21}$$

where λ_s is the inverse Thomas Fermi screening length. Hence

$$U_{\text{int}} = \frac{4\pi e^2}{q} \Big/ 1 + \frac{\lambda_s^2}{q^2} \tag{22}$$

so

$$U_{\text{int}} = \frac{4\pi e^2}{q^2 + \lambda_s^2} \tag{23}$$

Fourier transforming we have

$$U_{\text{int}}(r) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} U_{\text{int}}(q) \exp iqrdq \tag{24}$$

$$U_{\text{int}}(r) = \frac{1}{r} \exp\left(-\lambda_s r\right) \tag{25}$$

The effective interaction between an electron on the Fermi surface and the test charge is given [6] as

$$U_{eff} = Z(k_f)\Lambda(k_f, q)U_{\text{int}}(r) \tag{26}$$

where $Z(k_f)$ is the vertex function, $\Lambda(k_f, r)$ is the quasi particle renormalization factor.

Since the two electrons exchange with the screening electrons independently, each electron acquires a vertex correction and the approximate effective interaction between electrons with opposite spins is

$$U_{eff} = \left[Z(k_f)\Lambda(k_f, q)\right]^2 U_{\text{int}}(r) \tag{27}$$

Since Thomas-Fermi screening is used in this work, both $Z(k_f)$ and $\Lambda(k_f,q)$ are taken to be unity.

The compressibility of the uniform electron gas is determined by the second derivative of the total energy with respect to volume.

$$k = \left(V \frac{\partial^2 E}{\partial V^2} \right) \tag{28}$$

The compressibility of the ratio of the non-interacting electron gas k_{free} to that of the interacting electron gas, k is given [12] as

$$\frac{k_{free}}{k} = \left(1 - \frac{4}{\pi} \alpha r_s \gamma_0 \right) \tag{29}$$

where $$\gamma_0 = \frac{1}{4} - \frac{\pi\alpha}{24} r_s^5 \frac{d}{dr_s}\left(r_s^{-2} \frac{dE_c(r_s)}{dr_s} \right)$$

r_s is electron density parameter, $\alpha = \left(4/9\pi\right)^{1/3}$ and E_c is the correlation energy per electron.

The correlation energy used in this work is that of Caperley and Alder [13] as parameterized by Perdew and Zunger [14] expressed as

$$E_c = \frac{-0.1423}{1+1.0529r_s^{1/2}+0.3334r_s} \quad (30)$$

In the long wavelength limit, the effective interaction is determined by the compressibility i.e

$$U_{eff} = \frac{4\pi}{\lambda_s^2}\left[\frac{k}{k_{free}}\right] \quad (31)$$

where λs is the screening parameter expressed as [15]

$$\lambda_s = \frac{r^{1/2}}{1.56318} \quad (32)$$

The thermal resistivity, compressibility ratio, screening parameter of metals will be computed and the effects of screening on the thermal resistivity and compressibility ratio will be studied.

3.0 Results and Discussion

3.1 Thermal Resitivity

The variation of thermal resistivity computed in this work with electron density parameter r_s is shown in Figure 1. As reveled by Figure 1, for the transition metals and inner transition metals in the high-density limit, $r_s \leq 2.75$ a.u, the computed thermal resistivity of metals in the region is small and varies from one metal to another. But for $3 \leq r_s \leq 5.8$ a.u, the thermal resistivity of metals in this density region increases from one metal to another and their thermal resistivities are high compared to metals in the high-density region. This may be due to the large number of valence electrons found in metals in the low-density region. Furthermore, the results show in Figure 1 reveals that the thermal resistivity of metals is highly affected by the valence electrons in the metals showing that the number of valence electrons in the metals directly affects their thermal resistivities.

Figure 2 shows the variation of thermal resistivity with screening parameter for metals. Figure 2 exhibits the same trend as Figure 1. Figure 2 reveals that the thermal resistivity of metals increases slowly with screening parameter till when the screening parameter is 0.55Å. But when the screening parameter is above 0.57Å, the thermal resistivity increases exponentially with the screening parameter. Figure 2 seems to suggest that the screening between the electrons affects the thermal resistivity of the metals as metals with small screening parameter have small thermal resistivities and metals with high screening parameter have high thermal resistivities.

Figures 3 shows the variation of thermal resistivity with temperature for alkali metals. As the temperature increases, the thermal resitivity of alkali metals increases. The variation of thermal resistivity with temperature obtained in this work is in good agreement with the results of [2]. This may be due to the fact that increase in temperature causes an increase in electron-electron interaction with a consequential increase in the thermal resitivity of the metals.

3.2 Compressibility Ratio

Figure 4 shows the variation of compressibility ratio with electron gas parameter for different metals calculated using equation (29). Figure 4 reveals that the compressibility ratio decreases with an increase in the electron gas parameter. The decrease in compressibility ratio as the electron gas parameter increases seem to suggest that electrons in metals in the high density limit have lower polarizability and higher compressibility while electrons in metals in the low-density limit have high polarizability and low compressibility. The trend exhibited by the compressibility ratio suggests that the higher the number of valence electrons the smaller is the compressibility ratio. The compressibility ratio obtained in this work is in perfect agreement with the theoretical prediction of [6].

Figure 5 shows the compressibility ratio as a function of screening parameter. As revealed in Figure 5, the compressibility ratio decreases with increase in the screening parameter. This suggests that metals with high screening parameters like the alkali metals has small compressibility ratio. Also, this seems to suggest that compressibility ratio of metals is inversely affected by screening in the metals.

The results obtained for thermal resistivity of metals in this work follows the same trend as the results obtained by Iwamoto [7]. The difference between our results and that of Iwamoto [7] may be due to the band mass which he put into put into consideration which we did not put into consideration. The results obtained for compressibility ratio in this work is an improvement over the work of Browen [12] and that of Kukkonen and Wilkins [6]. The improvement arises from the correlation energy used in this work as the correlation energy affects compressibility ratio.

4.0 Conclusion

The effects of screening on the thermal resistivity and the compressibility ratio of metals have been successfully studied. From the study, it was found that the thermal resistivity of metals increases with an increase in temperature, also, thermal resitivity of metals if affected directly by electron-electron interaction and the thermal resistivity of metals is directly affected by the screening parameter. The compressibility ratio depends inversely on the polarizability of the metal and it decreases with an increase in the screening parameter.

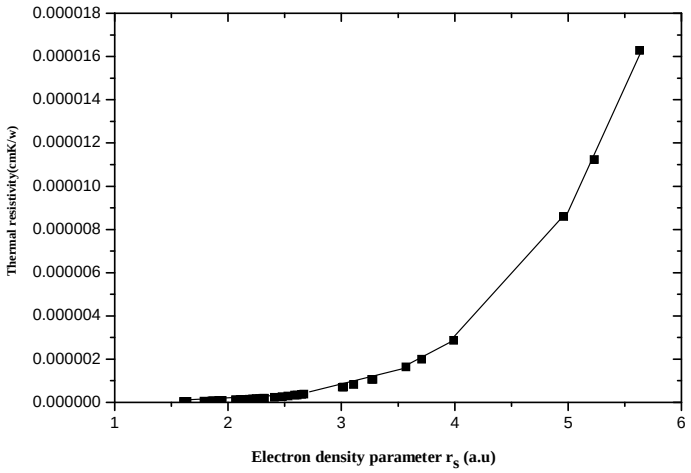

Fig. 1: Variation of thermal resitivity with electron density parameter of metals.

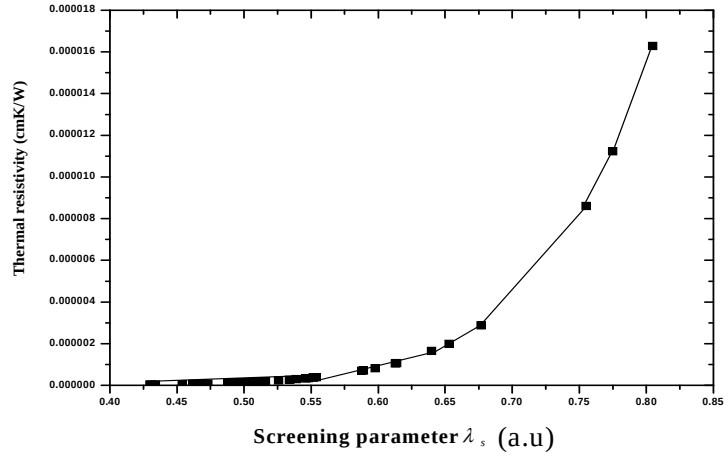

Fig.2: Variation of thermal resistivity with screening parameter

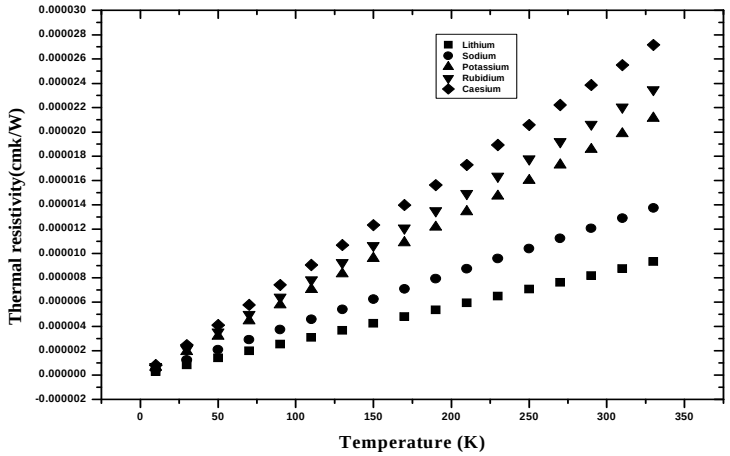

Fig.3: Variation of thermal resistivity with temperature for alkali metals.

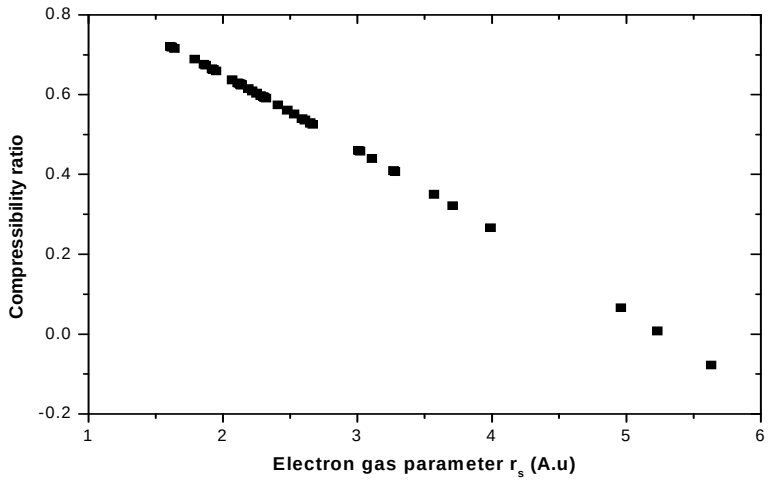

Fig. 4: Variation of compressibility ratio with electron gas parameter

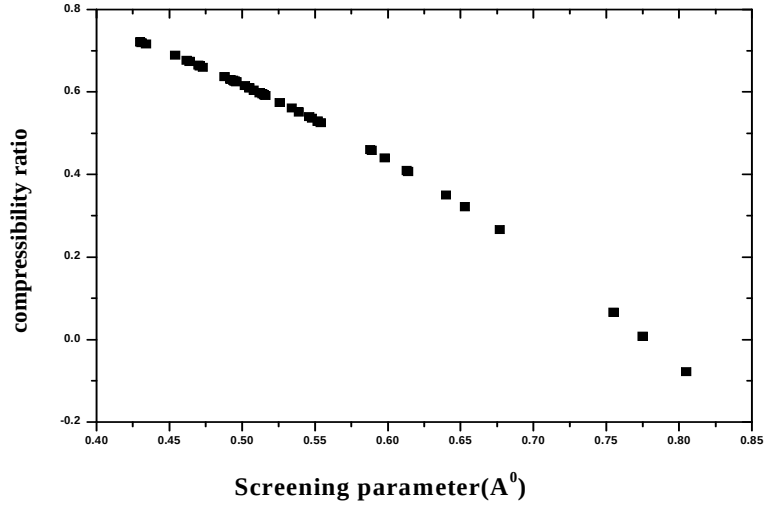

Fig. 5: Variation of compressibility ratio with screening parameter

References

[1] Duan, F. and Guojun, J. (2005) Introduction to Condensed Matter Physics, Vol. 1, World Scientific Publishing Co. Pte.Ltd. P. 199.

[2] Pecheur, P. and Toussaint, G. (1973) Thermal resistivity anisotropy of Zinc and Cadmium. Physical Review B, Vol. 7, No.4, 1223 – 1226.

[3] Prakash, J. and Hemkar, M.P. (1974) Electrical and Thermal Resistivities of Alkali Metals. Journal of Physics F: Metal Physics, Vol. 4, 1015 – 1023.

[4] Kus, F.W. (1976) Electronic thermal resistivity of potassium and lithium. Journal of Physics F: Metal Physics Vol.6, No.1, 59 – 71.

[5] MacDonald A.H. and Geldart D.J.W. (1980) Electron-electron scattering and thermal resistivity of simple metals. Journal of Physics F: Metal Physics, Vol. 10, 677 -692.

[6] Kukkonen, C. A. and Wilkins, W.J. (1979) Electron-electron scattering in simple Metals. Physical Review B, Vol. 19, No. 12, 6075 – 6093.

[7] Iwamoto N. (1999) Effect of screening on thermal resistivity of metals due to electron-electron scattering. Physical Review B, Vol. 59, No. 15, 9687 -9690.

[8] Lundmark, L. (1996) The exchange and correlation contribution to the electron-electron scattering part of the thermal resistivity in alkali metals. Journal of Physics: Condensed Matter, Vol. 8, 1021 – 1040.

[9] Lundmark, L. (1990) The Umkplapp Scattering contribution to the electron-electron scattering part of the thermal resistivity in alkali metals. Journal of Physics: Condensed Matter Vol. 2, 9309 – 9322.

[10] Jensen, H.H., Smith H. and Wilkins J.W. (1969) Upper and lower bounds on transport coefficients arising from a linearized Boltzmann Equation. Physical Review Vol. 185, No. 1, 323 – 337.

[11] Kukkonen, C. A. and Smith, H. (1973) Validity of the Born Approximation as applied to electron-electron scattering in metals: Implications for thermal conductivity. Physical Review B, Vol. 8, No. 10, 4601 – 4606.

[12] Bowen, C., Sugiyama, G. and Alder B.T, (1974) Static response of the electron gas. Physical Review B, Vol. 50, No. 20, 14838 – 14848.

[13] Caperley, D. M, and Alder B.J. (1980) Ground state of the electron gas by a stochastic method. Physical Review letters 45, 566 -569.

[14] Perdew J.P and Zunger A. (1981) Self -interaction correction to density functional approximation for many electron systems. Physical Review B, vol. 23, No. 10, 5048 -5079.

[15] Kiejna, A. and Wojciechoski, K. F. (1996) Metal surface Electron Physics, Elsiever Science ltd. UK p. 275.

.