

Residual Resistivity of Some Metallic Elements

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In the present article, the residual resistivity of some metallic elements of the periodic table is reported on the basis of model potential formalism. Ashcroft's well known empty core (EMC) model potential is explored first time with five different types of the local field correction functions proposed by Hartree (H), Taylor (T), Ichimaru-Utsumi (IU), Farid et al (F) and Sarkar et al (S) to investigate the effect of the exchange and correlation on the aforesaid properties. The comparisons of presently computed results are found in qualitative agreement with available theoretical and experimental findings. Present investigation of the residual resistivity is found to be quite sensitive to the selection of local field correction function and showing a significant variation with the change in the function.

Keywords : Pseudopotential; residual resistivity; metallic elements

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I. INTRODUCTION

It is well known that lattice defects and impurities destroy the periodicity of the lattice. The defects are intrinsic to real crystals and determine or modify the properties of real materials. For example, the point defects such as vacancies and interstitials modify the electrical properties because they contribute to the residual resistivity. The main source of the residual resistivity is the scattering of conduction electrons by phonons. Other source of resistance due to lattice imperfections are : (i) replacement of one atomic species by another atomic species, (ii) disappearance of an atom (or ion) from one site with its emergence at another site, (iii) displacement of an atom around a distorted site and (iv) stacking fault. The resistance due to these static imperfections (and grain boundaries) is called residual resistance. At low temperatures, the residual resistance due to such imperfections can be significant. This is because at low temperatures the excited phonons carry little momentum and deflect the electron through a small angle, which makes little contribution to the resistivity. At high temperatures, the contribution due to imperfections is small compared to that due to scattering of the conduction electrons by phonons. The absence of an atom or an ion at a lattice site (i.e. a vacancy) also contributes to the residual resistivity or residual resistivity, which modifies the potential at that site and acts as a perturbation to the conduction electrons. These vacancies are among the static imperfection [1-10].

Recently, Vora et al [1-5] have reported the residual resistivity of some metallic elements and their dilute alloys.

In the present paper, we thought it worthwhile to undertake the investigation of the contribution of the residual, which is one of the point defects, to the resistivity of some metallic elements of the different groups of the periodic table. Ashcroft's well known empty core (EMC) model potential [11] along with five different types of the local field correction functions proposed by Hartree (H) [9], Taylor (T) [12], Ichimaru-Utsumi (IU) [13], Farid et al (F) [14] and Sarkar et al (S) [15] are used to study the screening dependence of the residual resistivity. The motivation of the present investigation comes from the fact that while there have been a few scattered attempts at studying the residual resistivity of metals [2-4, 8-10], yet nobody has fully explored the investigation for a large number of metallic elements on the basis of a single model potential, with the same criteria to determine the parameters of the potential.

II.COMPUTATIONAL METHODOLOGY

Within the framework of the pseudopotential formulation, for low vacancy concentration and neglecting lattice distortion, the formula for residual resistivity can be derived using standard scattering theory giving the pseudopotential associated with the vacancy as [1-5]

$$\rho_v = \frac{3}{16 \hbar n e^2 v_F^2} \int_0^2 \int_{\Omega'} x^3 |W(x)|^2 dx d\Omega'.$$

(1)

Where n is the ion number density, v_F the Fermi velocity, k_F the Fermi wave vector, Ω' the solid angle in the scattering vector space, $W(x)$ the screened form factor of electron-ion interaction and $x = q/k_F$ with q the momentum transfer wave vector. For the residual resistivity of metallic elements, the Eq. (1) is written as [1-4]

$$\rho_v = \frac{3 \pi m \Omega_o C}{8 \hbar e^2 E_F} \int_0^2 |W(x)|^2 x^3 dx.$$

(2)

Here, Ω_o , C and $W(x)$ are the atomic volume of the metallic elements, the atomic fraction of the impurity and form factor of metals, respectively.

In the present work, we have calculated ρ_v by applying Ashcroft's well known empty core (EMC) model potential [11] including five different types of the local field correlation functions [12-16]. The bare ion model potential $W_B(r)$ in r -space explored in the present investigation is of the form (in atomic units) [11],

$$W_B(r) = 0 \quad ; \quad \text{for } r < r_c$$

$$= -\frac{Ze^2}{r} \quad ; \quad \text{for } r \geq r_c.$$

(3)

Where Z is the valence, r_c the parameter of the model potential and e the electronic charge. This EMC model potential is a local pseudopotential which makes an effectively complete cancellation of the true potential in the region $r < r_c$. The Fourier transform of this EMC model potential is given by,

$$W(q) = \frac{-4\pi Ze^2}{\Omega_o q^2 \epsilon(q)} \cos(qr_c),$$

(4)

here, $\epsilon(q)$ is the modified Hartree dielectric function, which is written as [12]

$$\epsilon(q) = 1 + (\epsilon_H(q) - 1)(1 - f(q)).$$

(5)

Where $\epsilon_H(q)$ is the static Hartree dielectric function and the expression of $\epsilon_H(q)$ is given by [12],

$$\epsilon_H(q) = 1 + \frac{me^2}{2\pi k_F \hbar^2 q^2} \left(\frac{1-\eta^2}{2\eta} \ln \left| \frac{1+\eta}{1-\eta} \right| + 1 \right); \eta = \frac{q}{2k_F}$$

(6)

While $f(q)$ the local field correction function. In the present investigation, the local field correction functions due to H [12], T [13], IU [14], F [15] and S [16] are incorporated to see the impact of exchange and correlation effects. The details of all the local field corrections are below.

The H-screening function [12] is purely static, and it does not include the exchange and correlation effects. The expression of it is,

$$f(q) = 0.$$

(7)

Taylor (T) [13] has introduced an analytical expression for the local field correction function, which satisfies the compressibility sum rule exactly. This is the most commonly used local field correction function and covers the overall features of the various local field correction functions proposed before 1972. According to T [13],

$$f(q) = \frac{q^2}{4k_F^2} \left[1 + \frac{0.1534}{\pi k_F^2} \right].$$

(8)

The IU-local field correction function [14] is a fitting formula for the dielectric screening function of the degenerate electron liquids at metallic and lower densities, which accurately reproduces the Monte-Carlo results as well as it also, satisfies the self consistency condition in the compressibility sum rule and short range correlations. The fitting formula is

$$f(q) = A_v Q + B_v Q^3 + C_v + \left[A_u Q + \left(B_u + \frac{8A_v}{3} \right) Q^3 - C_u \right] \left[\frac{4-Q}{4Q} \ln \left| \frac{2+Q}{2-Q} \right| \right]$$

(9)

On the basis of IU [14] local field correction function, Farid et al. (F) [15] have given a local field correction function of the form

$$f(q) = A_F Q^4 + B_F Q^2 + C_F + [A_F Q^4 + D_F Q^2 - C_F] \left\{ \frac{4-Q^2}{4Q} \ln \left| \frac{2+Q}{2-Q} \right| \right\} \quad (10)$$

Based on Eqs. (9-10), Sarkar et al. (S) [16] have proposed a simple form of local field correction function, which is of the form

$$f(q) = A_S \left\{ 1 - (1 + B_S Q^4) \exp(-C_S Q^2) \right\}. \quad (11)$$

Where $Q = q/k_F$. The parameters $A_{IU}, B_{IU}, C_{IU}, A_F, B_F, C_F, D_F, A_S, B_S$ and C_S are the atomic volume dependent parameters of IU, F and S-local field correction functions. The mathematical expressions of these parameters are narrated in the respective papers of the local field correction functions [14-16].

III. RESULTS AND DISCUSSION

The input parameters and constants used in the present calculations are given in Table 1. The input parameters and constants used in the present calculations are given in Table 1. Most of the input parameters used in the present computation are in atomic units (au). The parameter of the model potential is determined using the first zero of the form factor [1-6]. The other input parameters are taken from the literature [17]. The residual resistivity of metallic elements are narrated using five local field correction functions viz; H [12], T [13], IU [14], F [15] and S [16] in Table 2 with other such available theoretical [2, 7, 9] and experimental [10] findings.

From the study of Table 2, it can be noted that, the present findings of the residual resistivity of some metallic elements are found to be quite comparable and compatible with other such theoretical [2, 5, 7] and experimental [8] data. It is noted from the Table 2 that, among the five employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives the minimum numerical value of the residual resistivity, while the local field correction function due to F gives the maximum value of the residual resistivity. The residual resistivity of 'Rb' element is found higher than other alkali elements because the atomic volume of 'Rb' element is larger than in comparison with other alkali metals.

In comparison with the static H-screening function, the percentile influences of various local field correction functions due to T, IU, F and S-local field correction functions for Li, Na, K, Rb, Cs, Cu, Ag, Au, Be, Mg, Ca, Zn, Cd, Hg, Al, Ga, In, Tl, Si, Ge, Sn, Pb, Sb and Bi are found of the order of 39.10%-83.17%, 46.53%-99.59%, 56.14%-125.44%, 59.59%-135.75%, 61.04%-136.36%, 27.91%-51.16%, 30.61%-53.06%, 28.57%-53.02%, 18.03%-39.34%, 30.06%-61.27%, 36.41%-71.84%, 25.00%-51.72%, 23.38%-59.38%, 29.25%-74.72%, 22.56%-46.62%, 23.64%-50.30%, 27.00%-56.96%, 28.35%-59.39%, 20.79%-47.03%, 22.07%-48.65%, 24.28%-51.44%, 25.00%-45.83%, 22.91%-49.09% and 23.75%-43.13%, respectively.

The calculated results of the residual resistivity for Al and Pb metallic elements deviate 11.36%-39.55% and 657.89%-1005.26% from the experimental findings [10], respectively. The presently computed results of the residual resistivity of 'Al' metal are found lower than the experimental data [10], while those for 'Pb' metal are found higher than the experimental data [10]. This may be due to the EMC model potential is not found suitable with H, T, IU, F and S-local field correction functions for these two metallic substances, while in the present case, the presently computed results of the residual resistivity for 'Al' and 'Pb' metallic elements are found in qualitative agreement with available theoretical data [2, 7, 9]. The present comparison with available theoretical [2, 7, 9] and experimental [10] data is highly encouraging. Out of 24 metallic elements, we do not have either theoretical or experimental comparison for 17 metals. The present yielding of the residual resistivity of the metallic elements of the different groups of the periodic table are highly affected by the impurity atoms because they contribute the point defects in the lattice structure of the metallic elements.

The quantitative difference between the present calculation and the experimental results, in spite of good qualitative agreement can be attributed to following conditions : (1) the sampling conditions of the experiments, (2) the short supply of data in the long wave vector region and (3) the low or high effectiveness of the dielectric screening functions used for the calculation of the residual resistivity of the metallic substances.

The H-dielectric function is purely static and it does not include the exchange and correlation effects. The IU-local field correction function is a fitting formula for the dielectric screening function of the degenerate electron liquids at metallic and lower densities, which accurately reproduces the Monte-Carlo results as well as it also satisfies the self consistency condition in the compressibility sum rule and short range correlations. On the basis of IU local field correction function, Farid et al. (F) have

given a local field correction function. Hence, F-function represents same characteristic nature.

The numerical value of the residual resistivity is found to be quite sensitive to the selection of the local field correction function and showing a significant variation with the change in the function.

Thus, the calculation of the residual resistivity is one of the sensitive test for the proper assessment of the form factor of the model potential and in the absence of experimental information such calculations may be considered as one of the guidelines for further investigations either theoretical or experimental.

In contrast with the reported studies, the present study spans the metallic elements of the different groups of the periodic table on a common platform of the model potential and common criteria for evaluating parameter of the model potential. This is very much essential for obtaining concrete conclusions.

IV.CONCLUSIONS

Lastly we concluded that, the residual resistivity of large number of metallic elements of the different groups of the periodic table using EMC model potential with five different types of local field correction functions is reported for the first time. The EMC model potential with more advanced IU, F and S-local field correction functions generate consistent results regarding the residual resistivity. Hence, the EMC model potential is found suitable for studying the residual resistivity of the metallic elements. Also, the present investigation predicts that the present study of the residual resistivity of metallic elements is sensitive to the selection of the proper local field correction function.

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Table 1. Input parameters and constants used in the present calculations.

Metal s	Z	Ω_o (au) \AA^3	k_F (au)	r_C (au)
Li	1	144.9	0.5890	0.7738
Na	1	254.5	0.4882	1.0765
K	1	481.4	0.3947	1.3880
Rb	1	587.9	0.3693	1.4837
Cs	1	745.5	0.3412	1.9108
Cu	1	79.4	0.7198	1.1540
Ag	1	115.0	0.6370	1.3449
Au	1	114.0	0.6382	1.3475
Be	2	54.4	1.0287	0.7153
Mg	2	155.9	0.7242	0.8568
Ca	2	290.0	0.5890	1.1658
Zn	2	102.0	0.8342	0.7915
Cd	2	144.8	0.7423	0.8483
Hg	2	157.8	0.7213	1.0658
Al	3	111.3	0.9276	0.7306
Ga	3	131.4	0.8776	0.7336
In	3	175.3	0.7972	0.7341
Tl	3	191.7	0.7738	0.7395
Si	4	134.3	0.9590	0.6364
Ge	4	151.8	0.9205	0.6605
Sn	4	181.5	0.8674	0.7120
Pb	4	203.4	0.8350	0.9637
Sb	5	204.0	0.8986	0.6990
Bi	5	239.4	0.8520	0.9751

Table 2. Residual resistivity (ρ_v) of metals (in $\mu\Omega - \text{cm} / \text{at} \%$).

Metals	Present results					Expt. [10]	Others [2, 7, 9]
	H	T	IU	F	S		
Li	2.02	3.39	3.66	3.70	2.81	—	0.20, 0.302, 0.359, 0.398, 0.40, 0.421, 0.469, 0.475, 0.495, 0.578, 0.592, 0.719, 0.763, 0.869, 0.88, 0.995, 0.964, 1.364, 1.466, 1.504, 2.724, 3.50
Na	2.45	4.42	4.82	4.89	3.59	—	0.204, 0.207, 0.242, 0.251, 0.406, 0.481, 0.491, 0.50, 0.602, 0.67, 0.737, 0.77, 0.774, 0.785, 0.798, 0.802, 0.895, 0.933, 1.061, 1.137, 1.138, 1.166, 1.276, 1.32, 1.376
K	3.42	6.87	7.59	7.71	5.34	—	0.172, 0.3, 0.323, 0.398, 0.452, 0.474, 0.534, 0.562, 0.759, 0.806, 0.85, 0.879, 0.927, 0.978, 0.98, 0.989, 1.0, 1.03, 1.188, 1.239, 1.45, 1.521, 1.53, 1.656, 1.66, 1.799
Rb	3.86	8.07	8.94	9.10	6.16	—	0.385, 0.414, 0.732, 0.84, 0.84, 0.893, 0.914, 0.95, 1.02, 1.06, 1.079, 1.095, 1.200, 1.24, 1.339, 1.401, 1.719, 1.878, 1.89, 2.046
Cs	3.08	6.44	7.17	7.28	4.96	—	0.21, 0.288, 0.383, 0.63, 0.711, 0.938, 1.140, 1.153, 1.451, 1.51, 1.747, 1.795, 1.824, 1.917, 1.931, 1.95, 2.512, 2.733, 3.230, 5.237
Cu	0.43	0.61	0.65	0.65	0.55	—	—
Ag	0.49	0.71	0.75	0.75	0.64	—	—
Au	0.49	0.70	0.74	0.74	0.63	—	—
Be	0.61	0.81	0.85	0.85	0.72	—	—
Mg	1.73	2.60	2.77	2.79	2.25	—	—
Ca	2.06	3.27	3.52	3.54	2.81	—	—
Zn	1.16	1.66	1.75	1.76	1.45	—	—
Cd	1.60	2.39	2.54	2.55	2.07	—	—
Hg	1.06	1.54	1.63	1.64	1.37	—	—
Al	1.33	1.85	1.94	1.95	1.63	2.2	0.455, 0.50, 0.50, 0.632, 0.659, 0.67, 0.68, 3.42
Ga	1.65	2.34	2.46	2.48	2.04	—	—
In	2.37	3.49	3.70	3.72	3.01	—	—
Tl	2.61	3.88	4.12	4.16	3.35	—	—
Si	2.02	2.81	2.95	2.97	2.44	—	—
Ge	2.22	3.11	3.28	3.30	2.71	—	—
Sn	2.43	3.47	3.66	3.68	3.02	—	—
Pb	1.44	1.99	2.09	2.10	1.80	0.19	0.15, 0.81, 0.86, 1.23, 1.793, 1.85
Sb	2.75	3.87	4.08	4.10	3.38	—	—
Bi	1.60	2.19	2.29	2.29	1.98	—	—