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Residual resistivity of simple metals and their dilute alloys

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Ashcroft's empty core (EMC) model pseudopotential is used to study the residual resistivity of simple metals viz. Li, Na, K, Rb, Cs, Al, Pb as well as Al and Pb based dilute alloys. Three different types of local field correction functions proposed by Hartree (H), Taylor (T) and Ichimaru-Utsumi (IU) are used to investigate the effect of the exchange and correlation on the aforesaid property. The presently obtained results are compared with the other such theoretical and experimental data wherever exists. The comparison is highly encouraging. The investigation of the residual resistivity is found to be quite sensitive to the selection of the local field correction function, showing significant variation with the change in the function. Our conclusion suggests that similar study could be extended to other metallic elements and dilute alloys.

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1. 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 defect such as vacancies and interstitials modify the electrical properties because they contribute to the residual resistivity. The main source of residual resistivity is the scattering of conduction electrons by phonons. The 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, (iv) stacking fault etc. The resistance due to these static imperfections (and grain boundary) is called residual resistance. At low temperature the residual resistance due to such imperfections can be significant. This is because at low temperatures the excited phonons which carry little momentum and deflect the electron through a small angle, makes little contribution to the resistivity. At high temperatures the contribution due to imperfections is small compared to that due to scattering the conduction electrons by phonons. The absence of an atom or an ion at a lattice site (i.e. vacancy) also contributes to the 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 [1-13].

Harrison [4] has reported residual resistivity of 43 dilute alloys by adopting point ion model potential. He has adjusted the potential parameters of the point ion model potential to optimize the agreement with experiment. Fukai [8], Kachhava-Parihar [9] and DuCharme-Edwards [10] have used Ashcroft's empty core (EMC) model potential [11]. Though they have used same potential, all of them have adopted different criterion for determining parameter of the potential. Taut and Paasch [12] have used Shaw's model while the phase shift method was adopted by Dickey et al [13] Recently, Vora et al [1, 2] and Gajjar et al [3, 4] have studied the residual resistivity of some simple metals and 122 dilute alloys using model potential [1-4].

In the present paper we have used pseudopotential method to examine the contribution of monovacancy, which is one of the point defects, to the resistivity of seven simple metals viz; Li, Na, K, Rb, Cs, Al and Pb with six Al and Pb based dilute alloys. The local field correction functions due to Hartree (H) [5], Taylor (T) [14] and Ichimaru-Utsumi (IU) [15] are used to study the screening dependence of the residual resistivity. We have applied here the pseudopotential technique to study vacancies because it simplifies the calculations by eliminating the core states and strong potential responsible for binding them. Therefore, the study of residual resistivity of metals and dilute alloys is an interesting one.

2. Theoretical 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 with the pseudopotential associated with the vacancy as [1-4]

$$\rho_v = \frac{3}{16\,\hbar n\, e^2\, v_F^{\,2}} \int_0^2 \int_{\Omega'} x^3 \left| W(x) \right|^2 dx\, d\Omega' . \tag{1}$$

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) is 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 dilute alloys, the equation (1) is modified as [1, 2]

$$\rho_v\,(\text{alloy}) = \frac{3\pi\, m\, \Omega_o\, C}{8\hbar\, e^2\, E_F} \int_0^2 \left| W_2(x) - W_1(x) \right|^2 x^3\, dx. \quad (2)$$

Here Ω_0 is the atomic volume of the host metal, C is the atomic fraction of impurity. $W_1(x)$ and $W_2(x)$ are the form factors of impurity and host metals, respectively.

In the present work we have calculated ρv by applying Ashcroft's empty core (EMC) model potential [11] including three different types of local field correction functions [5, 14, 15]. The form factor explored in the present investigation is of the form, [11]

$$W(q) = \frac{-4\pi Z e^2}{\Omega_o\, q^2\, \varepsilon(q)} \cos(q r_C), \quad (3)$$

were, Z is the valency, Ω_0 the atomic volume, r_C the parameter of the potential, and ε(q) the modified Hartree dielectric function [5].

Using equations (2) and (3), we have simplified the formula of residual resistivity of dilute alloys as

$$\rho_v\,(\text{alloy}) = \frac{4m^2e^2\Omega_0 C}{3\pi\hbar} \int_0^2 \frac{dx}{x\varepsilon(x)} \left[\frac{Z_1}{Z_2} \left(\cos(r_{C1} k_{F2} x)\right) - \left(\cos(r_{C2} k_{F2} x)\right) \right]^2. \quad (4)$$

Here C, r_{C1} and Z_1 are the atomic fraction, potential parameter and valency appropriate to the impurity and Ω_{02}, k_{F2}, ε(x), Z_2 and r_{C2} are the atomic volume, Fermi wave vector, modified Hartree dielectric function, valency and potential parameter of the host metal, respectively. Both integrals in equations (1) and (4) were performed in the physically valid range $0<q\leq 2k_F$ with the step size of 0.01 k_F.

3. Results and discussion

The input parameters i.e. valency Z, Fermi wave vector k_F, volume Ω_0 and parameter of the potential r_C for all metals, which are used in present computation are shown in Table 1. Tables 2-4 show presently calculated values of the residual resistivity of seven simple metals viz; Li, Na, K, Rb, Cs, Al , Pb as well as Al and Pb based dilute alloys using three local field correction functions proposed by H, T and IU along with other available theoretical [1-6] and experimental findings [16].

Table 1. Input Parameters (in au).

Metals	Z	k_F	Ω_o	r_C
Li	1	0.5890	144.9	0.7738
Na	1	0.4882	254.5	1.0765
K	1	0.3947	481.4	1.3880
Rb	1	0.3693	587.9	1.4837
Cs	1	0.3412	745.5	1.9108
Al	3	0.9276	111.3	0.7306
Pb	4	0.8350	203.4	0.9637

The experimentally observed values of residual resistivity are not available for most of the metals and alloys under consideration. From the studies of Tables 2-4 show that, the present findings are comparable and compatible with other such theoretical data [1-6]. It is noted from the Tables 2-4 that for simple metals and their dilute alloys, the local field correction function due to H (without exchange and correlation) gives the lowest numerical values of residual resistivities while the local field correction function due to IU gives the highest values. The relative influence of T and IU local field correction functions with respect to H-function on the residual resistivity of metallic elements is 30.93% – 86.17% and 34.42% – 94.39%, respectively. In the case of Al-based dilute alloys, these influences are found of the order of 30.34% – 49.03% and 34.07% – 56.13%, while in the case of Pb-based dilute alloys, those are found of the order of 20.53% – 48.30% and 38.52% – 62.69%, respectively.

Table 2. Residual resistivity of simple metals ($\mu\Omega$. cm / at %).

Metals	Present results			Expt.	Others
	H	T	IU	[16]	[2-6]
Li	0.8689	1.3648	1.4667	–	0.302, 0.359, 0.475, 0.398, 0.421, 0.495, 0.469, 2.724, 0.592, 0.995, 1.504,0.964, 0.20, 0.88, 3.50,0.40, 0.578, 0.719, 0.763
Na	0.8025	1.2759	1.3763	–	0.602, 0.737, 0.933, 0.785, 0.895, 1.137, 0.406, 0.207, 0.481, 0.204, 0.251, 0.491, 0.798,0.242, 1.166, 1.32, 0.5, 0.67, 0.77, 0.774, 1.061, 1.138
K	0.9899	1.6569	1.7992	–	0.759, 0.927, 1.239, 0.978, 1.188, 1.521, 0.806, 0.534, 0.3, 0.452, 0.879, 0.172, 0.398, 0.323, 0.562, 0.474, 1.66, 0.85, 1.0, 0.98, 1.03, 1.45, 1.53
Rb	1.0956	1.8783	2.0464	–	0.84, 1.02, 1.401, 1.079, 1.339, 1.719, 0.914, 0.732, 0.414, 0.385, 0.893, 1.200, 1.24, 1.89, 0.84, 0.95, 1.06
Cs	0.9388	1.7478	1.8249	–	1.451, 1.795, 2.733, 1.917, 2.512, 3.230, 1.153, 0.288, 0.383, 0.711, 1.95, 5.237, 1.51, 1.140, 1.931, 0.63, 0.21
Al	0.5040	0.6599	0.6775	2.2	0.50, 0.67, 0.632, 0.455, 3.4156
Pb	1.2382	1.7935	1.8513	0.19	0.81, 0.86, 0.150

Table 3. Residual resistivity of Al based alloys ($\mu\Omega$ - cm / at %).

Host	Al					
Impurity	Li	Na	K	Rb	Cs	Pb
H	0.2254	0.3765	0.7319	0.8622	1.4112	1.1785
T	0.2938	0.5056	1.0180	1.2063	1.9937	1.7564
IU	0.3022	0.5279	1.0700	1.2691	2.1030	1.8400
[1]	0.2254, 0.2936, 0.3022	0.3762, 0.5056, 0.5279	0.7318, 1.0178, 1.0700	–	–	1.1767, 1.7538, 1.8400
[4]	0.94	0.74	1.027	–	–	0.54

Table 4. Residual resistivity of Pb based alloys ($\mu\Omega$ - cm / at %).

Host	Pb					
Impurity	Li	Na	K	Rb	Cs	Al
H	0.9215	0.6031	0.4974	0.5049	0.696	0.8116
T	1.3666	0.8581	0.6746	0.6793	0.9411	0.9782
IU	1.4161	0.8838	0.6935	0.6994	0.9782	1.3204
[1]	0.9215, 1.3666, 1.4161	0.6031, 0.8581, 0.8838	0.4974, 0.6746, 0.6935	–	–	0.8116, 1.2564, 1.3204
[4]	0.82	0.77	0.86	–	–	0.28
[9]	–	0.67	–	–	–	–

The residual resistivity of Cs is found higher than that of the other alkali elements because the atomic volume of Cs element is larger in comparison with other alkali metals. Also in Al-based dilute alloys, Al-Cs dilute alloy is found higher results in comparison with other Al-based dilute alloys. While in the case of Pb-based dilute alloys, the Pb-Li dilute alloy is found higher results than other Pb-based dilute alloys. Hence, the impurity elements play an important role in the study of the residual resistivity of the host metals.

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 as one of the sensitive tests 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 some of the guidelines for further investigations either theoretical or experimental. In contrast with the reported studies, the present study spans the simple metals and their dilute alloys on a common platform of model potential and common criteria for evaluating parameter of the model potential. This is essential for drawing concrete remarks.

4. Conclusions

Lastly we concluded that, the present study reports the residual resistivity of simple metals and their dilute alloys using the single parametric model potential with three different types of local field correction functions. The EMC model potential with more advanced IU-local field correction function generates consistent results regarding the residual resistivity of simple metals and their dilute alloys. Hence, the EMC model potential is suitable for studying the residual resistivity of simple metals and their dilute alloys with H, T and IU local field correction functions. Also, the present investigation predicts that the study of residual resistivity is sensitive to the selection of proper local field correction function. Our conclusion also suggests that similar study could be extended to other metallic elements and dilute alloys.

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