Residual Resistivity of Some Metallic Elements by Pseudopotential

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Abstract

A well-established local pseudopotential is used to study the residual resistivity of some metallic elements. Three different types of local field correction functions viz. Hartree (H), Taylor (T) and Ichimaru-Utsumi (IU) are used to investigate the effect the exchange and correlation on the aforesaid studies. The presently obtained results are compared with the other such data wherever exists and found encouraging in nature. This is the first attempt to study the residual resistivity for large number of metallic elements on the basis of single parametric model potential, with the same condition to evaluate the parameter of the potential. This can be useful to judge the trends of the residual resistivity in metallic elements.

1. Introduction

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 monovacancy resistivity. Much attention has been drawn in recent years towards the study of properties of crystals containing point defects i.e. monovacancy [1-10]. Therefore, 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 some metallic elements. The screening function due to Hartree (H) [10], Taylor (T) [11] and Ichimaru-Utsumi (IU) [12] were used to study the screening dependence of the residual resistivity. It is well known that lattice defects and

impurities destroy the periodicity of the lattice. In many important cases the lattice distortion due to such defect can be neglected. 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 is a fascinating task.

2. Computational Technique

Within the framework of the second order pseudopotential formalism, the expression for residual resistivity of metals can be given, using the standard scattering theory as [1-10],

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

Here $x=q/k_F$, n is the ion number density, v_F the Fermi velocity, q the momentum transfer wave vector and Ω' the solid angle in the scattering vector space. The term $|W(q)|^2$ is the integrand indicates that the values of ρ_v will depend sensitively on the many-electron screening through the form factor. Also, the well-recognized model potential $|W(q)|$ is taken from [13, 14]. Here the integral in equation (1) was 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 calculations are given in Table 1.

Table 1 : Input Parameters (in a. u.)

Metals	Z	Ω_O (au)^3	k_F (au)	r_C (au)
Li	1	144.9	0.5890	1.6617
Na	1	254.5	0.4882	2.0049
K	1	481.4	0.3947	2.4796
Rb	1	587.9	0.3693	2.6504
Cs	1	745.5	0.3412	2.8687
Cu	1	79.4	0.7198	1.3598
Ag	1	115.0	0.6370	1.5385
Au	1	114.0	0.6382	1.5341

Be	2	54.4	1.0287	0.9515
Mg	2	155.9	0.7242	1.3515
Ca	2	290.0	0.5890	1.6621
Zn	2	102.0	0.8342	1.1733
Cd	2	144.8	0.7423	1.3186
Hg	2	157.8	0.7213	1.3570
Al	3	111.3	0.9276	1.0552
Ga	3	131.4	0.8776	1.2277
In	3	175.3	0.7972	1.2649
Tl	3	191.7	0.7738	1.1152
Si	4	134.3	0.9590	1.1284
Ge	4	151.8	0.9205	1.1721
Sn	4	181.5	0.8674	1.0632
Pb	4	203.4	0.8350	1.0892
Sb	5	204.0	0.8986	1.1488
Bi	5	239.4	0.8520	1.6617

Table 2 gives presently calculated values of monovacancy resistivity of some metals using three local field correction functions i.e. H, T and IU along with other available theoretical and experimental [2, 3, 4, 6, 7, 8, 10] and theoretical [9] findings.

Table 2 : Residual Resistivity of Alkali Metals (μ Ω - cm / at %)

Metals	Present results			Expt. [9]	Others [2, 3, 4, 6, 7, 8, 10]
	H	T	IU		
Li	0.40	0.61	0.65	–	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	0.46	0.73	0.79	–	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	0.52	0.91	0.99	–	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	0.54	0.97	1.07	–	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	0.57	1.05	1.16	–	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	0.34	0.49	0.52	–	–
Ag	0.38	0.56	0.60	–	–
Au	0.38	0.56	0.60	–	–

Be	0.51	0.67	0.70	–	–
Mg	0.69	0.98	1.04	–	–
Ca	0.80	1.22	1.30	–	–
Zn	0.61	0.85	0.89	–	–
Cd	0.67	0.96	1.01	–	–
Hg	0.69	0.99	1.04	–	–
Al	0.84	1.13	1.18	2.2	0.455, 0.50, 0.50, 0.632, 0.659, 0.67, 0.68, 3.42
Ga	0.95	1.33	1.40	–	–
In	0.97	1.37	1.45	–	–
Tl	0.88	1.20	1.26	–	–
Si	1.18	1.62	1.70	–	–
Ge	1.22	1.69	1.77	–	–
Sn	1.12	1.52	1.59	–	–
Pb	1.44	1.95	2.04	0.19	0.15, 0.81, 0.86, 1.23, 1.793, 1.85
Sb	1.50	2.07	2.17	–	–
Bi	0.40	0.61	0.65	–	–

The experimentally observed values of monovacancy resistivity are not available for most of the metals and alloys under consideration. Such study shows that, the present results are comparable and compitible with such other theoretical and experimental results. It can be noted that for all the metals, the screening function due to Hartree (H) (without exchange and correlation) gives the lowest numerical values of monovacancy resistivities while the screening function due to Ichimaru-Utsumi (IU) gives the highest values. The numerical value of the monovacancy resistivity is found to be quite sensitive to the selection of the local field correction function showing a significant variation with the change in the screening function. Thus the calculation of the monovacancy resistivity as one sensitive investigation for the proper assessment of the form factor and in the absence of experimental evidence such calculations may be considered as one of the procedures for further examinations either theoretical or experimental.

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