

Residual Resistivity of Some Dilute Alloys

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We report on the study of residual resistivity for 122 dilute alloys of 18 hosts of the different groups of the periodic table on the basis of model potential. Our well-established local pseudopotential is explored with three different local field correction functions viz; Hartree, Taylor and Ichimaru-Utsumi to investigate the effect of the exchange and correlation on the residual resistivity. The comparison of presently computed results with available theoretical and experimental findings is highly encouraging. The investigation of residual 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 function.

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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, point defects 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. Other sources 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 [1-3]. 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., a 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 imperfections.

In the present paper we have used the pseudopotential method to investigate the contribution of monovacancy, which is one of the point defects, to the resistivity of 122 dilute alloys. Our well recognized model potential [1, 2, 4, 5], along with the screening function due to Hartree (H)³, Taylor (T)⁶ and Ichimaru-Utsumi (IU)⁷ are used to study the screening dependence of the residual

resistivity. The motivation for the present investigation comes from the fact that while there have been a few scattered attempts at studying the residual resistivity of metals [1, 2] and alloys [8-18] yet nobody has fully explored the investigation for a large number of alloys on the basis of a single model potential, with the same criteria to determine the parameters of the potential.

II. Method of computation

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 [1-3]

$$\rho_v = \frac{3}{16\pi^2 e^2 v_F^2} \int_0^{2\pi} \int_0^\pi x^3 |W(x)|^2 dx \sin\theta d\theta \quad (1)$$

Here n is the ion number density, v_F the Fermi velocity, k_F the Fermi wave vector, $\int_0^{2\pi} \int_0^\pi$ the solid angle in the scattering vector space, $W(x)$ is the screened form factor of the electron-ion interaction and $x = q/k_F$ with q the momentum transfer wave vector. For the residual resistivity of dilute alloys, equation (1) is modified to [3]

$$\rho_v(\text{alloy}) = \frac{3/4 m_0 C}{8\pi^2 e^2 E_F} \int_0^{2\pi} \int_0^\pi |W_2(x) + W_1(x)|^2 x^3 dx \quad (2)$$

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

In the present work we have calculated ρ_v by applying our well-established local pseudopotential [1, 2, 4, 5] including three different types of exchange and correlation functions [3, 6, 7]. The form factor explored in the present investigation is of the form [1, 2, 4, 5]

$$W(q) = \frac{i 4/3 Z e^2}{\Omega_0 q^2 \epsilon(q)} \cos(qr_c) + \frac{q^2 r_c^2}{1 + q^2 r_c^2} \quad (3)$$

where Z is the valency, Ω_0 the atomic volume, r_c the parameter of the potential, and $\epsilon(q)$ the modified Hartree dielectric function.

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

$$\rho_v(\text{alloy}) = \frac{4m^2 e^2 \Omega_0 C}{3/4 \Omega_0} \int_0^{2\pi} \int_0^\pi dx \frac{Z_1}{Z_2} \cos(r_{c1} x k_{F2}) + \frac{x^2 k_{F2}^2 r_{c1}^2}{(1 + x^2 k_{F2}^2 r_{c1}^2)} \cos(r_{c2} x k_{F2}) + \frac{x^2 k_{F2}^2 r_{c2}^2}{(1 + x^2 k_{F2}^2 r_{c2}^2)} \quad (4)$$

Here C , r_{c1} and Z_1 are the atomic fraction, potential parameter and valency appropriate to the impurity and Ω_0 , k_{F2} , $\epsilon(x)$, 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.

TABLE I. Parameters and constants used in the present calculations.

Metals	Z	- ϕ (a.u.)	k_F (a.u.)	r_c (a.u.)
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

III. Results and discussion

The parameters and constants used in present calculations are given in Table I. The parameter of the potential is determined using the first zero of the form factor [1, 2, 4, 5]. Table II gives a comparison of the presently calculated values of residual resistivity of 122 dilute alloys investigated using three local field correction functions, i.e., H^3 , T^6 and IU^7 with the other available theoretical [3, 8-13] and experimental findings [3, 8, 9, 12-18].

From studying of Table II, it can be noted that, among the three employed screening functions, the screening function due to H^3 (without exchange and correlation) gives the minimum value of residual resistivity, while the screening function due to IU^7 gives the maximum value. The numerical value of the residual resistivity is found to be quite sensitive to the selection of the

TABLE II. Residual resistivity of 122 dilute alloys (in 10^{-4} cm / at %):

Dilute Alloys		Present Calculation				
Host	Impurity	H	T	IU	Expt.	Others
Li	Na	0.4134	0.7417	0.7962	–	0.028 [8], 0.24 [8], 0.43 [8], 0.47 [13]
Li	K	1.7126	3.0677	3.2954	–	2.1 [8], 0.79 [8], 1.4 [8], 5.69 [13]
Li	Rb	2.2766	4.0760	4.3796	–	7.20 [13]
Li	Cs	5.5087	9.8422	10.5903	–	11.48 [13]
Li	Cu	0.6225	1.1755	1.2621	–	2.25 [13]
Li	Ag	1.4826	2.6561	2.8530	–	1.62 [13]
Li	Au	1.4960	2.6801	2.8788	–	1.58 [13]
Na	Li	0.4064	0.8094	0.8757	–	0.04 [8], 0.05 [8], 0.33 [13]
Na	K	0.4697	0.9234	1.0006	–	2.0 [8], 1.55 [13]
Na	Rb	0.7952	1.5772	1.7095	–	2.48 [13]
Na	Cs	3.2570	6.4453	6.9934	–	8.0 [13]
Na	Cu	0.0285	0.0566	0.0613	–	1.16 [13]
Na	Ag	0.3451	0.6850	0.7423	–	0.74 [13]
Na	Au	0.3519	0.6984	0.7567	–	0.77 [13]
K	Li	1.6602	3.8054	4.1460	–	1.7 [8], 3.7 [8], 2.98 [8], 0.50 [13]
K	Na	0.4597	1.0516	1.1468	0.56 [8]	2.0 [8], 3.4 [8], 2.6 [8], 0.79 [10], 0.47 [10], 0.15 [11], 0.10 [11], 0.67 [13]
K	Rb	0.0452	0.1031	0.1125	0.11 [14]	0.07 [13]
K	Cs	1.3520	3.0762	3.3616	1.1 [18]	2.08 [13]
Rb	Li	2.1947	5.2904	5.7699	–	0.67 [13]
Rb	Na	0.7814	1.8793	2.0518	–	0.92 [13]
Rb	K	0.0449	0.1078	0.1178	0.04 [13], 0.13 [16]	0.05 [13]
Rb	Cs	0.9098	2.1763	2.3809	–	1.11 [13]
Cs	Li	5.7840	14.8368	16.1996	–	2.62 [13]
Cs	Na	3.3326	8.5297	9.3224	–	3.02 [13]
Cs	K	1.3548	3.4599	3.7847	–	1.24 [13]
Cs	Rb	0.9096	2.3213	2.5397	0.28 [16]	0.84 [13]
Cu	Li	0.6234	1.0179	1.0830	–	2.62 [13]
Cu	Ag	0.1500	0.2444	0.2605	0.14 [3]	0.04 [3], 0.10 [12], 0.06 [13]

TABLE II. (continual)

Dilute Alloys		Present Calculation					Others
Host	Impurity	H	T	IU	Expt.		
Cu	Au	0.1461	0.2381	0.2537	0.55 [3], 0.52 [18]	0.55 [3], 0.11 [13]	
Cu	Be	0.2802	0.3865	0.4006	0.62 [3]	1.03 [3]	
Cu	Mg	0.5810	0.9107	0.9474	0.65 [3]	3.0 [3]	
Cu	Zn	0.3577	0.5303	0.5478	0.32 [3]	0.63 [3], 0.32 [12]	
Cu	Cd	0.5437	0.8476	0.8810	0.30 [3]	0.60 [3], 1.13 [12]	
Cu	Hg	2.2737	3.7281	3.9294	1.0 [3]	1.8 [3], 0.61 [12]	
Cu	Al	1.2215	1.6839	1.7593	1.25 [3]	1.6 [3], 1.35 [12]	
Cu	Ga	1.2090	1.6654	1.7390	1.42 [3]	1.6 [3], 1.96 [12]	
Cu	In	1.2070	1.6624	1.7357	1.06 [3]	1.86 [3], 1.44 [12]	
Cu	Ge	4.1363	5.9416	6.2875	3.79 [3]	4.2 [3], 5.66 [12]	
Cu	Sn	3.2342	4.5297	4.7649	2.88 [3]	3.60 [3], 3.0 [12]	
Cu	Sb	6.4018	9.0685	9.5685	5.4 [3]	7.1 [3]	
Ag	Li	1.4516	2.5040	2.6802	–	1.46 [13]	
Ag	Cu	0.1606	0.2764	0.2961	0.077 [12], 0.08 [17]	0.09 [12], 0.06 [13]	
Ag	Au	0.00002	0.00004	0.00005	0.36 [12] 0.36 [17,18]	0.09 [12], 0.01 [13]	
Ag	Zn	3.1387	5.1787	5.5639	0.64 [12]	0.41 [12]	
Ag	Cd	2.4034	3.9271	4.2195	0.38 [12]	0.52 [12]	
Ag	Hg	0.6082	0.9051	0.9644	0.79 [12]	1.58 [12]	
Ag	Al	7.8333	12.7179	13.6609	1.95 [12]	2.67 [12]	
Ag	Ga	7.7404	12.5599	13.4912	2.36 [12]	4.25 [12]	
Ag	In	7.7250	12.5338	13.4630	1.78 [12]	3.03 [12]	
Ag	Ge	16.9434	27.4922	29.5269	5.5 [12]	11.0 [12]	
Ag	Sn	14.0394	22.5599	24.2242	4.36 [12]	4.21 [12]	
Au	Li	1.4631	2.5203	2.6973	–	1.46 [13]	
Au	Cu	0.1643	0.2824	0.3026	0.45 [12], 0.36 [13]	0.09 [13]	
Au	Ag	0.00002	0.00004	5.00005	0.36 [12]	0.09 [12]	
Au	Zn	3.1321	5.1642	5.5475	0.95 [12]	0.50 [12]	
Au	Cd	2.3985	3.9166	4.2076	0.63 [12]	0.82 [12]	
Au	Hg	0.6069	0.9029	0.9621	0.44 [12]	1.02 [12]	
Au	Al	7.7919	12.6414	13.5568	1.87 [12]	2.15 [12]	
Au	In	7.6840	12.4582	13.3799	1.39 [12]	2.41 [12]	

TABLE II. (continual)

Dilute Alloys		Present Calculation				
Host	Impurity	H	T	IU	Expt.	Others
Au	Ge	16.8347	27.2946	29.3103	5.2 [12]	22.4 [12]
Au	Sn	13.9443	22.3898	24.0379	3.36 [12]	3.89 [12]
Be	Li	0.0698	0.0894	0.0916	–	–
Be	Na	0.2379	0.3234	0.3384	–	–
Be	K	0.6394	0.8902	0.9346	–	–
Be	Mg	0.1476	0.2117	0.2216	–	–
Be	Tl	0.0999	0.1354	0.1389	–	–
Be	Pb	2.4271	3.5862	3.6296	–	–
Mg	Li	0.1338	0.1870	0.1930	0.75 [3]	0.27 [3], 0.33 [0.44] 0.48 [8], 0.60 [8], 0.16 [10]
Mg	Na	0.2986	0.4374	0.4643	–	–
Mg	K	0.8639	1.3405	1.4302	–	–
Mg	Ag	0.7731	1.1917	1.2711	0.8 [3]	1.2 [3]
Mg	Be	0.1720	0.2806	0.2982	–	–
Mg	Cd	0.00063	0.00102	0.00108	0.8 [3]	0.68 [3]
Mg	Al	0.5327	0.8119	0.8119	2.1 [3]	1.6 [3], 0.63 [8], 0.82 [8], 0.83 [8], 1.0 [8], 0.65 [10], 0.88 [10], 0.62 [11], 0.60 [11]
Mg	In	0.5137	0.7814	0.8325	2.5 [3]	2.4 [3]
Mg	Tl	0.4854	0.7362	0.7842	3.3 [3]	3.5 [3]
Mg	Sn	1.5343	2.2951	2.4418	5.4 [3]	2.1 [3]
Mg	Pb	0.7385	1.1112	1.1498	5.7 [3]	1.6 [3], 0.81 [10], 0.73 [10]
Cd	Al	0.4585	0.6893	0.7332	–	–
Al	Li	0.2254	0.2936	0.3022	–	–
Al	Na	0.3762	0.5056	0.5279	–	–
Al	K	0.7318	1.0178	1.0700	–	–
Al	Cu	0.4502	0.6115	0.6400	0.8 [3]	0.76 [3], 0.86 [9]
Al	Ag	0.6751	0.9359	0.9832	1.2 [3]	0.58 [3]
Al	Be	3.5947	4.8915	5.1257	–	–
Al	Mg	0.1375	0.1894	0.1981	0.33 [3]	0.78 [3], 0.38 [9], 0.17 [10], 0.24 [10], 0.15 [11], 0.14 [11]
Al	Ca	0.9870	1.4356	1.5130	>4.5 [3]	1.8 [3]
Al	Zn	0.0742	0.0980	0.1019	0.22 [3]	0.1 [3], 0.13 [8], 0.21 [9], 0.074 [10] 0.12 [10], 0.053 [11], 0.1 [11]

TABLE II. (continual)

Dilute Alloys		Present Calculation				
Host	Impurity	H	T	IU	Expt.	Others
Al	Cd	0.1267	0.1738	0.1821	0.51 [7]	0.4 [9]
Al	Ga	0.00010	0.0015	0.00016	0.22 [7]	0.22 [9]
Al	Si	0.2362	0.3342	0.3516		
Al	Ge	0.1548	0.2150	0.2258	0.98 [3]	1.0 [3], 0.77 [9]
Al	Pb	1.1767	1.7538	1.8400	–	–
In	Cd	0.2241	0.3260	0.3451	0.3 [3]	0.31 [3]
In	Ga	0.000003	0.000004	0.000005	0.15 [3]	0.14 [3]
In	Tl	0.00037	0.00057	0.00061	0.18 [3]	0.08 [3]
In	Sn	0.1222	0.1705	0.1794	0.37 [3]	0.30 [3]
In	Pb	1.0042	1.5824	1.6651	0.60 [3]	0.56 [3]
In	Bi	1.6899	2.6447	2.7714	1.77 [3]	2.0 [3]
Tl	Be	0.0849	0.1149	0.1195	–	–
Sn	Mg	0.3604	0.4971	0.5219	–	–
Sn	Cd	0.3463	0.4763	0.4997	1.42 [3]	0.31 [3]
Sn	In	0.0633	0.0850	0.0886	0.58 [3]	0.31 [3]
Sn	Pb	1.0211	1.5508	1.6352	–	–
Sn	Sb	0.0629	0.0844	0.0880	0.63 [3]	0.63 [3]
Sn	Bi	1.6249	3.4805	2.6078	0.87 [3]	0.76 [3]
Pb	Li	0.9215	1.3666	1.4161	–	–
Pb	Na	0.6031	0.8581	0.8838	2.9 [3],	0.77 [3], 0.67 [10]
Pb	K	0.4974	0.6746	0.6935	–	–
Pb	Be	0.8437	1.3672	1.4278	–	–
Pb	Mg	0.4955	0.7433	0.7721	3.34 [3]	3.05 [9]
Pb	Cd	0.5148	0.7736	0.8040		
Pb	Hg	0.2227	0.3061	0.3146	1.8 [3]	1.8 [3]
Pb	Al	0.8116	1.2564	1.3204	–	–
Pb	In	0.7928	1.2273	1.2897	1.2 [3]	0.50 [3], 1.11 [9]
Pb	Tl	0.7648	1.1838	1.2438	0.9 [3]	0.9 [3]
Pb	Sn	1.0403	1.6023	1.6921	0.3 [3]	0.04 [3], 0.28 [9]
Pb	Bi	0.9874	1.4613	1.5138	1.6 [3]	0.4 [3]
Sb	Mg	0.4918	0.6619	0.6913	–	–
Sb	Pb	1.0099	1.4942	1.5758	–	–
Bi	Pb	0.0987	0.1461	0.1514	–	–

local field correction function, showing a significant variation with the change in the function. In comparison with the H^3 function, the influence of the T^6 function is of the order of 28.08% to 156.51% while the influence for the IU^7 function is of the order of 31.23% to 180.08%. Out of 122 dilute alloys of 18 hosts, the maximum influence of the local field correction function is found for Rb based alkali metals dilute alloys, and the minimum influence observed is for Be based dilute alloys. The present comparison with available theoretical and experimental data is encouraging. Out of 122 dilute alloys, we do not have either theoretical or experimental comparisons for 25 dilute alloys.

Harrison [3] has reported residual resistivity of 43 dilute alloys by adopting a point ion model potential. He has adjusted the potential parameters of the point ion model potential to optimize the agreement with experiment. DuCharme [12], Kachhava [10] and Fukai [9] have used Ashcroft's empty core model potential. Although they have used the same potential, all of them have adopted different criterion for determining the parameter of the potential. Taut and Paasch [11] have used Shaw's model, while the phase shift method was adopted by Dickey *et al.* [13].

In contrast with the reported studies, the present study spans the dilute alloys of a large number of metallic elements of the periodic table on a common platform of model potential and a common criteria for evaluating the parameters of the model potential. This is very essential for obtaining concrete conclusions. Our investigation also predicts that the study of residual resistivity of dilute alloys is sensitive to the selection of the proper local field correction function.

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