

Contribution of a point defect to the electrical resistivity of simple and non-simple metals

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Recently proposed potential has been used to calculate the contribution of a point defect to the electrical resistivity of simple and non-simple metals including d and f-shell metals. The parameter of the potential has been determined using zero pressure condition while the exchange and correlation effect due to Taylor is incorporated. Our present findings for Al, Pb, Cu, Ag and Au are excellent in agreement with the experimental findings while alkali metals have comparable results with the other such theoretical findings. We could not find sufficient theoretical as well as experimental data for Ni, Pd, Pt, Rh, Ir, La, Yb, Ce and Th for the contribution of a point defect to the electrical resistivity (residual resistivity) in order to workout a quantitative comparison. It, therefore, seems difficult to give concrete remark about the present results; we conclude that the calculations of monovacancy resistivity based on pseudopotential theory can be regarded as a sensitive test for the proper assessment of the pseudopotential form factor.

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I. Introduction

A perfect crystal is an ideal concept, which is not correct for any crystal found in nature or fabricated in a laboratory. The types of imperfections, which may be found in the crystal, are:

- (1) A substitutional impurity atom present at a regular site,
- (2) A missing atom from a regular site which has diffused into the interstitial space,
- (3) A displaced atom which appears at some other site,
- (4) A stacking fault etc. It can be assumed that the atomic cores remain undisturbed in a distorted crystal. This means that these static imperfections can be regarded as “frozen” atomic vibrations, which may be treated adiabatically.

The effect of imperfections in a crystal is to contribute to the total resistivity of the crystal. The resistivity of a metal containing imperfections consists of two contributions. One is due to the thermal motion of the lattice and the other due to imperfections. The resistance due to static imperfections is called residual resistance. The absence of an atom or an ion at a lattice site (a vacancy) modifies the potential at that site. This modification then acts as a perturbation to the conduction electrons or alternatively it can be said that the vacancy scatter the conduction electrons.

The thermal contribution of the total resistivity of a crystal vanishes at $T = 0\text{K}$ and hence the residual resistance at low temperatures due to static imperfections may be significant. This is because at low temperatures the excited phonon spectrum consists of long wavelength phonons,

which carry little momentum and deflect the electron through a small angle, which makes little contribution to the resistivity [1]. At high temperatures the contribution due to imperfections is small compared to that due to the scattering of conduction electrons by phonons. Recently we have [3,4] proposed model potential depending on an effective core radius but otherwise parameter free. We have also reported a large number of physical properties of d and f-shell metals in the fcc phase very successfully [3,4] with the help of same potential along with local field correction function of Taylor (T). Very recently Vora [2] has reported residual resistivity of some metallic elements using Ascroft's empty core model potential along with five different local field correction function such as Hartree (H), Taylor (T), Ichimaru-Utsumi (IU), Farid et al (F) and Sarkar et al (S). Vora has used the parameter of the potential using the condition of first zero of the formfactor. Using the same potential [3,4] in the recent past Baria has also reported thermodynamic properties of liquid d and f-shell metals [5]. To testify the wide applicability of the model potential, in this paper we have reported the point defect to the electrical resistivity of simple and non-simple metals including d and f-shell metals.

1. Theory of point defect to the electrical resistivity (residual resistivity)

Within the framework of the second order pseudopotential formalism, the expression for the contribution of point defect to the electrical resistivity (residual resistivity) can be

given, using the standard scattering theory as [6,7],

$$\rho_v = \frac{3}{16 \hbar n e^2 v_F^2 k_F^4} \int_0^{2k_F} \int_{\Omega'} q^3 |W(q)|^2 dq d\Omega' \quad (1)$$

where n is the ion number density, v_F the Fermi velocity, k_F the Fermi wave vector, q the momentum transfer wave vector and Ω' the solid angle in the scattering vector space and $W(q)$ is the screened form factor used by Baria and Jani [3,4]. The term $|W(q)|^2$ in the integrand indicates that the values of ρ_v will depend sensitively on the many-electron screening through the form factor.

II. Results and discussion

The calculated values of residual resistivity is shown in table 1 and compared with available theoretical and experimental values. From table 1 it can be seen that for alkali metals our present findings are consistent, satisfactory and lying within the range of other theoretical findings [6-8] while experimental data for these metals are not available. The present results of residual resistivity are excellent in agreement with the experimental findings for Al, Pb, Cu, Ag and Au while for other d and f-shell metals we could not found sufficient theoretical as well as experimental data for the contribution to point defect to the electrical resistivity in order to workout a quantitative comparison. The calculation of residual resistivity of Vora [2] varies significantly from screening function to screening function, having highest value for Farid et al [F] screening function and lowest value for Hartree (H) screening function. Moreover, Vora [2] has not considered experimental values of Cu, Ag and Au. The

theoretical values of residual resistivity of Vora [2] for Cu, Ag and Au are inferior to that of experimental values. The research paper of Vora [2] does not suggest concrete logical explanation about selection of screening function and determination of potential parameter, which is most important in the pseudopotential formalism and applications. The present results of residual resistivity are better than Vora [2] and for Al, Pb, Cu, Ag and Au our results are extremely match with the experimental findings while for the rest of the metals in absence of experimental findings our calculation may be considered as one of the guideline for further investigations either theoretical or experimental. we conclude that the calculations of monovacancy resistivity based on pseudopotential theory can be regarded as a sensitive test for the proper assessment of the pseudopotential form factor.

III. Conclusion

It is very interesting to point out that in spite of relative simple application of the pseudopotential technique in the study of point defects (residual resistivity), there have been only few attempts [2,6-8] to calculate their contribution to electrical resistivity of different metals using the same pseudopotential. In the absence of experimental information such calculation may be considered as one of the guideline for further investigations either theoretical or experimental. A good agreement between theoretical investigations and experimental findings show the ability of our model potential [3-5] to reproduce wide class of properties of simple, non-simple transition and Lanthanide metals.

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[14] R. W. Siegel, Phil. Mag. **13** (1966) 359.[15] W. Desorbo, Phys. Rev. **117** (1960) 444.**Table 1.** Monovacancy resistivity of some simple and non-simple metals

Metal	Present results	Expt. [9, 12-15]	Others			
			[2]	[6,10]	[6,10]	[6,11]
Li	0.975	-	3.39	0.89935, 0.47532	0.49686	0.96473, 3.50629
Na	0.977	-	4.42	1.22997, 0.93357	0.40620	0.49125, 0.16656
K	1.412	-	6.87	1.65443, 1.23943	0.805527	0.17188, 0.47379
Rb	1.717	-	8.07	1.87720, 1.40139	0.91404	0.89307, 1.88931
Cs	2.240	-	6.44	3.65985, 2.73374	1.15344	1.95579, 1.93097
Al	2.147	2.2	1.85	-	-	-
Pb	0.216	0.19	1.99	-	-	-
Cu	1.296	1.2 ± 0.6	0.61	0.3790, 1.03995, 2.0948, 3.2859, 20.8555, 3.3824	1.09, 1.44, 3.21, 3.20	1.28
Ag	1.207	1.3 ± 0.7 1.6	0.71	0.4610, .85535, 1.4611, 4.15863, 7.0403, 6.5453	1.92, 2.31, 2.72, 2.48	1.45
Au	1.416	1.5 ± 0.3 2.0 ± 0.4 1.8 ± 0.4 1.8 ± 0.6	0.70	1.5696, 2.3413, 3.2595, 8.5089, 9.0691, 19.1731	1.95, 2.65, 2.45, 4.35,	1.45
Ni	1.141	-		-	-	-
Pd	0.851	-		-	-	-
Pt	0.831	-		-	-	-
Rh	0.908	-		-	-	-
Ir	0.884	-		-	-	-
La	2.092	-		-	-	-
Yb	1.750	-		-	-	-
Ce	1.704	-		-	-	-
Th	1.434	-		-	-	-