

Electrical Resistivity of Some f-shell Metals using Pseudo Potential

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Abstract: In the present communication using pseudopotential with only one adjustable parameter is used to study electrical resistivity of some divalence and trivalence (f-shell) FCC metals. We observe that presently used pseudopotential is predicting results which are in excellent agreement with experimental findings. Such studies encourage us to extent present scheme for examining different liquid state properties of these metals. The present study also confirms that s-p-d hybridization is accounted properly in the presently used pseudopotential.

Keywords: electrical resistivity, f-shell metals, pseudopotential.

1. Introduction

Interest in the study of the transport properties of liquid metals continues unabatedly. The hope is that the information so obtained will throw light on the interactions in the corresponding solid metals¹⁻⁵. When studying the electronic properties of metals, one immediately encounters the problem of knowing the effective electron – ion interaction, which gives rise to the scattering of electrons on the Fermi surface. People have invented a number of model potentials, which incorporate in a parametric way the various physical requirements²⁻³. There are also satisfactory ways of specifying this potential from first principles. It may be noted that description of a wide range of properties of metals (solids, liquids and glasses) is still beyond the capabilities of completely ab initio approaches. It is in this context, the importance of the development of the pseudopotential theory for metals, for which it is valid, appears indisputable⁶.

Transition metals have attracted continues attention of physicist and chemists because of their unusual electronic and structural properties. In transition metals, narrow d-bands are filled and lie below the Fermi energy. This group of metals often exhibit pronounced phonon anamolias as a result of complex Fermi surface geometries in conjunction with strong electron phonon coupling, whose consistent description still provides a challenge for theoretical approaches. Pseudopotential for f-shell transition metals have to be energy dependent and non-local if they are to fully all structural and transport properties and use of the non-local potential is not a serious hindrance in the most pseudopotential calculations. Looking at the literature, it is found that the theoretical works of f-shell metals using non-local pseudopotential are scattered. The transport properties computed by local pseudopotential by different authors have used different phenomenology to construct model.

In the present communication, we have computed liquid metal resistivity of f-shell metals using local pseudopotential. The pseudopotential proposed by Kumar⁷ and used to study lattice mechanical properties of Thorium⁸ is used in the present study.

The plane of the paper is as follows. In section-2, we describe necessary theory to compute pseudopotential and resistivity. The results with necessary discussions are given in section-3.

2. Theory

The expression for the liquid metal resistivity using pseudopotential form-factor is given by ¹

$$(2.1) \quad \rho_{Ziman} = \frac{3\pi^2 m}{4\pi^2 e^2 \hbar^3 n k_F^6} \int_0^\infty dq q^3 s(q) |v(q)|^2 \Theta(2k_F - q).$$

One of the essential ingredients for evaluating the electrical resistivity is the static structure factor $s(q)$ which involves the inter atomic interaction through statistical mechanics. In the present work, we have used hard-sphere solution of the Percus-Yevick equation with packing fraction 0.45. In any case, the theoretical values of the electrical resistivity are very sensitive to the accuracy of the structure factor. The conduction electron density (n) is related to the Fermi vector $k_F = (3\pi^2 n)^{1/3}$. The unistep function Θ which cuts off the integration at $2k_F$ corresponding to a perfectly sharp Fermi surface. It is defined as, for $q > 2k_F$ it is zero and it is 1 for $q \leq 2k_F$. The second important

term is electron-ion interaction. In the present communication, we use the model potential proposed by Kumar⁷, which has the following form in r-space.

$$\begin{aligned}
 v_{ion}(r) &= -\frac{ze^2}{R_m R_c}, \quad \text{For } 0 < r < R_m \\
 &= -\frac{ze^2}{R_m}, \quad \text{For } R_c < r < R_m \\
 &= -\frac{ze^2}{r}, \quad \text{For } R_m < r.
 \end{aligned}
 \tag{2.2}$$

Here z is the effective valency, R_m and R_c are potential parameters. The potential parameter R_c is computed using relation given in reference. In the present study by adjusting R_m for transition metals from the range ($R_m > R_c$), we achieve better agreement with the experimental resistivity for each metal. The presently obtained parameters are shown in Table-1.

Table-1 Pseudopotential parameters (all in a.u)

Metal	Z	R_c	R_m
La	3.0	1.40	1.68
Ce	3.0	1.35	1.64
Gd	3.0	1.39	1.46
Eu	2.0	1.8	1.55
Yb	2.0	1.70	1.92

In the q-space, pseudopotential due to Kumar is given by

$$\begin{aligned}
 v_{ion}(q) &= -\frac{4\pi Z^* e^2}{\Omega_0 q^2} \cos(qR_m) - \frac{4\pi Z^* e^2}{\Omega_0 q^4 R_c R_m} \left[-q^2 R_c^2 \cos(qR_c) + 2qR_c \sin(qR_c) \right] \\
 &\quad - \frac{4\pi Z^* e^2}{\Omega_0 q^3 R_m} \left[qR_c \cos(qR_c) - qR_m \cos(qR_m) + \sin qR_m - \sin(qR_c) \right]
 \end{aligned}
 \tag{2.3}$$

3. Results and Discussions

The presently computed pseudopotential form-factors for all metals are plotted in fig.1.

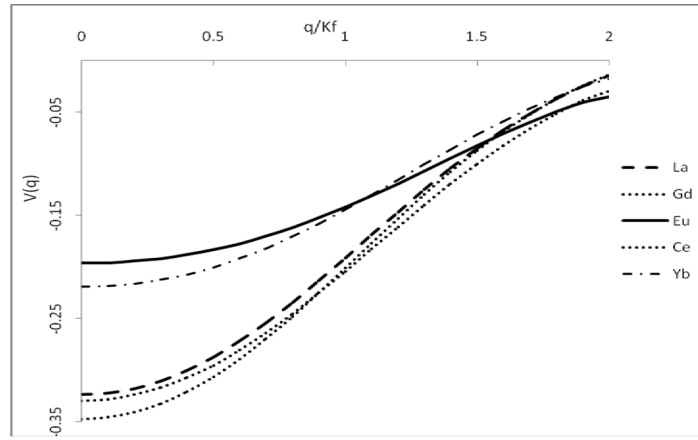


Fig.1. The pseudopotential form factors versus q/k_f for La, Ce, Gd, Eu and Yb.

The presently computed form factors do not have any spurious oscillations at large q , hence unphysical contribution to off shell elements are removed. The calculated results for resistivity are shown in table-2 along with experimental and theoretical results.

Table-2 The electrical resistivity (in $\mu\Omega\text{-cm}$) for various liquid f-shell metals. The values in the parentheses are experimental values taken from ref.⁸

Metals	Present	Other Theoretical results
La	140.95 (140)	133^{10} , 147.58^3
Ce	124.62 (125.83)	127.17^3
Gd	196.81 (195)	209^{10}
Eu	244.78 (244)	221^{10}
Yb	109.83 (110)	135^{10} , 118.56^3

The agreement with experiment is excellent. The experimental behavior of the resistivity data of liquid rare earth shows the following behavior. The resistivity increases across the series of trivalent RE's. The temperature coefficient changes from slightly positive from La to slightly negative for Lu. The divalent Eu and Yb behave exceptionally: Eu has the highest and Yb has the lowest ρ – values of all liquid RE's. They both have negative

temperature coefficient. Our results are better than Delley⁹ who have used renormalized muffin-tin potential using single site t-matrix approximation. Baria³ has computed resistivity of some d-band and f-shell metals using model potential depending on effective core radius but otherwise parameter free. He has used three different approaches to compute liquid metal resistivity and found that t-matrix formulation is better than usual Ziman's and self-consistent approach. For comparison, we have quoted only t-matrix formulation results in table.2. Comparison between our results with theoretical results due to Baria³ suggests that our model is superior, simple and more transparent. Concluding, we find that our calculation indeed shows that presently used pseudopotential and Ziman's free electron approach to compute liquid metal resistivity is appropriate for f-shell metals.

The present investigation is contradictory to strong emphasis by Esposito et al⁹ suggest that the Ziman's formula describes electrical transport properties correctly for simple liquid metals while self-consistent results of resistivity are over estimates if mean free paths are comparable or smaller than an interatomic distances, which happens in the d and f shell metals. Baria found that t-matrix approach gives better results of resistivity. The Kumar's pseudopotential, which was used previously to study transport properties of noble metals and lattice mechanical properties of Thorium by us⁸ can be used to study liquid state properties (thermo physical and static) of f-shell metals.

References

1. J. G. Gasser, *J. Phys.: Condens. Matter*, **20** (2008) 114103.
2. A. M. Vora, *J. Ovonic Res.*, **3** (2007) 57, *Russian Phys. J.*, **49** (2006) 834.
3. J. K. Baria, *Braz. J. Phys.*, **34** (2004) 1185; *Physica B*, **357** (2003) 245.
4. M. B. Pathak, N. K. Bhatt, P. R. Vyas, A. R. Jani and V. B. Gohel proc. of the 53rd DAE SSPS, (2008) 963.
5. M. B. Pathak, N. K. Bhatt, P. R. Vyas, A. R. Jani and V. B. Gohel proc. of the 54th DAE SSPS, 2010 proc. of the 55th DAE SSPS, (2009) 943.
6. L. Pollack, Y. P. Perdew, J. He, M. Marques, *et al*, *Phys. Rev.* **B55** (1997) 15554.
7. J. Kumar, *Solid State Communication*, **21** (1977) 945.

8. T. C. Pandya, P. R. Vyas, C. V. Pandya and V. B. Gohel, *Czecho. J. of Phys.*, **51** (2001) 49.
9. Y. Waseda, *the structure of non-crystalline materials.*, Mc Grow Hill Pub. C. New York (1980).
10. E. Esposito, H. Ehrenreich and C. D. Gelatt, *J. Phys. Rev. B*, **18** (1978), 3913.