The Comparative Study of Electrical Resistivity of bcc Liquid Transition Metals

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(Received 15 February 2020; revised manuscript received 15 April 2020; published online 25 April 2020)

In the present paper, we have used Ziman’s approach and transition matrix (t-matrix) approach to study the electrical resistivities of bcc liquid metals. By carrying out this study, we have verified the validity of our proposed pseudopotential extracted from generalized pseudopotential theory (GPT). Our theoretical results agree well with experimental results. Also, it has been verified that for transition metals t-matrix approach is more realistic and physically sound than Ziman approach.

Keywords: Pseudopotential, Liquid metal resistivity, Transition metal, T-matrix approach.

DOI: 10.21272/jnep.12(2).02020 PACS numbers: 72.15.Cz, 71.22.+i, 61.25.Mv

1. INTRODUCTION

Over the past few years there have been several theoretical and experimental investigations on electronic transport properties of liquid metals in order to understand its structure and atomic interactions occurring in the similar solid state metals [1-6]. These studies can help to establish relation between the electronic state theory and liquid state theory in metals as liquid state theory is complicated and physically more transparent in comparison with solid state theory [9]. The t-matrix and Ziman’s approach requires pseudopotential phenomenology. It can be used to study the electrical resistivity of bcc liquid transition metals which can further explain the electron-ion interaction. According to the past studies, it has been established that t-matrix is more suitable and can provide accurate information about the interactions occurring in liquid metals whereas Ziman’s approach, that is based on electron-ion interactions, is not applicable to transition metals due to the strong resonant scattering caused by empty d states [10].

In present communication, we have computed electrical resistivity of molybdenum, tungsten, niobium, chromium and iron (Mo, W, Nb, Cr and Fe) at a given temperature using Ziman and t-matrix approach and have proposed a transition metal pseudopotential (TMPP) by using generalized pseudopotential theory (GPT).

The present paper is organized in a given manner: In section 2 we have described necessary mathematical equation to calculate liquid metal resistivity. Section 3 is devoted for comparison of our computed results with other theoretical data and experimental findings. We have also discussed merits and demerits of present approach in this section. The paper is concluded with concluding remarks in section 4.

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2. THEORY

We use t-matrix of pseudopotential to calculate the relevant scattering cross-section. The transition matrix for the scattering on the energy shell can be written as [11]

\[ t(k,k') = \frac{-2\pi v^2}{\partial m(2\epsilon k)\epsilon^2} \times \sum_i (2l + 1) \sin \Delta_i(E_F) e^{i\Delta_i(E_F)} P_i(\cos \theta), \]

(1)

The t-matrix is normalized to atomic volume \( \Omega \) and it has dimension of energy. The values of phase shifts (\( \Delta_0, \Delta_1, \Delta_2 \)) are calculated using method described in reference [1]. The electrical resistivity computed using t-matrix approach takes the following form

\[ \rho_t = \frac{3na}{c^2\pi^2} \int_0^\infty dy \int_0^\infty |t(k,k')|^2 dy, \]

(2)

where \( y = q/k_F \). Here, we have used Percus-Yeckin equation for \( S(q) \) with packing fraction \( \eta = 0.45 \).

The form of bare-ion pseudopotential, directly extracted from generalized pseudopotential theory (GPT), with having three parameters core radius (\( r_c \)) radius of d-electron (\( r_d \)) and hybridization parameter (\( \beta \)) has the following form in q-space (in a.u.) [12]

\[ V_{DQ}(q) = \frac{1}{\eta} \left[ \frac{-8\pi^2}{q^2} \right. \times \cos q r_c + \left. \frac{\beta}{1 + q^2 r_d^2} \right], \]

(3)

Z is the valency and \( \Omega \) is the atomic volume at melting temperature. To obtain screened pseudopotential we have adopted method suggested by Wallace [13]. The present calculation consist of exchange and correlation function due to Hubbard and Sham [14, 15].

3. RESULTS AND DISCUSSION

In present work, we have proposed a simple scheme to determine pseudopotential parameter in which three parameters are reduced to two. Here, \( r_d/r_c \), i.e. ratio of d-electron along with the core radius is kept within the range of 1.1 to 1.5 and hybridization parameter \( \beta \) for all metals is tuned in such a manner that first zero (\( V(q_0) = 0 \))
are found between 1 kx and 1.5 kx. The values of the input parameters used in the calculation of pseudopotential are tabulated in Table 1.

Table 2 exhibits the computed values of phase shifts $\Delta_0$, $\Delta_1$, and $\Delta_2$ (in radian) at $q = 2kx$. In addition, it shows the calculated values of liquid metal resistivity using Ziman approach and t-matrix approach compared with the experimental findings and other theoretical values. From the detailed analysis in Table 2, we observe that our results are in good agreement with the experimental values at a given temperature. In addition, it has been found that our results for molybdenum, niobium, chromium and iron are far more superior in comparison with the theoretical values obtained by Ononiwu [10] and Waseda [11]. We would like to elaborate these studies in detail. Waseda have used muffin tin potential to determine theoretical values obtained by Ononiwu [10] and Waseda um and iron are found that our results for molybdenum, niobium, chromium and iron are far better than nearly free electron Ziman approach. Such observation is in agreement with Bhatia et al. [1] who have used both the approaches to carry out comparative study of liquid metal resistivities for 16 transition metals.

For further detailed explanation of the given calculation, we have also presented the variation of $\Delta_0$, $\Delta_1$, $\Delta_2$ up to $q = 2kx$ (up to fermi surface) for chromium and iron in Fig. 1 and Fig. 2, respectively. During computation, we observe that the maximum value of the phase shift for each metal is found to be less than $\pi$ radian. Such observation goes in the favor of application of the perturbation expansion and born approximation. The main ingredient for the calculation of t-matrix resistivity is t-matrix form factor $t(k,k')$ (see Eq. (1)). We have also examined the behavior of t-matrix form factor $t(k,k')$ for all the five metals and presented the behavior of $t(k,k')$ for Cr and Fe in Fig. 3 and Fig. 4, respectively.

Table 1 – The input parameters and pseudopotential parameters (in a.u.). The quantity shown in parenthesis represents temperature (in °C) at which atomic volume ($\Omega$) is used

<table>
<thead>
<tr>
<th>Metal</th>
<th>Z</th>
<th>$\Omega$ (in 10$^{26}$cm$^3$)</th>
<th>$\beta$</th>
<th>$\rho_{\text{Ziman}}$ (in $\mu\Omega\text{cm}$)</th>
<th>$\rho_{\text{exp}}$ (in $\mu\Omega\text{cm}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo</td>
<td>6</td>
<td>115.27 (2617)</td>
<td>63</td>
<td>91.05</td>
<td>97 [16]</td>
</tr>
<tr>
<td>W</td>
<td>6</td>
<td>116.47 (3410)</td>
<td>60</td>
<td>81.92</td>
<td>131 [16]</td>
</tr>
<tr>
<td>Nb</td>
<td>5</td>
<td>137.02 (2741)</td>
<td>52</td>
<td>96.11</td>
<td>92.97 [17]</td>
</tr>
<tr>
<td>Cr</td>
<td>3</td>
<td>95.04 (1900)</td>
<td>35</td>
<td>77.52</td>
<td>80 [11]</td>
</tr>
<tr>
<td>Fe</td>
<td>3</td>
<td>89.35 (1550)</td>
<td>24</td>
<td>137.88</td>
<td>140 [11]</td>
</tr>
</tbody>
</table>

Table 2 – The computed results of phase shifts $\Delta_0$, $\Delta_1$, and $\Delta_2$ (in radian) and liquid metal resistivity $\rho_{\text{Ziman}}$ and $\rho_{\text{exp}}$ (in $\mu\Omega\text{cm}$)

<table>
<thead>
<tr>
<th>Metal</th>
<th>$\Delta_0$</th>
<th>$\Delta_1$</th>
<th>$\Delta_2$</th>
<th>$\rho_{\text{Ziman}}$</th>
<th>$\rho_{\text{exp}}$</th>
<th>Other theoretical results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo</td>
<td>2.3529</td>
<td>2.0233</td>
<td>0.9135</td>
<td>32.97</td>
<td>91.05</td>
<td>94 [10]</td>
</tr>
<tr>
<td>W</td>
<td>2.7415</td>
<td>1.9374</td>
<td>0.8938</td>
<td>40.96</td>
<td>81.92</td>
<td>96 [10]</td>
</tr>
<tr>
<td>Nb</td>
<td>2.6938</td>
<td>1.7071</td>
<td>0.7284</td>
<td>56.27</td>
<td>96.11</td>
<td>110 [10]</td>
</tr>
<tr>
<td>Cr</td>
<td>1.5412</td>
<td>1.0655</td>
<td>0.4421</td>
<td>14.04</td>
<td>77.52</td>
<td>56 [10]; 120 [11]</td>
</tr>
<tr>
<td>Fe</td>
<td>1.9075</td>
<td>1.0483</td>
<td>0.4146</td>
<td>40.27</td>
<td>137.88</td>
<td>92 [10]; 182 [11]</td>
</tr>
</tbody>
</table>

Fig. 1 – The variation of phase shift for Cr

Fig. 2 – The variation of phase shift for Fe
found near Fermi surface (within the range (1-1.2) kF). By taking the limit of Eq. (1) as q → 0, the values of the t-matrix form factors at q = 0 can be found. This limiting value can be represented by following form in the atomic unit:

\[
t(k,k') = -\frac{4\pi}{mk_F} [\sin \Delta_1 \cos \Delta_0 + 3\sin \Delta_1 \cos \Delta_1 + 5\sin \Delta_2 \cos \Delta_2].
\] (4)

4. CONCLUSIONS

The current study establishes that the local pseudopotential method extracted from the generalized pseudopotential theory (GPT) can help in understanding the transport properties of bcc liquid transition metals. From the comparative studies, we observe that the values of the liquid metal resistivities for transition metals t-matrix approach is satisfactory and far more realistic than nearly free electron (NFE) Ziman approach occurring due to weak scattering. In addition, it has been found that our results agree very well with the experimental investigations compared to other theoretical values. Encouraged by present method, we would like to extend it for the study of other bcc metals and their alloys.

ACKNOWLEDGEMENTS

On behalf of all authors, the corresponding author states that there is no conflict of interest. Authors are thankful for the computational facilities developed at the Department of Physics, Gujarat University, Ahmedabad by using financial assistance of (i) Department of Sciences and Technology (DST), New Delhi through the DST-FIST (Level 1) project (SR/FST/PSI-001/2006) (ii) University Grant Commission (UGC), New Delhi through DRS SAP (AP-I) project (F.530/10/DRS/2020), (iii) Department of Sciences and Technology (DST), New Delhi through the DST-FIST project (SR/FST/PSI-198/2014).

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