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The Comparative Study of Electrical Resistivity of bcc Liquid Transition Metals

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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.

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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 shows dual behavior, metallic as well as fluidic. Pseudopotential approach has been an important area of research for investigations of nearly all physical properties such as static, dynamic and electronic properties of metallic solids, liquids, alloys and glasses [7, 8]. This approach is found to be simple in computation, less complicated and physically more transparent in comparison with first principles method [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.

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]

$$t(k,k')=\frac{-2\pi\hbar^3}{\Omega m(2mE_F)^{\frac{1}{2}}} \times [\sum_l (2l+1)\sin\Delta_l(E_F)e^{i\Delta_l(E_F)}P_l(\cos\theta)], \quad (1)$$

The *t*-matrix is normalized to atomic volume Ω and it has dimension of energy. The values of phase shifts (Δ_0, Δ_1, Δ_2) are calculated using method described in reference [1]. The electrical resistivity computed using *t*-matrix approach takes the following form

$$\rho_t = \frac{3\pi\Omega}{e^2\hbar^2v^2}\int_0^1 4y^3S(q)\ |t(k,k')|^2\ dy, \quad (2)$$

where $y = q/k_F$. Here, we have used Percus-Yevick 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 (β) has the following form in *q*-space (in a.u.) [12]

$$V_{ion}(q) = \frac{1}{\Omega}\left[\frac{-8\pi Z}{q^2}\times cosqr_c + \frac{\beta}{[1+q^2r_d^2]^4}\right], \quad (3)$$

Z is the valency and Ω 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 β for all metals is tuned in such a manner that first zero ($V(q_0) = 0$)

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are found between 1 k_F and 1.5 k_F. 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 Δ_0, Δ_1 and Δ_2 (in radian) at $q = 2k_F$. 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 phase shifts at fermi energy and by using these phase shifts, he has constructed *t*-matrix form factor as a function of q/k_F. Also by utilizing experimental structural data, he has calculated the potential. Ononiwu have used Ziman's theory updated by Evan's et al. (for details see [1]) to study the transport properties of liquid transition metals. In nearly free electron approximation, he has simulated the effect of the *d*-band resonance. Here, *t*-matrix form factor replaces the ordinary *V*-matrix pseudopotential form factor.

In comparison with both the theoretical researchers, we find that present form of pseudopotential with simple method to determine potential parameter yields better results. One more thing emerging from the present study is that the values of t-matrix resistivity of all the five metals molybdenum, tungsten, 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 Δ_0, Δ_1, Δ_2 up to $q = 2k_F$ (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 π 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 pseudopotental parameters (in a.u.). The quantity shown in parenthesis represents temperature (in °C) at which atomic volume (Ω) is used

Metal	Z	Ω	β	r_c	r_d
Mo	6	115.27 (2617)	63	0.227	0.255
W	6	116.47 (3410)	60	0.275	0.3063
Nb	5	137.02 (2741)	52	0.2725	0.3025
Cr	3	93.04 (1900)	35	0.25636	0.282
Fe	3	89.35 (1550)	24	0.215	0.2365

Table 2 – The computed results of phase shifts Δ_0, Δ_1 and Δ_2 (in radian) and liquid metal resistivity ρ_{ziman} and ρ_t (in μΩcm)

Metal	Δ_0	Δ_1	Δ_2	ρ_{ziman}	ρ_t	ρ_{exp}	Other theoretical results
Mo	2.3529	2.0233	0.9135	32.97	91.05	97 [16]	94 [10]
W	2.7415	1.9374	0.8938	40.96	81.92	131 [16]	96 [10]
Nb	2.6938	1.7071	0.7284	56.27	96.11	92.97 [17]	110 [10]
Cr	1.5412	1.0655	0.4421	14.04	77.52	80 [11]	56 [10]; 120 [11]
Fe	1.9075	1.0483	0.4146	40.27	137.88	140 [11]	92 [10]; 182 [11]

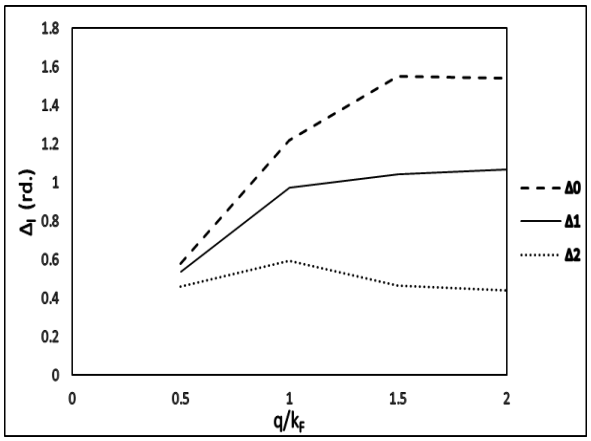

Fig. 1 – The variation of phase shift for Cr

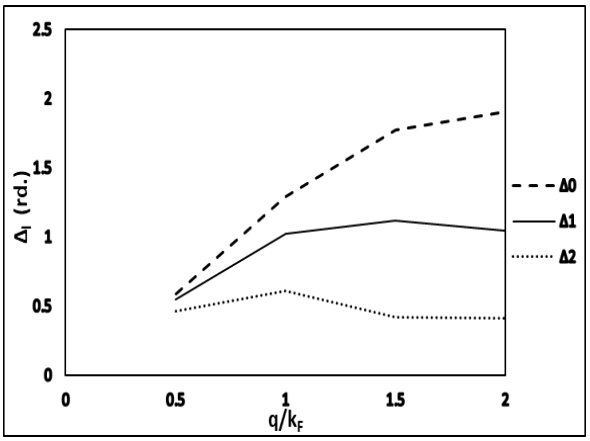

Fig. 2 – The variation of phase shift for Fe

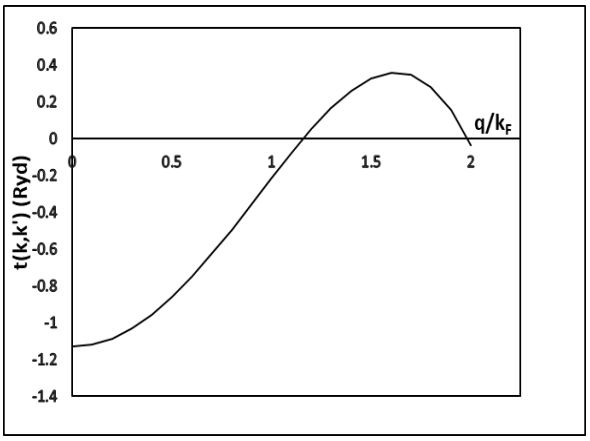

Fig. 3 – The variation of t-matrix form factor for Cr

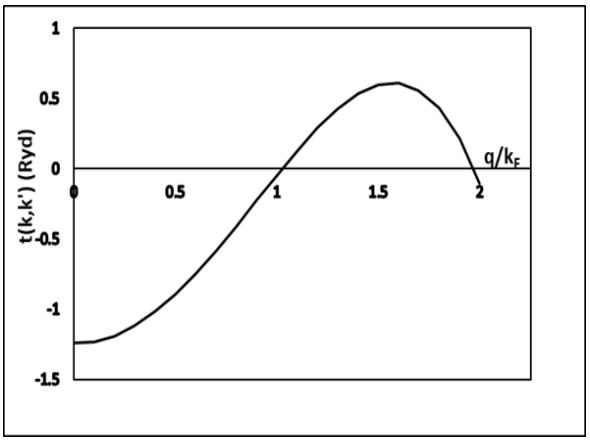

Fig. 4 – The variation of t-matrix form factor for Fe

It is interesting to note that the behavior of t-matrix form factors are identical to screened pseudopotential $V(q)$. From the present study, we can observe one interesting observation that the first zero of t-matrix form factor for all the metals (Mo, W, Nb, Cr and Fe) are found near Fermi surface (within the range (1-1.2) k_F). By taking the limit of Eq. (1) as $q \to 0$, 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:

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

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.

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