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Impact of eigenvalues on the pesudopotential calculation of superconducting parameters of Mg, Al and Zn

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ABSTRACT

In the present paper some superconducting (SC) state parameters of simple metals Mg, Al and Zn have been studied through Harrison's First Principle[HFP] pseudopotential technique using McMillan's formalism. The impact of choosing two different sets of core energy eigenvalues viz, Herman-Skillman and Clementi has been studied. It has been observed that the choice of eigenvalues has appreciable impact on the form factor and consequently on the SC state transition parameter viz, electron-phonon coupling strength (λ) and superconducting transition temperature Tc. Hence the choice of suitable eigenvalues is essential for these computations .Reasonable agreement with experimental and theoretical data have been obtained.

KEYWORDS

Superconductivity;
Pseudopotential;
Multivalent metals.

INTRODUCTION

One of the thrust areas in the field of condensed matter physics is the theoretical and experimental studies of metals and alloys in respect of their superconducting behaviors. The pseudopotential technique has been used by different workers in the past decades[1-3]. In the resent years also some attempts have been done in this direction and they have been reported in the literature[4-7].

The theoretical studies of the superconducting parameters of metals and alloys are based on the famous BCS theory and McMillan formalism[1]. In the present paper the Harrison's First Principle[HFP] pseudopotential technique has been used which has some inherent advantages over the model potential technique. In this technique no arbitrary model of potential is proposed, no arbitrary adjustable parameter is incorporated to give agreement with experimental data. The number of input parameters required are minimum viz,the valence Z, atomic volume Ω_0, Fermi wave vector k_F, core energy eigenvalues $\in_{nl}$, and radial wave function $P_{nl}(r)$. The HFP technique has been widely used in the past for the study of atomic, electronic and other physical properties of metals and alloys with reasonable success. Hence we have been encouraged to use this technique for the present investigation .In the next section we present the formalism, followed by results and figures and conclusion.

Formalism

Within the pseudopotential model the Hamiltonian of the metal is the sum of kinetic energy of the electrons, the Coulomb interaction between electrons, the kinetic energy of bare ions, the coulomb interaction between ions and the bare electron-ion interaction given by the pseudopotential.

This ionic pseudopotential is screened by the conduction electrons and in momentum space the screen-

ing potential is $1/\in(q)$ times the bare pseudopotential, where $\in(q)$ is the dielectric screening function .McMillan[1] on the basis of the pseudopotential theory has obtained the expansion for the Coulomb pseudopotantial μ^* which has been expressed by Gupta and Tripathi[9] as

$$\mu^* = \frac{\mu}{1+\mu \ln (E_F / k_B \theta_D)} \quad (1)$$

where $\mu = \frac{1}{\pi k_F} \int_0^{2k_F} \frac{dq}{q \in (q)}$ (2)

Here θ_D is the Debye temperature, E_f is the Fermi energy, k_f is the Fermi wave vector, $\in(q)$ is the dielectric screening function.

Various other expressions have been proposed with different modification[6-8].

In the present paper we have used the expression of Gupta and Tripathi[9] which has also be used by various authors.

From McMillan's formalism the electron-phonon coupling strength λ is given by

$$\lambda = 2 \int d\omega \alpha^2(\omega) F(\omega) / \omega$$
$$= N(o) \langle I^2 \rangle / M \langle \omega^2 \rangle \quad (3)$$

where $\langle \omega^2 \rangle$ is an average of the square of the phonon frequency.

$$\langle \omega^2 \rangle = \int d\omega \, \alpha^2(\omega) F(\omega) / d\omega \alpha^2(\omega) F(\omega) / \omega \quad (4)$$
$$\cong \int d\omega \, \omega F(\omega) / \int d\omega \, F(\omega) / \omega \quad (5)$$

where $F(\omega)$ is the phonon density of states, $\alpha^2(\omega)$ is the average of electron-phonon interaction. In pseudopotential approach the average I^2 over the Fermi Surface is given by

$$\langle I^2 \rangle = \sum_v \int_0^{2k_F} \frac{(\in_{qv},q)^2 v_q^2 q dp}{\int_0^{2k_F} q dq} \quad (6)$$

$$= 8/9 \, k_F^2 E_F^2 \langle Vq^2 \rangle \quad (7)$$

where E_F and k_F are the Fermi energy and wave number respectively. A dimensionless average of the pseudopotential is given by

$$\langle V_q^2 \rangle = \frac{\int_0^{2k_F} v_q^2 q^3 dq}{\int_0^{2k_F} v_0^2 q^3 dq} \quad (8)$$

Form this the final expression for λ has been obtained as -

$$\lambda = \frac{12 m^* Z^*}{M \langle \omega^2 \rangle} \int_0^2 \eta^3 \, | w(k,q) |^2 d\eta \quad (9)$$

where,

$$\langle \omega^2 \rangle^{1/2} = (\omega_L + \omega_T) / 2 \quad (10)$$

where ω_L & ω_T are the most representative maximum frequencies of longitudinal and transverse modes of phonon spectra as measured by neutron inelastic scattering experiment. This expression as well as other equivalent expressions has been widely used by various authors[4,7]. From μ^* and λ the superconducting transition temperature Tc is computed through the well known McMillan formula[1].

$$T_C = \frac{\theta_D}{1.4} \exp[-(\frac{1.04(1+\lambda)}{\lambda - \mu^* (1+0.62\lambda)})] \quad (11)$$

Computation

In the present work we have studied the impact of the core energy eigenvalues on the computation of the form factor w (k, q) and consequently on the SC state parameters.

It should be mentioned that the core energy eigenvalues are one of the most important input parameters for the computation of the form factor through the HFP technique. The eigenvalues and corresponding eigen functions have been computed through different methods using the self consistent field[SCF] approximation by authors like Herman-Skillman[10] and Clementi[11]. The form factor using these sets of eigenvalues are denoted by $w(k,q)_H$ and $w(k,q)_C$ respectively. Their natures have been shown in figure 1 for Mg, Al and Zn respectively. The computed SC parameters along with the theoretical and experimental data of other authors have been presented in TABLE 1 for comparison.

The computation of form factor has been done through Vashishta-Singwi (V-S) form of dielectric

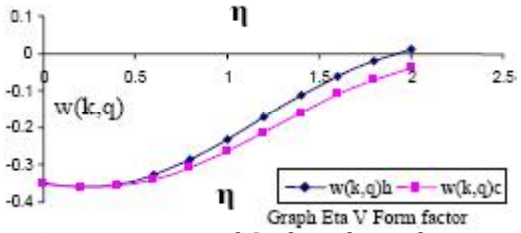

Figure 1 : Nature of the form factor for Mg

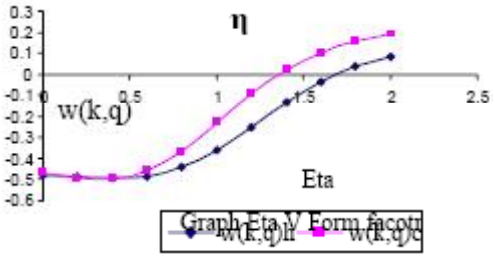

Figure 1 : Nature of the form factor for Al

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TABLE 1

(a): Coulomb pseudopotential μ* of metals using V-S exchange-correlation

Metals	μ* (present)	μ* (others)
Mg	0.11	0.15-0.17[4] 0.12[8], 0.15[12],
Al	0.10	0.14[12], 0.10[8,9,13]
Zn	0.07	0.12[1,12], 0.13–0.14[4],0.09[8,13]

(b): Computed electron-phonon coupling strength λ of metals

λ (present)	λ (others)		λ (others)
	H	C	
Mg	0.24	0.40	0.33-0.49[7],0.23[8],0.39[9] 0.35[12],0.32[13]
Al	0.43	0.50	0.38[1], 0.31-0.47[4], 0.53[12], 0.33[13]
Zn	0.17	0.28	0.38[1],0.31-0.44[7],0.27[12],0.25[13]

(c): Transition temperature T_c K of metals

Metals	T_c (present)		T_c (Expt.)	T_c (others)
	H	C		
Mg	0.0112	1.5172	0.017	0.08-0.009[12], 0.891[7]
Al	2.2789	4.9953	1.196	2.6- 3.0[12],1.16[1], 0.089-2.260[4]
Zn	0.24	0.3499	0.85	0.013[1], 0.782[8], 0.85[2], 0.852[4], 0.0329-0.6051[7], 0.9[3]

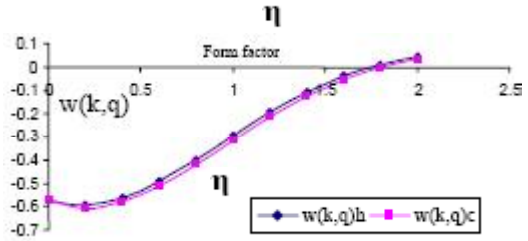

Figure 1 : Nature of the form factor for Mg, Al and Zn

screening function. The Xα- exchange parameter α_{vt} satisfying viral theorem has been used along with the orthogonalisation hole parameter β=1 as originally used by Harrison[2].

RESULT AND FINDINGS

From figure 1 the impact of different sets of eigenvalues viz, those of Herman – Skillman and Clementi are clearly visualized. There is appreciable variation in the magnitude in the higher region of $\eta = q/k_F$ for Mg and Zn while there is almost uniform variation in the form factor of Al .For Mg the $w(k,q)_H$ crosses over the η-axis for $\eta > 1.8$ while $w(k,q)_c$ remains negative throughout .For Al and Zn both the form factors cross over the η- axis with different cross-over points.

TABLE 1 presents the computed electron–phonon coupling strengths λ using these form factors. It is observed that reasonable agreement has been obtained with the previous theoretical data.

TABLE 1 summarizes the computed T_c of the metals under experiment alongwith the experimental data and theoretical data of previous authors. It is observed that $w(k, q)_H$ predicates the Tc = 0.112 against $(Tc)_{expt.}$ = 0.017 K. For Al although experimental data has not been reproduced the value Tc = 2.27 against $(Tc)_{expt.}$ =1.196 K has been obtained with $w(k, q)_H$ which lies within the range of previous theoretical results. Lastly for Zn none of the form factors could satisfactorily reproduce the experimental T_c although λ is within reasonable limit. However, using shaw form of dielectric screenings the result has been improved to 0.35 K and 0.24 K with $w(k,q)_c$ and $w(k,q)_H$ respectively against experimental T_c =0.85 K.

CONCLUSION

The HFP technique has been applied to the study of superconducting transition temperature and other related parameters through the well known McMillan's formalism. With the choice of suitable input parameters and form of dielectric screening the SC parameters may be satisfactorily reproduced.

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