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Impact of core energy eigenvalues on the superconducting parameters of MgB_2

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ABSTRACT

In the present paper we have studied the superconducting parameters viz. electron-phonon coupling strength (λ), Coulomb pseudopotential (μ^*) and transition temperature (T_c) of MgB_2 on the basis of Mc. Millan's formalism. We have applied the Harrison's first principle pseudopotential technique which has been a favorite theoretical framework within which various physical properties of metals and alloys have been studied since past decades. In this paper we have studied the impact of two different sets of core energy eigenvalues and observed that the measured transition temperature can be obtained through the choice of proper core energy eigenvalues ($\in_{nl}$). Reasonable agreement has been obtained using Faber-Ziman formalism.

KEYWORDS

Superconductivity;
Pseudopotential theory;
Magnesium diboride.

1. INTRODUCTION

In the present years, the discovery of superconductivity in magnesium diboride (MgB_2) with remarkably high transition temperature (T_c = 39K) has sparked renewed interest in this system[1] all over the world. This has prompted a large amount of research work on this system both on theoretical and experimental fronts. It is a simple type superconducting material which adopts a simple primitive hexagonal crystal structure comprising of interleaved two dimensional magnesium and boron layers. This simple system does not contain transition metal. The appearance of high T_c superconductivity in such a simple system which does not contains any transition metal has lead to considerable optimism among workers from theoretical and experimental point of view. It has generated an optimism for achieving the high value of T_c in this system with simple constituents.

Loui and Cohen and their coworkers used the well established phonon mediated BCS theory to explain SC state parameters of MgB_2[2]. This theory is a good tool for theoretical studies of such a binary system using Mc Millan's formalism[3] in which Harrrison's first principle pseudopotential (HFPP) technique[4] is used. In this technique, the pseudopotential form factor (PFF) is needed to study the SC state parameters. Recently such attempts are being made[5-8] and we have also persued our investigation along these lines using Harrison's first principle pseudopotential[HFPP] technique[4].

2. Formalism

The SC state parameters under investigations are the electron-phonon coupling strength (λ), Coulomb pseudopotential (μ^*) and SC transition temperature (T_C) represented by

$$\lambda = \frac{12m^*Z^*}{M<\omega^2>}\int_0^1 |w(k,q)|^2 q^3 dq \qquad (1)$$

$$\mu^* = \frac{\mu}{\left[1+\mu\ln\left(\frac{E_F}{k_B\theta_D}\right)\right]} \qquad (2)$$

where $\mu = \frac{m_b}{\pi k_F}\int_0^1 \frac{dq}{q \in *(q)}$ (3)

and $T_C = \frac{\theta_D}{1.45}\exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu*(1+0.62\lambda)}\right]$ (4)

In the above equations the m* is the effective mass of the electron, Z* the effective valence, M the atomic mass, $<\omega^2>$ the averaged phonon frequency, k_B the Boltzmann's constant, θ_D the Debye temperature, m_b the band mass of the electron from the specific heat measurements, E_F the Fermi energy, k_F the Fermi wave vector, q the phonon wave vector, k the electronic wave vector (π/λ) and $\eta = q/2k_F$. $<\omega^2>$ has been estimated by $(k_B\theta_D)^2$ as done by other workers.

The non-local screened form factor of the alloy[9] using Faber-Ziman formalism is given by

$$|w(k,q)_{12}|^2 = c_1|w(k,q)_1|^2 + c_2|w(k,q)_2|^2 + 2(c_1c_2)^{1/2}|w(k,q)_1||w(k,q)_2| \quad (5)$$

where, c_1 and c_2 = Concentration fractions of Mg and B respectively, $w(k, q)_1$ and $w(k, q)_2$ = Form factors of Mg and B respectively, $w(k, q)_{12}$ = Form factor of MgB_2

The basic needs for the computation of the parameters λ and μ * are the form factor w(k,q) and the modified Hartree dielectric screening function $\in$*(q) which has to be computed for the system under investigation through equation (5).

The screened form factor of the constituent metals is given by

$$w(k,q) = \left[\left(v_q^{a,b} + v_q^c + v_q^d\right)/\in *(q)\right] + \left[\{1-G(q)\}v_q^f/\in *(q) + W^R\right] \quad (6)$$

where, $v_q^{a,b}$ is the valence charge and core electron potential, v^c_q the conduction band–core exchange potential, v^d_q the conduction electron potential, v^f_q the screening potential and W^R the repulsive potential.

The modified Hartree dielectric screening function is represented by

$$\in * = [1+G(q)][\in(q)-1]+1 \quad (7)$$

The hartree dielectric screening function is given by

$$\in = 1 + \frac{2}{\pi k_F \eta^2}\left[1 + \frac{4-\eta^2}{4\eta}\ln\left|\frac{2+\eta}{2-\eta}\right|\right] \quad (8)$$

The exchange correlation function is given by

$$G(q) = A\left[1 - e^{-Bn^2}\right] \quad (9)$$

in the (V-S) form[10] of exchange-correlation function. A and B are (V-S) constants. The modified Hartree dielectric screening function $\in$* is also involved in the expression for Coulomb coupling strength μ*.

3. Computation

The core energy eigenvalues ($\in_{nl}$) have been taken from Herman-Skillman (H-S)[11] and Clementi (C)[12]. These eigenvalues of the constituents metals Mg and B obtained from two different sources have been presented in TABLE 1. The computation of the (HFPP) form factor w(**k**,**q**) has been done through equation (6) and the modified Hartree dielectric screening function $\in$*(q) is carried on through equation (7, 8 and 9). From these computed form factors $w(\mathbf{k},\mathbf{q})_1$ and $w(\mathbf{k},\mathbf{q})_2$ of the constituent metals Mg and B, the form factor $w(\mathbf{k},\mathbf{q})_{12}$ of the system MgB_2 is obtained through equation (5). The computed form factors of MgB_2 obtained using two sets of core - energy eigenvalues viz. those of Herman-Skillman (H) and Clementi (C) using Xα-exchange parameter ($\alpha = \alpha_{vt}$) and orthogonalisation hole parameter ($\beta = 1$) and V-S exchange-correlation function[10] have been presented in TABLE 2. The computed SC state parameters have been presented in TABLE 3 alongwith the theoretical data of the other authors as well as the experimental data wherever available. The nature of the computed form factors have been shown in figure 1 for comparison.

4. RESULT AND DISCUSSION

From TABLE 1 we observe that in case of Mg, the H eigenvalues are smaller than C eigenvalues for 1s state. But for 2s and 2p-states, the H eigenvalus are greater than C eigenvalues. The relative deviations $\Delta\in_{nl} = (\in_{nl})_H - (\in_{nl})_C$ are -1.11, 0.972 and 1.24 (Ryd.) for 1s, 2s and 2p-states respectively. In case of B, the H eigenvalues are samaller than C eigenvalues for 1s-state. The relative deviation is -1.017 for 1s-state. It is observed that there are both negative and positive devia-

TABLE 1 : Comparative table of eigenvalues of Mg and B (in Ryd.)

Metals	Sources	Energy eigenvalues			$\Delta\in_{nl}$		
		$\in_{10}$	$\in_{20}$	$\in_{21}$	$\Delta\in_{10}$	$\Delta\in_{20}$	$\Delta\in_{21}$
Mg	H	94.95	6.552	4.144	-1.11	0.972	1.124
	C	96.06	5.58	30.02	-	-	-
B	H	14.373	-	-	-1.017	-	-
	C	15.390	-	-	-	-	-

$\Delta\in_{nl} = (\in_{nl})_H - (\in_{nl})_C$

Full Paper

TABLE 2: Selected form factors of MgB_2 (in Ryd.) using two sets of eigenvalues H and C with $\alpha = \alpha_{vt}$, $\beta = 1$ and (V-S) exchange-correlation function

$\eta = q/k_F$	$w((k, q)_H$	$w(k, q)_C$	$\Delta w = w(k, q)_H - w(k, q)_C$
0.0	-1.0089	-1.0089	0
0.2	-1.0378	-1.0394	-0.0016
0.4	-0.9746	-0.9779	-0.0033
0.6	-0.8635	-0.8688	-0.0053
0.8	-0.7250	-0.7329	-0.0079
1.0	-0.5790	-0.5899	-0.0109
1.2	-0.4409	-0.4546	-0.0137
1.4	-0.3206	-0.3366	-0.0160
1.6	-0.2250	-0.2400	-0.0175
1.8	-0.1470	-0.1048	-0.0178
2.0	-0.1018	-0.1059	-0.0041

TABLE 3 : Computed SC state parameters

Form factors	SC state parameters				
	μ^*	λ(Present)	λ(Previous)	T_C(Present)	T_C(Expt.)
$w(k,q)_H$	0.11	0.73	0.7 - 0.9	30.3	39K
$w(k,q)_C$	0.11	0.79	-	36.1	-

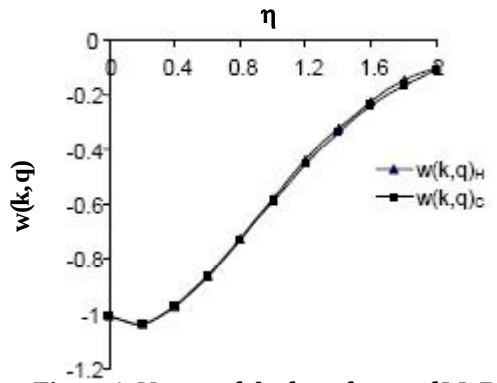

Figure 1: Nature of the form factor of MgB_2

tions in the two sets of eigenvalues of Mg while there is only negative deviations in the two sets of eigenvalues of B.

From TABLE 2 and figure 1 it is found that inspite of significant differences in the two sets of eigenvalues, namely those of Herman-Skillman (H) and Clementi (C), the form factors have not been so significantly affected. This is due to the positive and negative deviations of the two sets of eigenvalues. The maximum percentage variation of the form factors due to the two sets of eigenvalues is nearly 12%.

TABLE 3 reveals that the Coulomb coupling strength (μ^*) is found to be order of 0.1 as obtained by previous authors. The electron-phonon coupling strength (λ) are $\lambda_H = 0.73$ and $\lambda_C = 0.79$ respectively. The value of λ lies in the range 0.7 – 0.9 as obtained by other authors[13-21]. The SC transition temperature (T_C) are $(T_C)_H = 30.3$K and $(T_C)_C = 36.1$K respectively against the experimental value of $T_C = 39$K[1]. The impact on λ is about 0.06[$\lambda_H = 0.73$, $\lambda_C = 0.79$]. The impact on T_C is about 5.8K[$(T_C)_H = 30.3$K, $(T_C)_C = 36.1$K]. Thus C eivenvalues give better agreement with $(T_C)_{Expt} = 39$K.

5. CONCLUSION

From the above investigation it may be concluded that the Harrison's First principle pseudopotential technique in conjunction with the Faber-Ziman formalism is successful in reproducing the SC state transition parameters of MgB_2 on the basis of BCS theory and Mc.Millian's formalism.

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