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Screening dependence of Superconducting State parameters of Carbon doped MgB_2

Gargee Sharma

Abstract— The screening dependence of superconducting state parameter (λ, μ*, T_c, α and N_0V) of four alloys of carbon doped MgB_2 system has been studied in the BCS-Eliashberg-McMillan framework by employing five forms of dielectric screening function in conjunction with Ashcroft's potential. It is observed that electron-phonon coupling strength (λ) and Coulomb pesudopotential (μ*) are quite sensitive to the form of dielectric screening , whereas the transition temperature (T_c), isotope effect exponent (α) and effective interaction strength(N_0V) show weak dependence on screening function. The Random phase approximation (RPA) form of dielectric screening function is observed to yield best results for all the alloys of carbon doped MgB_2 system studied in the present work. Present computation yield quadratic variation of T_c with concentration(x) in the carbon doped MgB_2 system, which is in good agreement with the experimental data. A quadratic T_c equation is proposed by fitting the present results for Random phase approximation (RPA) screening, which is in conformity with other results for the experimental data.

Index Terms— MgB_2, Pseudopotential, superconductivity, transition temperature, electron-phonon coupling strength, isotope effect, interaction strength.

1 INTRODUCTION

he pseudopotential theory [1] has successfully contributed Tin the advancement of microscopic theory of various properties of metals, alloys and metallic glasses viz. atomic structure, electronic, thermal and superconducting properties etc. The method followed in this theory is simple and straight forward and has been applied to calculate binding energy, elastic constants, phonon spectrum, resistivity and superconducting state parameters etc. of various metals, alloys and metallic glasses. In the pseudopotential theory any solid can be thought of as a set of rather tightly bound spherical ions assembled in the system of electron gas formed by valence or conduction electrons, separated from the ions and which are mainly responsible for most of the physical and chemical properties of the solid. The ions interact with each other by direct Coulombian repulsive forces and indirect attractive forces acting through the electron gas permeating through the ions. The effective way of representing interaction between the conduction electron and the ion core is known as pseudopotential (PP) [2,3].The atomic pseudopotential is the sum of two terms, the attractive Coulomb potential of the ion experienced by the conduction electrons and a repulsive potential arising due to exclusion of conduction electrons from the bound electrons in the core-region but a conduction electron also experiences an additional potential due to electron-electron interaction i.e. the interaction of a conduction electron with the other conduction electrons. The above problem can be viewed differently by saying that the electron gas formed by conduction electrons provides a dielectric medium for electron-ion interaction. Thus, an ion interacts with an electron through the medium of electron gas and other ions. The electron-ion interaction is accounted for by the pseudopotential and electron-electron interaction is involved through a dielectric screening function, so for successful prediction of the properties of a system, careful selection of pseudopotential and screening function is essential.

Empty core model pseudopotential due to Ashcroft [4] is a simple one parameter potential, which has been found to work well for metallic systems [5, 6, 7] and binary alloys [8, 9]. This potential when used with suitable form of dielectric screening has also been found to yield good results in predicting superconducting state parameters of metallic systems [10, 11,12] As such we decided to employ this potential in the present work. In order to determine the best form of dielectric screening to be used with Ashcroft's potential for predicting the superconducting state parameters carbon doped MgB_2 system we use five different forms of dielectric screening in conjunction with Ashcroft's potential, viz. Random phase approximation (RPA) [13], Harrison [14], Geldart and Vosko [15] Hubbard [16], and Overhauser [17].

In the present investigation we decided to study alloys of carbon doped MgB_2 system for the following reasons: MgB_2 has an unusual high critical temperature of about 40K among binary compounds, with an AlB_2-type structure and the substitutions are important from several points of view. First, it may increase the critical temperature of one compound. Secondly, it may suggest the existence of a related compound with higher T_c. Thirdly; the doped elements which do not lower the T_c considerably may act as pinning centers and increase the critical current density. And last but not least, there has been extensive experimental study of lattice, electronic, thermal, resistive, and superconducting and other properties of $MgB_{2-x}C_x$ [18-20]. However there are few theoretical investigations [21-22] reported in the literature, and in particular the screening dependence of superconducting state parameters has not been reported so far.

• *Gargee Sharma,Government Dungar College, Bikaner, India .*
E-mail: gargeesharma9@gmail.

2 Theory

The electron phonon coupling strength (λ) and Coulomb pseudopotential (μ^*) [23-24] for the alloy of the $MgB_{2-x}C_x$ system may be written by extending the relevant formula as:

$$\lambda = \frac{12\, m^* z^*}{M\langle\omega^2\rangle}\int_0^1 x^3\, |\, Vs\,(x)|^2\ dx\,, \qquad (1)$$

where Vs(x) is the screened potential. The relevant expression of Ashcroft's potential is given (in a.u.) by:

$$V_s(x) = \frac{-\pi z^*\ \cos(2\, k_F\ r_c x)}{\Omega_0\, k_F^2\, x^2\, \mathcal{E}(x)}\ , \qquad (2)$$

where

$$x = \frac{q}{2\, k_F}, \quad \text{and} \quad \Omega_0 = \frac{3\,\pi^2 z^*}{k_F^3}, \qquad (3)$$

$$\mu^* = \frac{\frac{m_b}{\pi\, k_F}\int_0^1 \frac{dx}{x\, \varepsilon(x)}}{\left[1+\frac{m_b}{\pi\, k_F}\ln\left(\frac{k_F^{\ 2}}{20\ \theta_D}\right)\int_0^1 \frac{dx}{x\ \varepsilon(x)}\right]}\ , \qquad (4)$$

And the symbols m*, $\langle\omega^2\rangle$, z*, Ω_0, k_F, M, and θ_D) denote the effective mass, most representative average square phonon frequency, effective valence, Fermi wave vector, ionic mass and Debye temperature for the alloys, respectively. $\mathcal{E}(x)$ in Eq. 2 and Eq. 3 is modified Hartree screening function, which is written as [25]:

$$\mathcal{E}(x) = 1 + \{\,(1 - f\,(x))\,(\mathcal{E}_H(x) - 1)\} \qquad (5)$$

where $\mathcal{E}_H$ is the static Hartree dielectric function [25] and f(x) is the local field correction function. In the present investigation, to know the dielectric dependence of superconducting state parameters, we consider the dielectric screening function due to Random phase approximation (RPA) [13], Harrison [14], Geldart and Vosko [15] Hubbard [16], and Overhauser [17]. Hartree screening function is purely static, and it does not include the exchange and correlation effects and is thus expressed as f (x) = 0.

$$\mathcal{E}_H(x) = Q(x) + 1\,, \qquad (6)$$

where

$$Q(x) = \frac{m}{\pi\, k_F x^2}\ f(x)\,, \qquad (7)$$

The Hartree screening function can be modified by replacing the free electron mass by effective mass m* which is known as RPA dielectric function and is given by [13]:

$$\mathcal{E}_{RPA}\,(x) = \frac{m^*}{\pi\, k_F x^2}\ f(x) + 1, \qquad (8)$$

where

$$f(x) = 0.5 + \frac{(1-x^2)}{4\,x}\ln\left|\frac{(1+x)}{(1-x)}\right|, \qquad (9)$$

The relevant forms of dielectric screening function due to Harrison (Ha) and Geldart-Vosko (GV), and are as given below:

$$f_{Ha}\,(x) = \frac{1}{2}\left[\frac{x^2}{x^2+\ \frac{1}{3}}\right], \qquad (10)$$

$$f_{GV}\,(x) = \left[\frac{2x^2}{4x^2+v}\right], \qquad (11)$$

with

$$v = \frac{2}{\left[1 + 0.153\left(\frac{m^*}{\pi\ k_F}\right)\right]}, \qquad (12)$$

The relevant forms of dielectric screening function due to Hubbard (HB) and Overhauser (OH) are as given below [1]:

$$\varepsilon(x) = 1 + \frac{Q(x)}{1-f(x)Q(x)}, \qquad (13)$$

where

$$Q(x) = \mathcal{E}_H(x) - 1\,, \qquad (14)$$

$$f_{HB}\,(x) = \frac{2x^2}{1+4x^2+\frac{4\,m^*}{\pi k_F}}\ , \qquad (15)$$

and

$$f_{OH}\,(x) = \frac{1.1\ x^2}{(\,1+10\,x^2+\ 1.50\ \ x^4\,)^{\frac{1}{2}}}\ , \qquad (16)$$

The relevant expression for the transition temperature (T_c), isotope effect exponent (α), and effective interaction strength (N_0V) [26-27] for $MgB_{2-x}C_x$ is taken as:

$$T_c = \frac{\theta_D}{1.45}\left\{\exp\left(\frac{-1.04\ \ (1+\ \lambda)}{\lambda - \mu^*\,(1+0.62\ \ \lambda)}\right)\right\}, \qquad (17)$$

$$\alpha = \frac{1}{2}\left[\,1 - \left(\mu^*\ln\frac{\theta_D}{1.45\ T_C}\right)^2\ \frac{1\ +\ 0.62\ \lambda}{1.04\ \ (1+\lambda)}\right], \qquad (18)$$

$$N_0V = \frac{\lambda - \mu^*}{1+\ \left(\frac{10}{11}\right)\ \lambda}\ , \qquad (19)$$

3 Result And Discussion

The values of input parameters relevant to the components of the $MgB_{2-x}C_x$ have been assembled in Table 1. In the present work we use m_b=m* for the sake of uniformity. The values of m*, $\langle\omega^2\rangle$, z*, M for the $MgB_{2-x}C_x$systemunder investigation are obtained from the relevant values for the component by using Vegard's rule [28], viz.

$$V_s = \frac{1}{3}[V_s(Mg) + (2-x)V_s(B) + x\,V_s(C)], \qquad (20)$$

The value of θ_D for the $MgB_{2-x}C_x$ system is computed from the relevant values by using Grimvall's formula [32], viz.

$$\frac{1}{\theta_D^2} = \frac{1}{3}\left[\frac{1}{\theta_{DMg}^2} + \frac{2-x}{\theta_{DB}^2} + \frac{x}{\theta_{DC}^2}\right], \qquad (21)$$

Table 2 shows the computed values of electron-phonon coupling strength (λ) for $MgB_{2-x}C_x$ system with Ashcroft's potential using five different forms of dielectric screening. Fig.1 shows the variation of electron-phonon coupling strength (λ) with the different concentration of carbon (x=0.00, 0.03, 0.11, 0.20) for different forms of dielectric screening. It is observed from the table as well as Fig.1 that the value of electron-phonon coupling strength (λ) for $MgB_{2-x}C_x$ system decreases continuously by increasing carbon concentration for all five different forms of dielectric screening. The values obtained using different forms of dielectric screening yield different results that vary from 1.213 to 1.719 for concentration x = 0.00 and 1.028 to 1.423

for concentration x=0.20. These results show that e-ph coupling constant is quite sensitive to the form of dielectric screening used. The computed results obtained are in accordance with the experimental and other reported values. On increasing the concentration of carbon electron-phonon coupling strength (λ) decreases which shows change of strong coupling behavior of MgB_2 to intermediate coupling behavior with doping.The present electron phonon coupling strength (λ) values are also well within the limit 0.65 to 1.2 prescribed by Hinks et al. [38]. Fig.1 and Table 2 shows that the G.V screening yields the highest values of λ, whereas the values obtained from other screenings are almost same. G.V screening is suitable for metals and elements where as it is not suitable for binary glasses and alloys [1] [39-41].

TABLE1.

VALUES OF INPUT PARAMETERS [29-31]

Data	Component metals		
	Mg	B	C
m*	1.01	1.394	0.87
M(au)×10^4	4.4345	1.8440	2.1908
K_F (au)	0.7242	1.2177	1.4594
Ω_0(au)	156.819	51.824	38.363
z^*	2	3	4
$<\omega^2>$(au)×10^{-6}	0.76389	7.45985	16.521
θ_D(K)	400	1250	1860

TABLE2

Computed values of λ for $MgB_{2-x}C_x$system for five different screening.

x	λ					
	RPA	Ha	G V	HB	OH	0thers [33-37]
0.00	1.291	1.344	1.719	1.246	1.213	1.7-1.4 ,1.08, 0.90,0.87
0.03	1.258	1.316	1.686	1.221	1.189	
0.11	1.199	1.242	1.592	1.150	1.132	
0.20	1.087	1.124	1.423	1.042	1.028	

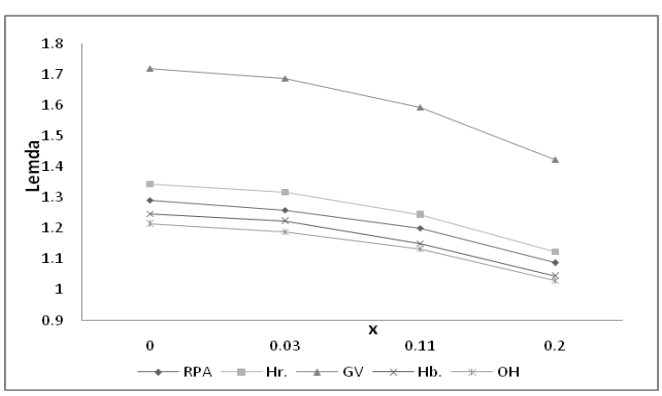

Fig.1 Variation of electron phonon coupling strength (λ) with C-conc.x (at.%) for five dielectric screening.

The values of Coulomb pseudopotential (μ^*), which accounts for the Coulomb interaction between the conduction electrons, obtained from five different forms of dielectric screening are tabulated in Table 3. Fig. 2 shows the variation of Coulomb pseudopotential (μ^*), with the different concentration of Carbon (x = 0.00, 0.03, 0.11, 0.20) for different forms of dielectric screening, which shows the strong dependence of μ^*on dielectric screening. It is observed from the table as well as Fig.2 that the value of Coulomb pseudopotential (μ^*), for $MgB_{2-x}C_x$ system decreases continuously by increasing carbon concentration for all five different forms of dielectric screening. The results obtained from all five different forms of dielectric screening yield different values. The computed results obtained are in accordance with the experimental and others [43-44] and also by Allen and Cohen [45].

TABLE3

Computed values of values of μ^* for $MgB_{2-x}C_x$system for five different screening

x	μ^{*-}					
	RPA	Ha	G V	HB	OH	0thers [42-44]
0.00	0.172	0.184	0.267	0.157	0.152	0.15,0.14, 0.13-0.12
0.03	0.171	0.183	0.267	0.157	0.152	
0.11	0.170	0.182	0.266	0.156	0.151	
0.20	0.169	0.180	0.265	0.155	0.151	

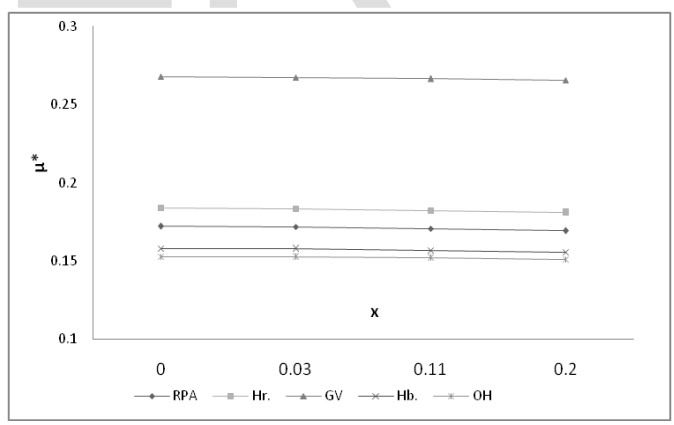

Fig.2 Variation of Coulomb pseudopotential (μ^*) with C-conc.x (at.%) for five dielectric screening

Table 4 contains computed values of transition temperature (T_c) for the $MgB_{2-x}C_x$system obtained from five different forms of dielectric screening along with experimental transition temperature (T_c) values [46].The values of T_c with varying concentration of carbon in $MgB_{2-x}C_x$ system have been plotted for dielectric screening in Fig.3.The graph also include experimental values [46]. It is observed from the table as well as Fig.3 that the value of transition temperature (T_c) for $MgB_{2-x}C_x$ system decreases continuously by increasing carbon concentration for all

five different forms of dielectric screening. However the results obtained using RPA dielectric screening are in best agreement with the experimental data, as the relevant curve for RPA screening almost overlaps the experimental curve. It is interesting to know that the values of T_c obtained using different screening functions are almost same for all carbon concentration showing its insensitivity towards form of dielectric screening function. Formula for T_c consists of both λ & μ^* terms and they both are sensitive to the form of dielectric screening function; so it is possible that they cancel each other's effect in $MgB_{2-x}C_x$ system.

TABLE4

Computed values of values of Tc for $MgB_{2-x}C_x$system for five different screening.

x	T_c(K)					
	RPA	Ha	GV	HB	OH	Expt.[46]
0.00	38.41	38.60	38.51	38.82	38.19	38.40
0.03	37.05	37.58	37.52	37.75	37.10	37.05
0.11	34.56	34.59	34.53	34.55	34.54	34.50
0.20	29.38	29.31	29.90	29.35	29.38	29.30

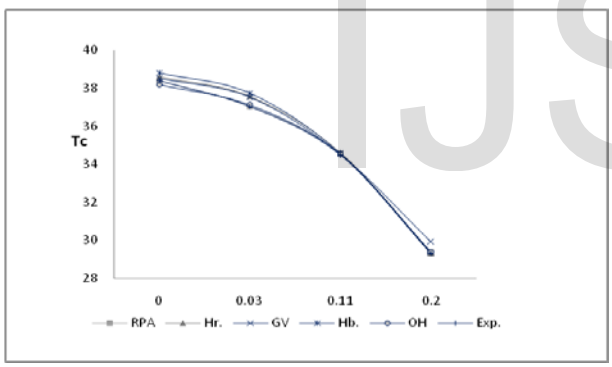

Fig 3. Variation of transition temperature T_c with C-conc. x (at.%) for five dielectric screening.

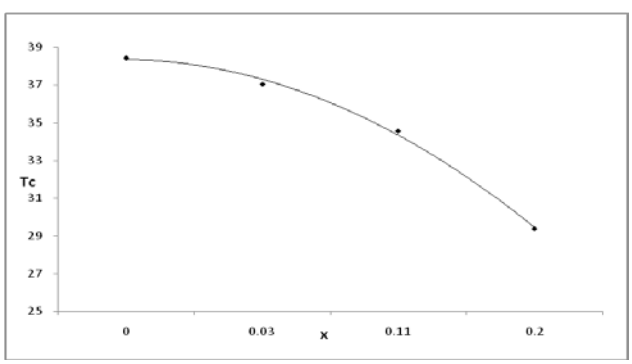

Fig 4. Fitted T_c equation showing variation T_c with C- conc. x (at.%) .
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The plot of fitted T_c equation is represented in Fig. 4, which indicates that T_c drops in quadratical manner with increasing C content. A wide extrapolation predicts a T_c = 37.28 K for the hypothetical case of "amorphous pure MgC_2".The composition dependence can be described by quadratic regression of the data obtained for RPA screening for different values of x, which yields.

$$T_c(K) = -0.955x^2 + 1.817x + 37.47, \qquad (22)$$

The values of isotope effect exponent (α) for $MgB_{2-x}C_x$ system for the five different forms of dielectric screening are tabulated in Table 5.Fig.5 shows the variation of isotope effect exponent (α) with carbon concentration (x) for different screenings. It is observed from the table as well as Fig. 5 that the value of isotope effect exponent (α) for $MgB_{2-x}C_x$ system decreases continuously by increasing carbon concentration for all five different forms of dielectric screening which suggests that the superconductivity is suppressed as the relative concentration of Carbon increases in MgB_2.The values obtained from all screening functions are almost same, however the values obtained using Geldart & Vosko screening yields slightly lower than the other screenings .The values of isotope effect exponent (α) show a weak dependence on the form of dielectric screening function.

TABLE5

Computed values of α for $MgB_{2-x}C_x$system for five different screening.

x	α					
	RPA	Ha	GV	HB	OH	Other [22]
0.00	0.434	0.425	0.346	0.444	0.447	0.462
0.03	0.432	0.422	0.342	0.443	0.446	
0.11	0.428	0.419	0.331	0.439	0.443	
0.20	0.419	0.409	0.323	0.431	0.435	

TABLE6

Computed values of N_0V for $MgB_{2-x}C_x$system for five different screening.

x	N_0V					
	RPA	Ha	GV	HB	0.504	Other [22]
0.00	0.514	0.522	0.566	0.510	0.498	0.407
0.03	0.507	0.512	0.560	0.504	0.483	
0.11	0.492	0.497	0.541	0.485	0.453	
0.20	0.461	0.469	0.508	0.455	0.504	

The values of interaction strength (N_0V) for $MgB_{2-x}C_x$ system for the five different forms of dielectric screening are tabulated in Table 6.Fig.6 shows the variation of interaction strength (N_0V) with carbon concentration (x) for different screenings. It is observed from the table as well as Fig.6 show that the value of interaction strength (N_0V) for $MgB_{2-x}C_x$ system decreases continuously by increasing carbon concentration for all five different forms of dielectric screening. The val-

ues obtained from all screening functions are almost same, however with Geldart & Vosko screening function we get slightly higher results than other screening functions .The values of interaction strength (N_0V) obtained again show a weak dependence on dielectric screening.

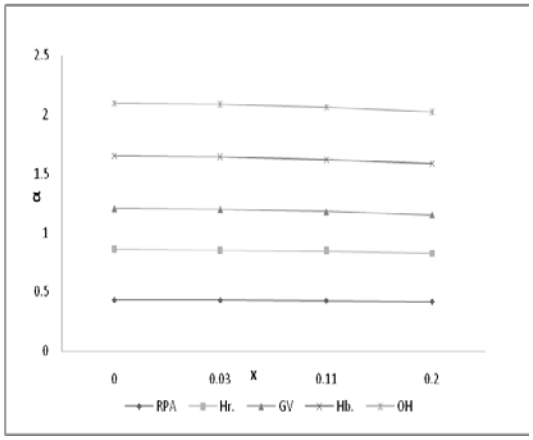

Fig 5. Variation of isotope effect exponent (α) with C-conc x (at. %) for five dielectric screening.

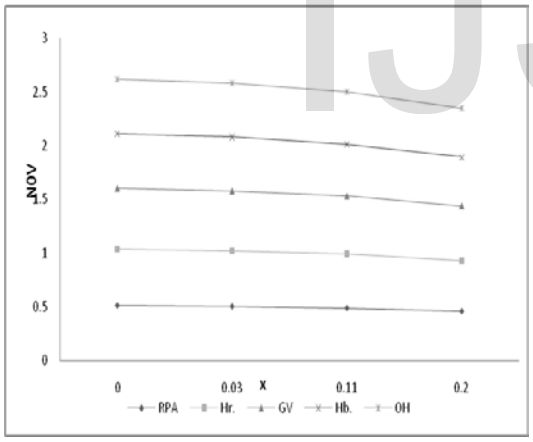

Fig 6. Variation of interaction strength (N_0V) with C-conc. x (at. %) for five dielectring screening.

4 Conclusion

The present study shows that electron-phonon coupling strength(λ) and Coulomb pseudo potential (μ*) are quite sensitive to the form of dielectric screening, whereas the transition temperature (T_c), isotope effect exponent (α) and effective interaction strength(N_0V) show weak dependence on screening function. It is observed that the superconducting parameters of carbon doped MgB_2 system are composition dependent i.e. they vary with the change in concentration of component metals. The study also proves that the RPA form of dielectric screening when used with Ashcroft's potential provides best explanation for the superconductivity in carbon doped MgB_2 system. A quadratic T_c equation is proposed by fitting the present results for RPA screening, which is in conformity with other results for the experimental data.

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