Screening dependence of Superconducting State parameters of Carbon doped MgB₂

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Abstract— The screening dependence of superconducting state parameter (λ, μ*, Tc, α and N/V) of four alloys of carbon doped MgB₂ 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 pseudopotential (μ*) are quite sensitive to the form of dielectric screening , whereas the transition temperature (Tc), isotope effect exponent (α) and effective interaction strength(N/V) 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 MgB₂ system studied in the present work. Present computation yield quadratic variation of Tc with concentration(x) in the carbon doped MgB₂ system, which is in good agreement with the experimental data. A quadratic Tc 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— MgB₂, Pseudopotential, superconductivity, transition temperature, electron-phonon coupling strength, isotope effect, interaction strength.

1 INTRODUCTION

The pseudopotential theory [1] has successfully contributed in 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 straightforward 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 MgB₂ 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 MgB₂ system for the following reasons: MgB₂ has an unusual high critical temperature of about 40K among binary compounds, with an AlB₂-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 Tc. Thirdly; the doped elements which do not lower the Tc 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 MgB₂-Cx [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.
2 Theory

The electron phonon coupling strength (λ) and Coulomb pseudopotential (μ∗) [23-24] for the alloy of the MgB2-xCx system may be written by extending the relevant formula as:

\[ \lambda = \frac{12 m_e^*}{\text{Mg}_2^*} \int_0^1 x^3 |V_s(x)|^2 \, dx, \quad (1) \]

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

\[ V_s(x) = -\frac{\mu^* \cos(2k_Fr_\alpha x)}{0.2k_F^2 \varepsilon(x)}, \quad (2) \]

where

\[ x = \frac{q}{2k_F} \quad \text{and} \quad \Omega_0 = \frac{3m_e^*}{k_F^2}, \quad (3) \]

\[ \mu^* = \frac{m_b}{\pi k^2} \int \frac{dx}{[1 + 20^{0.25}] \varepsilon(x)}, \quad (4) \]

And the symbols \( m^*, \langle \omega^2 \rangle, z^*, \Omega_0, k_F, \text{M}, \text{and} \theta_0 \) denote the effective mass, most representative average square phonon frequency, effective valence, Fermi wave vector, ionic mass and Debye temperature for the alloys, respectively. \( \varepsilon(x) \) in Eq. 2 and Eq. 3 is modified Hartree screening function, which is written as [25]:

\[ \varepsilon(x) = 1 + \left\{ \left(1 - f(x)\right) \left( \varepsilon_{H} - 1 \right) \right\} \quad (5) \]

where \( \varepsilon_{H} \) 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 \( f(x) = 0 \).

\[ \varepsilon_{H}(x) = Q(x) + 1, \quad (6) \]

\[ Q(x) = \frac{m}{\pi k_F^2} f(x), \quad (7) \]

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]:

\[ \varepsilon_{RPA}(x) = -\frac{m}{\pi k_F^2} f(x) + 1, \quad (8) \]

where

\[ f(x) = 0.5 + \frac{1-(x^2)}{4x} \ln \left[ \frac{1+(x)}{1-(x)} \right]. \quad (9) \]

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

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

\[ f_{GV}(x) = \frac{2x^2}{4x^2 + 1}, \quad (11) \]

with

\[ \nu = \frac{2}{1 + 0.153 \left( \frac{m^*}{\pi k_F} \right)^2}. \quad (12) \]

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

\[ \varepsilon(x) = 1 + \frac{q(x)}{1-f(x)Q(x)}, \quad (13) \]

where

\[ Q(x) = \varepsilon_{H}(x) - 1, \quad (14) \]

\[ f_{HB}(x) = \frac{2x^2}{1+4x^2+4 \pi m^*}, \quad (15) \]

and

\[ f_{OH}(x) = \frac{1.1x^2}{(1+10x^2+1.5x^4)^2}, \quad (16) \]

The relevant expression for the transition temperature (\( T_c \)), isotope effect exponent (\( \alpha \)), and effective interaction strength (\( N_0 \varepsilon \)) [26-27] for MgB2-xCx is taken as:

\[ T_c = \frac{0.15}{1+0.153 \left( \frac{m^*}{\pi k_F} \right)^2} \exp \left( \frac{-1.04 (1 + \lambda)}{\lambda - \mu^* (1+0.62 \lambda)} \right), \quad (17) \]

\[ \alpha = \frac{1}{2} \left[ 1 - (\mu^* \ln \left( \frac{0.15}{1+0.153 \left( \frac{m^*}{\pi k_F} \right)^2} \right) 2 + 1 + 0.62 \lambda \right], \quad (18) \]

\[ N_0 \varepsilon = \frac{\lambda - \mu^*}{1 + (\mu^*/\pi)^2 \lambda}, \quad (19) \]

3 Result and Discussion

The values of input parameters relevant to the components of the MgB2-xCx have been assembled in Table 1. In the present work we use \( m=m^* \) for the sake of uniformity. The values of \( m^*, \langle \omega^2 \rangle, z^*, M \) for the MgB2-xCx system under investigation are obtained from the relevant values for the component by using Vegard’s rule [28], viz.

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

The value of \( \theta_0 \) for the MgB2-xCx system is computed from the relevant values by using Grimvall’s formula [32], viz.

\[ \frac{1}{\theta_0} = \frac{1}{3} \left[ \frac{1}{\theta_{BO}}, \frac{2-x}{\theta_{DO}} + \frac{x}{\theta_{DC}} \right], \quad (21) \]

Table 2 shows the computed values of electron-phonon coupling strength (\( \lambda \)) for MgB2-xCx system with Ashcroft’s potential using five different forms of dielectric screening. Fig.1 shows the variation of electron-phonon coupling strength (\( \lambda \)) 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 (\( \lambda \)) for MgB2-xCx 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 ($\lambda$) decreases which shows change of strong coupling behavior of MgB$_2$ to intermediate coupling behavior with doping. The present electron phonon coupling strength ($\lambda$) 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 $\lambda$, 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]

<table>
<thead>
<tr>
<th>Data</th>
<th>Component</th>
<th>metals</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m^*$</td>
<td>Mg</td>
<td>B</td>
</tr>
<tr>
<td>$M(au)\times 10^4$</td>
<td>4.4345</td>
<td>1.8440</td>
</tr>
<tr>
<td>$K_e(au)$</td>
<td>0.7242</td>
<td>1.2177</td>
</tr>
<tr>
<td>$Q(au)$</td>
<td>156.819</td>
<td>51.824</td>
</tr>
<tr>
<td>$&lt;\omega^2&gt;(au)\times 10^{-6}$</td>
<td>0.76389</td>
<td>7.45985</td>
</tr>
<tr>
<td>$\theta_d(K)$</td>
<td>400</td>
<td>1250</td>
</tr>
</tbody>
</table>

**TABLE2**

Computed values of $\lambda$ for MgB$_{2-x}$C$_x$ system for five different screening.

<table>
<thead>
<tr>
<th>$x$</th>
<th>RPA</th>
<th>Ha</th>
<th>G V</th>
<th>HB</th>
<th>OH</th>
<th>Others [33-37]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>1.291</td>
<td>1.344</td>
<td>1.719</td>
<td>1.246</td>
<td>1.213</td>
<td>1.7-1.4,1.08, 0.90,0.87</td>
</tr>
<tr>
<td>0.03</td>
<td>1.258</td>
<td>1.316</td>
<td>1.686</td>
<td>1.221</td>
<td>1.189</td>
<td></td>
</tr>
<tr>
<td>0.11</td>
<td>1.199</td>
<td>1.242</td>
<td>1.592</td>
<td>1.150</td>
<td>1.132</td>
<td></td>
</tr>
<tr>
<td>0.20</td>
<td>1.087</td>
<td>1.124</td>
<td>1.423</td>
<td>1.042</td>
<td>1.028</td>
<td></td>
</tr>
</tbody>
</table>

**TABLE3**

Computed values of $\mu^*$ for MgB$_{2-x}$C$_x$ system for five different screening.

<table>
<thead>
<tr>
<th>$x$</th>
<th>$\mu^*$</th>
<th>RPA</th>
<th>Ha</th>
<th>G V</th>
<th>HB</th>
<th>OH</th>
<th>Others [42-44]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.172</td>
<td>0.184</td>
<td>0.267</td>
<td>0.157</td>
<td>0.152</td>
<td>0.15,0.14, 0.13-0.12</td>
<td></td>
</tr>
<tr>
<td>0.03</td>
<td>0.171</td>
<td>0.183</td>
<td>0.267</td>
<td>0.157</td>
<td>0.152</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.11</td>
<td>0.170</td>
<td>0.182</td>
<td>0.266</td>
<td>0.156</td>
<td>0.151</td>
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<td></td>
</tr>
<tr>
<td>0.20</td>
<td>0.169</td>
<td>0.180</td>
<td>0.265</td>
<td>0.155</td>
<td>0.151</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

The values of Coulomb pseudopotential ($\mu^*$), 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 ($\mu^*$), 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 $\mu^*$on dielectric screening. It is observed from the table as well as Fig.2 that the value of Coulomb pseudopotential ($\mu^*$), 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].

**TABLE4**

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 $\lambda$ & $\mu^*$ 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 $\text{MgB}_2\text{C}_x$ system.

\[ T_c(K) = -0.955x^2 + 1.817x + 37.47, \quad (22) \]

The values of isotope effect exponent ($\alpha$) for $\text{MgB}_2\text{C}_x$ system for the five different forms of dielectric screening are tabulated in Table 5. Fig. 5 shows the variation of isotope effect exponent ($\alpha$) 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 ($\alpha$) for $\text{MgB}_2\text{C}_x$ 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 $\text{MgB}_2$. 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 ($\alpha$) show a weak dependence on the form of dielectric screening function.

\[ \text{TABLE5} \]

Computed values of $\alpha$ for $\text{MgB}_2\text{C}_x$ system for five different screening.

<table>
<thead>
<tr>
<th>$x$ (at.%)</th>
<th>RPA</th>
<th>Ha</th>
<th>GV</th>
<th>HB</th>
<th>OH</th>
<th>Expt. [46]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.434</td>
<td>0.425</td>
<td>0.346</td>
<td>0.444</td>
<td>0.447</td>
<td>0.462</td>
</tr>
<tr>
<td>0.03</td>
<td>0.432</td>
<td>0.422</td>
<td>0.342</td>
<td>0.443</td>
<td>0.446</td>
<td></td>
</tr>
<tr>
<td>0.11</td>
<td>0.428</td>
<td>0.419</td>
<td>0.331</td>
<td>0.439</td>
<td>0.443</td>
<td></td>
</tr>
<tr>
<td>0.20</td>
<td>0.419</td>
<td>0.409</td>
<td>0.323</td>
<td>0.431</td>
<td>0.435</td>
<td></td>
</tr>
</tbody>
</table>

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 $\text{MgC}_2$". The composition dependence can be described by quadratic regression of the data obtained for RPA screening for different values of $x$, which yields.

\[ T_c(K) = -0.955x^2 + 1.817x + 37.47, \quad (22) \]

The values of interaction strength ($N_0V$) for $\text{MgB}_2\text{C}_x$ 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 that the value of interaction strength ($N_0V$) for $\text{MgB}_2\text{C}_x$ 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.

![Graph](image1)

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

![Graph](image2)

**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 ($\lambda$) and Coulomb pseudo potential ($\mu^*$) are quite sensitive to the form of dielectric screening, whereas the transition temperature ($T_c$), isotope effect exponent ($\alpha$) 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 metal.

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### References


