A study of carbon substitutions in MgB$_2$ within the two-band Eliashberg theory

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We study the effects of C substitutions in MgB$_2$ within the two-band model in the Eliashberg formulation. We use as input the $B-B$ stretching-mode frequency and the partial densities of states $N_n^\sigma(E_F)$ and $N_n^\pi(E_F)$, recently calculated for Mg(B$_{1-x}$C$_x$)$_2$ at various $x$ values from first-principles density functional methods. We then take the prefactor in the Coulomb pseudopotential matrix, $\mu$, and the interband scattering parameter, $\Gamma^{\sigma\pi}$, as the only adjustable parameters. The dependence on the C content of $T_c$ and of the gaps ($\Delta_\sigma$ and $\Delta_\pi$) recently measured in Mg(B$_{1-x}$C$_x$)$_2$ single crystals indicate an almost linear decrease of $\mu$ on increasing $x$, with an increase in interband scattering that makes the gaps merge at $x = 0.132$. In polycrystals, instead, where the gap merging is not observed, no interband scattering is required to fit the experimental data.

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In spite of its simple structure, the intermetallic compound MgB$_2$ — discovered to be superconducting at about 40 K in 2001 [1] — soon revealed a number of surprising features that could not be explained within a picture of conventional superconductivity. Bandstructure calculations [2] showed that the energy bands of MgB$_2$ can be grouped into two sets: the quasi-2D $\sigma$ bands, and the 3D $\pi$ bands, originating from the superposition of in-plane and out-of-plane boron orbitals, respectively. As a matter of fact, most of the physical properties of this superconductor have found a clear and relatively simple explanation within an effective two-band model [3, 4, 5] in which the two bands interact via a phonon-mediated interband coupling. The result is that superconductivity develops in both bands at the same $T_c$, but with energy gaps of different amplitude, $\Delta_\sigma$ and $\Delta_\pi$, and thus different values of the gap ratio $2\Delta/k_BT_c$. The success of the two-band model in describing the features of MgB$_2$ naturally opens the question whether it can predict (or at least explain a posteriori) the effects of induced disorder, irradiation and, over all, chemical substitutions on the physical properties of the compound. As far as substitutions are concerned, the experimental test of theoretical predictions has been delayed or even prevented by the technical difficulties in obtaining good-quality samples of partially substituted MgB$_2$ [6]. Recently, point-contact measurements of the gap amplitudes as a function of $T_c$ have been reported in state-of-the-art Mg(B$_{1-x}$C$_x$)$_2$ polycrystals [7] and single crystals [8]. The availability of these results (that for some aspects contrast with each other) gives a good opportunity to test the two-band model. In this paper we will show that both the experimental data concerning $T_c$ and the gaps as a function of $x$ can be well explained within the two-band model in the Eliashberg formulation. We will use as input the frequencies of the B-B stretching mode (which is strongly coupled to the holes in the $\sigma$ band) and the partial densities of states at the Fermi level, $N_n^\sigma(E_F)$ and $N_n^\pi(E_F)$, calculated from first-principle density functional methods adopting the viewpoint of ordered supercells [6] instead of the virtual-crystal approximation. Then, we will show that the experimental $x$ dependence of $T_c$ and of the gaps $\Delta_\sigma$ and $\Delta_\pi$ can be very well reproduced by admitting a reasonable $x$ dependence of the prefactor in the Coulomb pseudopotential matrix [4, 10] and, in the case of single crystals, an increase in the interband scattering $\Gamma^{\sigma\pi}$ on increasing the C content.

Let us start from the generalization of the Eliashberg theory [11, 12] for systems with two bands [13], that has already been used with success to study the MgB$_2$ system [14, 15, 16, 14, 17, 10]. To obtain the gaps and the critical temperature within the s-wave, two-band Eliashberg model one has to solve four coupled integral equations for the gaps $\Delta_i(\omega_n)$ and the renormalization functions $Z_i(\omega_n)$, where $i$ is a band index and $\omega_n$ are the Matsubara frequencies. We included in the equations (explicitly reported elsewhere [14]) the non-magnetic impurity scattering rates in the Born approximation, $\Gamma^\delta$.

The solution of the Eliashberg equations requires as input: i) the four (but only three independent [15]) electron-phonon spectral functions $\alpha_{ij}^x(\omega)F(\omega)$; ii) the four (but only three independent [15]) elements of the Coulomb pseudopotential matrix $\mu_{ij}^x(\omega)$; iii) the two (but only one independent [15]) effective impurity scattering rates $\Gamma^\delta$. None of these parameters or functions has been calculated for C-substituted MgB$_2$, and in many cases their determination is a very difficult task, at least at the present moment. Hence, we are left with a problem with too many degrees of freedom. However, we will now show how some reasonable approximations allow reducing the number of adjustable parameters to 2, with no significant loss of generality.

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them with the electron-phonon coupling constants functions does not change with of since we showed in a previous paper [14] that the details of the phonon spectrum, that were calculated for pure MgB$_2$ in ref. [18]. As a first approximation, and as we did in the case of Al substitution [14], we will assume that also the average matrix element of the electron-ion interaction $<I^2>$ is constant, because it is basically determined by the deformation potential which is almost independent of $x$ [18].

Let’s start with the four spectral functions $\alpha^2_{ij}(\omega)F(\omega)$, that were calculated for pure MgB$_2$ in ref. [14]. For simplicity, we will assume that the shape of the $\alpha^2_{ij}(\omega, x)$ functions does not change with $x$, and we will only rescale them with the electron-phonon coupling constants $\lambda_{ij}$:

$$\alpha^2_{ij}(\omega, x) = \frac{\lambda_{ij}(x)}{\lambda_{ij}(x=0)} \alpha^2_{ij}(\omega, x=0)$$

Neglecting the effect of C substitution on the shape of the e-ph spectral functions is not a dramatic simplification, since we showed in a previous paper [14] that the details of $\alpha^2F(\omega)$ do not significantly affect the resulting $T_c$. To determine the scaling factor in eq. [1] let us remind that, from the definition of electron-phonon coupling constant [17]:

$$\lambda = \frac{N_N(E_F)}{\Omega_0^2} < I^2 >$$

where $M$ is the ion mass, $\Omega_0$ is a frequency representative of the phonon spectrum, $N_N(E_F)$ is the density of states at the Fermi level and $<I^2>$ is the average matrix element of the electron-ion interaction [17]. In our case, $M$ is the boron mass [3] and does not depend on $x$. As a first approximation, and as we did in the case of Al substitution [14], we will assume that also the average matrix element of the electron-ion interaction $<I^2>$ is constant, because it is basically determined by the deformation potential which is almost independent of $x$ [18].

FIG. 1: (a) Calculated density of states at the Fermi energy, $N_N^0(E_F)$ (solid line) and $N_N^7(E_F)$ (dashed line) as a function of $x$ (From Ref. 14). (b) Calculated frequency of the B-B bond stretching mode (the $E_{2g}$ mode in pure MgB$_2$) as a function of $x$ (From Ref. 14).

The partial densities of states at the Fermi level, $N^\sigma_N(E_F)$ and $N^\pi_N(E_F)$, have been recently calculated from first principles by using a supercell approach [4] for different values of the C content $x$, and are reported in Fig.1(a). The frequency $\Omega_0$ can be identified with the frequency of the B-B bond-stretching phonon mode (the $E_{2g}$ mode), that has been recently calculated as a function of $x$ from first principles [13], and is reported in Fig 1(b). Since this mode couples strongly with the holes on top of the $\sigma$ band, from eq. 2 we will have for $\lambda_{\sigma\sigma}$ (which gives the most important contribution to superconductivity in our system):

$$\lambda_{\sigma\sigma}(x) = \frac{N^\sigma_N(E_F, x)\omega^\sigma_{E_{2g}}(x=0)}{N^\sigma_N(E_F, x=0)\omega^\sigma_{E_{2g}}(x=0)}\lambda_{\sigma\sigma}(x=0)$$

In this way, we assume that the change in the frequency of the $E_{2g}$ phonon affects the coupling constant, while we neglect its influence on the shape of the electron-phonon spectral function. For the other coupling constants, we will instead assume for simplicity

$$\forall(i, j) \neq (\sigma, \sigma) \quad \lambda_{ij}(x) = \frac{N^i_j(N(E_F, x))}{N^i_j(N(E_F, x=0))}\lambda_{ij}(x=0)$$

where $\lambda_{\sigma\sigma}(x=0)=1.017$, $\lambda_{\pi\pi}(x=0)=0.448$, $\lambda_{\sigma\pi}(x=0)=0.213$ and $\lambda_{\pi\pi}(x=0)=0.155$ [4, 10]. Fig. 2 shows the calculated electron-phonon coupling constants $\lambda_{ij}$ as a function of $x$.

As far as the Coulomb pseudopotential is concerned, let us start from its expression in pure MgB$_2$ [4, 17, 19]:

$$\mu^*(x) = \begin{vmatrix} \mu_{\sigma\sigma}^* & \mu_{\sigma\pi}^* \\ \mu_{\pi\sigma}^* & \mu_{\pi\pi}^* \end{vmatrix} = \mu(\omega_c, x)N_N^{tot}(E_F, x) \begin{vmatrix} 2.23 & 1 \\ -1 & 2.48 \end{vmatrix}$$

where $\mu(\omega_c, x)$ is a free parameter and $N_N^{tot}(E_F, x)$ is the total normal density of states at the Fermi level. The
numbers 2.23 and 2.48 in the Coulomb matrix have been calculated for pure MgB\(_2\) but, as a first approximation, we will suppose them not to depend on \(x\). In this way, the elements of the Coulomb pseudopotential matrix, \(\mu_{ij}^\ast\), depend on \(x\) only through the densities of states at the Fermi level and through the common prefactor \(\mu(\omega_c, x)\), that could also take into account the effects of disorder.

As far as the scattering rates are concerned, let us remind that, due to Anderson’s theorem, intraband scattering does not affect neither \(T_c\) nor the gaps [21], so we will disregard both \(\Gamma^{\sigma\sigma}\) and \(\Gamma^{\pi\pi}\). The remaining interband scattering parameters are related to each other since [13]

\[
\frac{\lambda_{ij}(x)}{\lambda_{ji}(x)} = \frac{\mu_{ij}^{\ast}(x)}{\mu_{ji}^{\ast}(x)} = \frac{\Gamma_{ij}(x)}{\Gamma_{ji}(x)} = \frac{N_i^j(E_F, x)}{N_j^i(E_F, x)}
\]

and thus we will always refer only to \(\Gamma^{\sigma\pi}\). Finally, we can fix the cut-off energy (e.g., \(\omega_c = 700\) meV) so as to reduce the number of adjustable parameters to two: the prefactor in the Coulomb pseudopotential, \(\mu(\omega_c)\) (that we will call simply \(\mu\) from now on) and the interband scattering parameter \(\Gamma^{\sigma\pi}\).

As already pointed out, the aim of the present work is to show that the experimental dependence of \(T_c\) and of the gaps, \(\Delta_\sigma\) and \(\Delta_\pi\), on the C content in Mg(B\(_{1-x}\)C\(_x\))\(_2\) can be explained within the two-band Eliashberg theory. The experimental \(T_c(x)\) curves measured in single crystals [21] and polycrystals [8] are reported in Fig. 3. The corresponding \(x\) dependencies of the gaps measured by point-contact spectroscopy (PCS) are reported in Fig. 4 and Fig. 5 respectively (symbols). In single crystals (Fig. 3), the two gaps approach each other on increasing \(x\), until at \(x = 0.132\) they become experimentally indistinguishable. This means that, at this doping content, their amplitudes are equal to each other within the experimental uncertainty. In polycrystals, instead, the two gaps remain clearly distinct up to \(x = 0.10\), where \(\Delta_\sigma\) is much smaller than in single crystals with the same C content (see Fig. 5).

Let us focus for the time being on single crystals. The \(T_c(x)\) curve (solid circles in Fig. 3) can be exactly reproduced by adjusting only one of the two free parameters of the model, or both of them at the same time (but, in this case, the choice of their values is not univocal unless one adds another constraint).

For example, one can keep \(\mu\) equal to its value in pure MgB\(_2\) (i.e., \(\mu(x) = \mu(0)\)), and view the substituted compound as a “disordered” version of MgB\(_2\), as if the only effect of C substitution was an increase in interband scattering. This implies neglecting also the phonon hardening and the electron-doping effects (that actually play a leading role in determining the observed \(T_c(x)\) curve [22]) so that the \(T_c(x)\) curve is reproduced by only varying \(\Gamma^{\sigma\pi}\). The resulting trend of the interband scattering rate is shown in Fig. 3(a) (open squares). Notice that with this approach one cannot obtain critical temperatures lower than \(T_c = 25.8\) K, that corresponds to the isotropic “dirty” limit in which the two gaps merge into one of amplitude \(\Delta = 4.1\) meV [5]. This is clearly seen in the \(x\) dependence of the gaps calculated with these values of \(\Gamma^{\sigma\pi}\), which is reported in Fig. 4 as a dashed line. In spite of a rather good agreement between experimental and theoretical values of \(\Delta_\sigma\), the model predicts an increase in \(\Delta_\pi\) which is not observed, and the merging of the two gaps at a much lower C content with respect to the actual one.

The opposite case consists in taking into account all the effects of substitutions (i.e. phonon hardening and electron doping), with no increase of interband scattering. In this case, one can keep \(\Gamma^{\sigma\pi} = 0\), and vary \(\mu\).
and $\mu$ are reported as solid symbols in Fig. 5(a) and (b), respectively.

As shown in Fig. 5(a), the interband scattering remains smaller than 2 meV (which is a value reasonable even for pure MgB$_2$) up to $x = 0.10$ and then increases to make the gaps approach each other until they become indistinguishable. The point at $x = 0.132$ in Fig. 5(a) represents the minimum value of $\Gamma^\sigma\pi$ that gives gap values differing less than 0.3 meV (which is approximately the best experimental resolution of PCS at 4.2 K). Greater values of $\Gamma^\sigma\pi$ are allowed as well, since they would give rise to gaps even closer to each other. Although the point at $x = 0.132$ might depend on the approximations we are using in the present paper, there is no doubt that $\Gamma^\sigma\pi$ has to increase to reproduce the experimental gap values.

This increase is thus a general prediction of the two-band Eliashberg theory, but its origin in C-substituted MgB$_2$ is still debated at the moment. According to Ref. 22, carbon substitutions should not change the high lattice point symmetry and therefore the interband scattering should remain very small as in pure MgB$_2$. However, a $\sigma$-$\pi$ hybridization might also arise, above $x = 0.10$, from the presence of superstructures or even short-range order in the substituted compound. It must be said, however, that high-resolution TEM has shown no superstructures in these single crystals even, if the possibility of short-range order is not ruled out. An alternative explanation is based on the observed increase in flux pinning and in the normalized resistance on increasing $x$.

These effects suggest the existence of microscopic defects in the single crystals, acting as scattering centers. As indicated by magnetization data, these defects might be local inhomogeneities in the C distribution on a length scale comparable to $\xi$, that may well give rise also to $\sigma - \pi$ scattering.

The values of the Coulomb pseudopotential prefactor, $\mu$, that allow reproducing both the $T_c$ and the gap amplitudes, are reported in Fig. 5(b) (solid circles) as a function of $x$. The resulting $\mu(x)$ curve is almost linear up to $x = 0.10$, where a change in slope reflects the analogous feature of the experimental $T_c$ (see Fig. 5). Fig. 5 reports the values of the components of the Coulomb pseudopotential matrix, $\mu_{ij}^*$, calculated from eq. 9 by using the densities of states ($N^\sigma_N(E_F, x)$ and $N^\pi_N(E_F, x)$) from density-functional methods, and the values of $\mu(x)$ that allow best-fitting the experimental gaps (solid symbols in Fig. 5(b)). It is clear that all the components of the $\mu^*$ matrix monotonically decrease on increasing the C content. The large decrease (by a factor of two) of $\mu$ or, similarly, of $\mu_{\sigma\pi}^*$ between $x = 0$ and $x = 0.1$, suggests large changes in the electronic screening, that seem to be incompatible with the much smaller changes in the partial densities of states (Fig. 1). Giving an explanation of this puzzle within the two-band model is a very difficult task. However, a tentative and qualitative explanation can be given in the much simpler single-band case. Let us therefore consider the $\sigma$-band quantities alone. Let $\mu^* \equiv \mu_{\sigma\sigma}^*$ be the renormalized Coulomb pseudopotential, given by

FIG. 5: (a) Open squares: the $x$ dependence of $\Gamma^{\sigma\pi}$ necessary to reproduce the $T_c$ of single crystals, if $\mu(x) = \mu(0)$. Solid squares: the $\Gamma^{\sigma\pi}(x)$ curve that allows fitting both $T_c$ and the gaps when also $\mu$ is varied with $x$. Lines are only guides to the eye. (b) Open circles: the $x$ dependence of the prefactor in the Coulomb pseudopotential, $\mu$, that gives the $T_c(x)$ curve measured in single crystals (solid symbols in Fig. 3), when $\Gamma^{\sigma\pi} = 0$. Solid circles: the $\mu(x)$ curve that allows fitting both $T_c$ and the gaps ($\Delta_\sigma$ and $\Delta_\pi$) in single crystals, when also $\Gamma^{\sigma\pi}$ is varied.

with $x$ so as to reproduce the experimental $T_c(x)$ curve. With the resulting values of $\mu(x)$, shown in Fig. 5(b) as open circles, one obtains the $x$ dependence of the gaps indicated in Fig. 3 as thin solid lines. It is clear that the $\mu(x)$ curve that reproduces the experimental $T_c$ for any C content gives values of the large gap $\Delta_\pi$ that agree rather well with the experimental ones (open circles in Fig. 1) but gives rise to a decrease in the small gap which is not observed experimentally.

The analysis of the previous two cases suggests that the experimental $\Delta_\sigma(x)$ and $\Delta_\pi(x)$ curves could be explained as due to the interplay between a decrease in $\mu$ (that makes $\Delta_\pi$ decrease) and an increase in $\Gamma^{\sigma\pi}$ (that instead makes $\Delta_\pi$ increase). This result has been recently anticipated by an analysis of the effects of band filling and interband scattering. Hence, we will now try to fit the experimental $x$ dependence of $T_c$ and of the gaps $\Delta_\sigma$ and $\Delta_\pi$ by varying both $\mu$ and $\Gamma^{\sigma\pi}$. The best-fitting curves for the gaps (actually, the values of $\Delta(E, n_{\sigma\pi})$ at $T = T_c/4$, for the two bands) are reported as thick solid lines in Fig. 4. The choice of the parameters is univocal, and the resulting $x$ dependencies of $\Gamma^{\sigma\pi}$
\[\mu^* = \mu[1 + \mu \ln(E_F/\omega_{\text{log}})]^{-1}.\]

Starting from the value \(\mu^*(x=0) \simeq 0.17\) (see Fig. 4) and using \(E_F=500\) meV \(^{24}\) and \(\omega_{\text{log}}=\omega_{\text{2g}}\), the value of the bare Coulomb pseudopotential \(\mu = 0.26\) is obtained. From the Morel-Anderson definition \(^{25}\) of \(\mu\), i.e.:

\[
\mu = \frac{1}{2 a/r_0} \ln \left[ 1 + \left( \frac{2k_F}{k_S} \right)^2 \right] \tag{7}
\]

where \(k_S\) is the screening wavevector, and using as a first approximation the free-electron relationship between \(k_F\) and \(E_F\), one gets \(k_S(x=0)=0.47\) Å\(^{-1}\). The same calculation gives, for \(x = 0.1\), \(k_S(x=0.1)=0.16\) Å\(^{-1}\), so that \([k_S(x=0)/k_S(x=0.1)]^2 = 8.56\). Since in the Morel-Anderson model \(k_S^2 \propto k_T^2\) (where \(k_T\) is the Thomas-Fermi screening wavevector) and \(k_T^2\) is proportional to \(N(E_F)\), this value has to be compared to the ratio \(N_0^0(E_F, x=0)/N_0^0(E_F, x=0.1) = 1.11\). The comparison confirms that the change in the DOS alone cannot explain the observed reduction in \(\mu^*\). However, a large increase in the residual resistivity is observed on increasing the C content \(^{21}\), so that \(\rho_0(x=0.1) \approx 5\rho_0(x=0)\). This suggests that, for some \(x > 0.1\), a metal-to-insulator (MIT) transition might be expected. In the hypothesis that at \(x = 0.1\) the system already lies somewhere between the Fermi liquid and the critical regime where the MIT occurs, a generalization of the Morel-Anderson model \(^{24}\) has to be used to describe the \(x = 0.1\) case. Within this scenario, \(k_S^2(x=0.1) \propto k_T^2 \left[ 1 + (a/\alpha r)^2 \right]^{-1}\), where \(r = [\rho_0(x=0.1) - \rho_c]/\rho_c\), \(\rho_c\) is the critical value of the residual resistivity and \(a, \alpha\) are constants defined in Ref. \(^{24}\). Hence one gets

\[
\left[ \frac{k_S(x=0)}{k_S(x=0.1)} \right]^2 = \frac{N_0^0(x=0)}{N_0^0(x=0.1)} \cdot \left[ 1 + \left( \frac{a}{\alpha r} \right)^2 \right] \tag{8}
\]

from which \((a/\alpha r) = 2.78\). The parameter \(\alpha r\) expresses the distance from criticality (i.e. from the MIT) and can be obtained from \(N_0^0(E_F, x=0)/N_0^0(E_F, x=0.1) = 1 - \exp(-\alpha r)\), that gives \(\alpha r = 2.3\). According to Ref. \(^{26}\), this value is perfectly compatible with a strongly disordered Fermi liquid. Finally, the value of the constant \(a\) turns out to be \(a = 6.4\) that falls in the range of values allowed in Ref. \(^{27}\) and is correctly of the order of the cell parameter. In conclusion, the observed drop of \(\mu^*_{\sigma\pi}\) is due to a change in the screening length that, in turns, can be justified by the transition to a disordered Fermi liquid on increasing the C content. Incidentally, this result might further justify the observed increase in interband scattering \(\Gamma^\pi\) at high doping levels.

At this point, all the parameters entering the two-band model in Eliashberg formulation have been determined as a function of the C content, so that in principle any relevant physical property of the superconducting state of Mg(B\(_{1-x}\)C\(_x\))\(_2\) single crystals can be calculated. For the time being, we can calculate the temperature dependence of the gaps at different C contents, that can be easily tested by performing PCS measurements as a function of temperature. Fig. 7 reports the calculated values of \(\Delta_\pi(i\omega_n=0)\) and \(\Delta_\sigma(i\omega_n=0)\) as a function of \(T\) given by the solution of the Eliashberg equations in four different cases: \(x = 0\) (solid lines), \(x = 0.055\) (dashed lines), \(x = 0.1\) (dotted lines) and \(x = 0.132\) (dashed-dotted lines).

![Fig. 6: The elements of the Coulomb pseudopotential matrix, \(\mu_{ij}\), calculated from equation by using the densities of states from first-principles calculations and the prefactor \(\mu(x)\) that best fits the experimental data (\(T_c\) and gaps) in Mg(B\(_{1-x}\)C\(_x\))\(_2\) single crystals.](image)

![Fig. 7: The temperature dependence of \(\Delta_\pi(i\omega_n=0)\) and \(\Delta_\sigma(i\omega_n=0)\) calculated by solving the Eliashberg equations in four different cases: \(x = 0\) (solid lines), \(x = 0.055\) (dashed lines), \(x = 0.1\) (dotted lines) and \(x = 0.132\) (dashed-dotted lines).](image)
Let us now turn our attention to the experimental results obtained in Mg(B$_{1-x}$C$_x$)$_2$ polycrystals. As we did in the case of single crystals, we start by trying to reproduce the experimental $T_c(x)$ curve (open circles in Fig. 3) keeping $\Gamma^{\sigma\pi}$ = 0 and varying the prefactor in the Coulomb pseudopotential, $\mu$. Once determined the values of $\mu$ that give exactly the experimental $T_c$, we can calculate the gaps $\Delta(i\omega_n=0)$ at $T = T_c/4$ for the $\sigma$ and $\pi$ bands. The results are reported as a function of $x$ in Fig. 8 (solid lines). Surprisingly, the calculated gaps agree very well with those measured by PCS (symbols), with no need of interband scattering. This result indicates that the strong difference between the trend of the gaps measured in single crystals and polycrystals is very likely to be due to the different nature of the samples. Unfortunately, a more detailed discussion would require a deeper knowledge of the mechanisms that give rise to interband scattering in C-substituted samples, which is lacking at the present moment - even though some hypotheses for the increase in $\Gamma^{\sigma\pi}$ in single crystals have been presented above.

In conclusion, we have studied the Mg(B$_{1-x}$C$_x$)$_2$ system within the effective two-band Eliashberg model, that was already shown to be well suited for the description of unsubstituted MgB$_2$. In the analysis of the C-substituted system, we have used as input parameters the frequency of the B-B stretching mode and the partial densities of state at the Fermi level, calculated as a function of $x$ by first-principles density-functional methods. Adopting some reasonable approximations, we have come to a simplified model with only two adjustable parameters (the prefactor in the Coulomb pseudopotential and the interband scattering rate), whose dependence on $x$ has been determined so as to reproduce the experimental values of $T_c$ and of the gaps $\Delta_{\sigma}$ and $\Delta_{\pi}$.

The success of the model in describing the experimental findings shows that C-substituted MgB$_2$ is a weak-coupling two-band system as the parent compound. In details, the results indicate that: i) the experimental behaviour of $T_c$ on increasing $x$ is the results of the decrease in the $\sigma - \sigma$ intraband coupling (due to the filling of the $\sigma$ bands) and of a decrease in all the elements of the Coulomb pseudopotential matrix, in particular $\mu_{\sigma\pi}$. Without the contribution from $\mu^*$, the $T_c(x)$ curve would be steeper than experimentally observed \(^{22}\); ii) the different trend of the gaps observed experimentally in single crystals (where the gaps become indistinguishable at $x = 0.132$) and polycrystals (where there is no tendency to gap merging) only arises from the different amount of interband scattering in the two cases. The increase in $\Gamma^{\sigma\sigma}$ above $x \simeq 0.10$ might arise from short-range order in the single crystal structures, or from local inhomogeneities in the C content on a microscopic scale. \(^{21}\)

Finally, these results give an indication of what an ideal substitution, capable of increasing the $T_c$ of the MgB$_2$ system, should do, i.e. increase $\lambda_{\sigma\pi}$, decrease $\mu_{\sigma\pi}^*$, and keep the interband scattering as small as in pure MgB$_2$. According to eqs. \(^{4}\) and \(^{6}\) this is possible if $N_{\sigma}^E(E_F)$ increases and $N_{\pi}^E(E_F)$ decreases.

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