Pressure dependence of critical temperature in MgB$_2$ and two bands Eliashberg theory

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The variation of the superconducting critical temperature $T_c$ as a function of the pressure $p$ in the magnesium diboride MgB$_2$ has been studied in the framework of two-bands Eliashberg theory and traditional phonon coupling mechanism. I have solved the two-bands Eliashberg equations using first-principle calculations or simple assumptions for the variation, with the pressure, of the relevant physical quantities. I have found that the experimental $T_c$ versus $p$ curve can be fitted very well and information can be obtained on the dependence of the electron-phonon interaction matrix $<I^2>$ by pressure. The pressure dependence of the superconductive gaps $\Delta_x$ and $\Delta_x$ is also predicted.

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In the last few years, there is a noticeable increase of the study of superconductivity in many elements under pressure [1], such as sulphur ($T_c = 17$ K), oxygen ($T_c = 0.5$ K), carbon in nanotube ($T_c = 15$ K) and diamond forms ($T_c = 4$ K), a non-magnetic state of iron ($T_c = 1$ K), and the light elements lithium ($T_c = 20$ K) and boron ($T_c = 11$ K). The application of external pressure to superconductors can drive the compounds towards or away from lattice instabilities by varying the principal parameters determining the superconducting properties (the electronic density of states at the Fermi energy, the characteristic phonon frequency, and the electron-phonon coupling constant), and it can be used to tune the $T_c$ and the superconducting properties. Almost all of the superconducting metallic materials, unlike the previous simple elements, show a decrease of $T_c$ with pressure. This negative pressure coefficient was attributed to the volume dependence of the electronic density of states at the Fermi energy and of the effective interaction between the electrons mediated by the electron-phonon coupling. Measurements of the influence of pressure on the transition temperature and critical field yield information on the interaction causing the superconductivity. Indeed, the pressure would seem to be a variables whose effects might be capable of immediate theoretical interpretation. The binary alloy MgB$_2$, superconductor [2], at ambient pressure, at $T = 40$ K has, under pressure, a behaviour similar to metallic materials. The magnesium diboride has stimulated intense investigation, both from the theoretical and the experimental point of view. Now the electronic structure of MgB$_2$ is well understood and the Fermi surface consists of two three-dimensional sheets, from the $\pi$ bonding and antibonding bands, and two nearly cylindrical sheets from the two-dimensional $\sigma$ bands [3]. There is a large difference in the electron-phonon coupling on different Fermi surface sheets and this fact leads to a multiband description of superconductivity. Theory indicates that the strongest coupling is realized for the near-zone center in-plane optical phonon ($E_{2g}$ symmetry) related to vibration of the B atoms [4]. The superconductivity in MgB$_2$ has been deeply studied in the past three years and so also the effect of pressure on the superconducting properties. The effect of pressure on the superconductive properties of MgB$_2$ has been studied by several groups. All groups observed a decrease of $T_c$ with increasing pressure [4, 5] and I want show that this decrease can be very well explained in the framework of the two bands Eliashberg theory. In the following I will refer to the paper of A.F.Goncharov [5] because in there are present both measurement of the variation of critical temperature and of phonon mode by means of Raman measurement, with the pressure and so I mainly refer to these experimental data. In fact only in this work there are all input parameters necessary to my model.

Let us start from the generalization of the Eliashberg theory [6] for systems with two bands [4]. There is a large difference in the electron-phonon coupling on different Fermi surface sheets and this fact leads to a multiband description of superconductivity. Theory indicates that the strongest coupling is realized for the near-zone center in-plane optical phonon ($E_{2g}$ symmetry) related to vibration of the B atoms [4].

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FIG. 1: The spectral functions of the two-band model for the MgB$_2$: $\sigma \pi$ (solid line), $\pi \pi$ (dashed line), $\sigma \sigma$ (dotted line) and $\pi \pi$ (dashed dotted line), taken from ref. 11.

$$N^\alpha_j(i\omega_m) = \frac{\Delta_j(i\omega_m)Z_j(i\omega_m)}{\omega_n^2Z_j^2(i\omega_m) + \Delta_j^2(i\omega_m)Z_j^2(i\omega_m)}$$ (4)

$$N^\sigma_j(i\omega_m) = \frac{\omega_mZ_j(i\omega_m)}{\omega_n^2Z_j^2(i\omega_m) + \Delta_j^2(i\omega_m)Z_j^2(i\omega_m)}$$ (5)

where $\omega_n = \pi T(2n - 1)$ and $n, m = 0, \pm 1, \pm 2, \ldots$.

The solution of Eqs. 1, 2 requires as input: i) the four (but only three independent[9]) electron-phonon spectral functions, $\alpha_{ij}^2(\omega)F(\omega)$; ii) the four (but only three independent[9]) elements of the Coulomb pseudopotential matrix $\mu^\sigma(\omega_c)$.

Let’s start with the four spectral functions $\alpha_{ij}^2(\omega)F(\omega)$, that were calculated in ref. 11 (see Fig. 1).

For simplicity, I will assume that the shape of the $\alpha_{ij}^2F(\omega, p)$ functions does not change with the pressure, and I will only rescale them with the electron-phonon coupling constants $\lambda_{ij}$:

$$\alpha_{ij}^2F(\omega, p) = \frac{\lambda_{ij}(p)}{\lambda_{ij}(0)}\alpha_{ij}^2F(\omega, 0)$$ (6)

Let me remind the definition of electron-phonon coupling constant [14, 15, 18]:

$$\lambda = \sum_{q,i} \frac{\gamma_i(q)}{\pi N^\alpha(\epsilon^F)}$$ (7)

where $\gamma_i(q)$ is the phonon linewidth which is the width in energy of a phonon of momentum $q$, mode index $i$ and energy $\epsilon^F(q)$ and $N^\alpha(\epsilon^F)$ is the normal density of states at the Fermi level. The frequency $\Omega_i$ can be identified with the frequency of the B-B bond-stretching phonon mode (the $E_{2g}$ mode), that has been recently measured as a function of pressure [13], and is reported in Fig. 2. In the insert of Fig. 2 the experimental Raman linewidth that here is used as phonon linewidth, is shown. Since this mode couples strongly with the holes on top of the $\sigma$ band, from eq. [4] I will have for $\lambda_{\sigma\sigma}$ (which gives the most important contribution to superconductivity in our system):

$$\lambda_{\sigma\sigma}(p) = \frac{1}{\pi N^\sigma(\epsilon^F,p)} \gamma_{E_{2g}}(p) + \sum_{q,i} \frac{\gamma_i(q)}{\Omega_i(q)}$$ (8)

$$\lambda_{\sigma\sigma}(p) = \frac{1}{\pi N^\sigma(\epsilon^F,p)} \gamma_{E_{2g}}(p) + C(0)$$ (9)

where

$$C(0) = \pi \lambda_{\sigma\sigma}(0)N^\sigma(\epsilon^F,0) - \frac{\gamma_{E_{2g}}(0)}{\Omega_{E_{2g}}(0)}$$ (10)

When the lattice parameters of MgB$_2$ are modified by chemical substitutions the normal density of states, at
the Fermi level, in the $\pi$-band changes relatively little \[14\] and so I assume that, in the first approximation,

$$N^\sigma_N(E_F,p) = N^\sigma_N(E_F,0)$$

(11)

and

$$N^\sigma_N(E_F,p) = N^\sigma_N(E_F,0) + p \frac{\partial N^\sigma_N(E_F,p)}{\partial p} |_{p=0}$$

(12)

I use the values calculated in ref. 10: $N^\sigma_N(E_F,0) = 0.30061 \ (eV \text{unitcell})^{-1}$ and $N^\sigma_N(E_F,0) = 0.40359 \ (eV \text{unitcell})^{-1}$ for the $MgB_2$. So $\frac{\partial N^\sigma_N(E_F,p)}{\partial p} |_{p=0}$ is the only true free parameter of the model. In this way, I assume that the change in the frequency of the $E_{2g}$ phonon affects the coupling constant, while I neglect its influence on the shape of the electron-phonon spectral function \[14\]. For the other coupling constants, I will instead assume for simplicity

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

(13)

with \[10\] \[11\] \[14\] \[15\] $\lambda_{\sigma\sigma}(0) = 1.017$, $\lambda_{\pi\pi}(0) = 0.448$, $\lambda_{\sigma\pi}(0) = 0.213$ and $\lambda_{\pi\sigma}(0) = 0.155$. At the end, in this approximate model of electron-phonon coupling constants only $\lambda_{\sigma\sigma}$ and $\lambda_{\pi\pi}$ change with the pressure. This fact is in agreement with the results of ref. 20 where the authors find that $\lambda_{\pi\pi}$ is almost constant. Fig. 3 shows the calculated electron-phonon coupling constant $\lambda_{\sigma\sigma}$ as a function of the pressure.

As far as the Coulomb pseudopotential is concerned, let us start from its expression in pure $MgB_2$ \[10\] \[11\] \[12\]:

$$\mu^*(p) = \left| \begin{array}{c} \mu^*_{\sigma\sigma} \\ \mu^*_{\pi\pi} \end{array} \right| = \left| \begin{array}{c} \frac{2.23}{N^\sigma_N(E_F,p)} \\ \frac{1}{N^\sigma_N(E_F,p)} \end{array} \right| = \mu(\omega_c) N^\sigma_N(E_F,p)$$

(14)

where $\mu(\omega_c)$ is a free parameter and $N^\sigma_N(E_F,p)$ 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 the $MgB_2$ in ambient pressure but, as a first approximation, I will suppose them not to depend on the pressure. In this way, the elements of the Coulomb pseudopotential matrix, $\mu^*_i$, depend on the pressure only through the densities of states at the Fermi level. Now I can fix the cut-off energy (e.g., $\omega_c = 700 \text{ meV}$) so as to reduce the number of adjustable parameters to two: the prefactor in the Coulomb pseudopotential, $\mu(\omega_c)$ and $\frac{\partial N^\sigma_N(E_F,p)}{\partial p} |_{p=0}$. For having $T_c = 40.2 \text{ K}$ I fix $\mu(\omega_c)$ equal to 0.00315 so there is only more a free parameter for fitting the experimental critical temperature as a function of pressure. Before of examining the fit of experimental data with the my $\lambda_{\sigma\sigma}$ model I can check the other possible choices for the electron-phonon coupling constants.

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**FIG. 4:** The measured critical temperature $T_c$ as function of the pressure (open circles) and theoretical fits obtained by different assumptions on the electron-phonon coupling constant $\lambda_{\sigma\sigma}(p)$.

$$\lambda_{\sigma\sigma}(p) = \frac{\eta}{\Omega^2_{E_{2g}}(p)}$$

(15)

where $\eta$ is a constant \[18\] \[22\] and so

$$\lambda_{\sigma\sigma}(p) = \Omega^2_{E_{2g}}(0) \lambda_{\sigma\sigma}(0)$$

(16)

The result is in very poor agreement with experimental data (see dotted line in Fig. 4).

The second possibility is of that the effect of the pressure is similar to chemical substitutions as $Al$ and $C$ and so I assume that \[14\]

$$\lambda(p) = \frac{N_N(E_F,p)}{M \Omega^2_{E_{2g}}(p)}$$

(17)

where $M$ is the ion mass \[13\] and $< I^2 >$ does not depend from the pressure. Consequently

$$\lambda_{\sigma\sigma}(p) = \frac{N^\sigma_N(E_F,p) \Omega^2_{E_{2g}}(0)}{N^\sigma_N(E_F,0) \Omega^2_{E_{2g}}(p)}$$

(18)

$\frac{\partial N^\sigma_N(E_F,p)}{\partial p} |_{p=0} = -0.003 \ (eV \text{GPa})^{-1}$. Also in this case the result is in very poor agreement with experimental data (see dashed line in Fig. 4).
The last possibility is suggested by recent bandstructure calculations that show MgB$_2$ is a traditional $sp$ metal superconductor\cite{3}. The pressure dependence of $I$ has long been an interesting issue in the research of $sp$ metals\cite{26}. Zimans calculation of the electron-phonon interaction led to $<I^2>$ of the $sp$-band as a function of pressure is in agreement with experimental data (see short dashed line in Fig. 4). I can see that, after $\simeq 25$ GPa the Hopfield parameter $\lambda_{\sigma\sigma}(p)$ is almost constant. Now I can see that my simple model is the only one that explains the experimental critical temperatures because other possible models for electron-phonon coupling constant $\lambda_{\sigma\sigma}$ are incompatible with experimental data. I obtain the best fit of experimental data (solid line in Fig. 4) with $\frac{\partial N_N^{\sigma}(E_F,p)}{\partial p}|_{p=0} = 0.00584$ (eV GPa)$^{-1}$. The fact that $N_N^{\sigma}(E_F)$ increases with the pressure is in agreement with theoretical calculations\cite{24}. The only free parameter of this model is $\frac{\partial N_N^{\sigma}(E_F,p)}{\partial p}|_{p=0}$ and so when I have fixed the optimal value from the $T_c$ fit I can calculate, in principle, all other physical quantities. In Fig. 5 the theoretical dependence of the $\sigma$ and $\pi$ gaps from the pressure is shown. Now from the following equality

$$\frac{N_N^{\sigma}(E_F,p)}{M\Omega_{E_{2g}}^2(p)} < I^2(p) > = \frac{1}{\pi N_N^{\sigma}(E_F,p)\Omega_{E_{2g}}(p)} \sum_{q,i} \frac{\gamma_i(q)}{\Omega_i(q)} \quad (21)$$

it is possible determine the dependence of $N_N^{\sigma}(E_F) < I^2 >$ and of $< I^2 >$ from the pressure as it is shown in Fig 6. It can see that, after $\simeq 25$ GPa the Hopfield parameter $\lambda_{\sigma\sigma}(E_F)$ $< I^2 >$ is almost constant.

At the end it is possible to use this model for explaining the experimental upper critical field\cite{20} in function of pressure without free parameters. For the sake of completeness, I give here the linearized gap equations under magnetic field, for a superconductor in the clean limit (negligible impurity scattering), as can be found in ref. 20. In the following, $v_{Fj}$ is the Fermi velocity of band $j$, and $H_{c2}$ is the upper critical field:

$$\omega_n Z_i(i\omega_n) = \omega_n + \pi T \sum_{m,j} \Lambda_{ij}(i\omega_n - i\omega_m)\text{sign}(\omega_m)$$

$$\lambda_{\sigma\sigma}(p) = \frac{N_N^{\sigma}(E_F,0)\Omega_{E_{2g}}^2(0)}{N_N^{\sigma}(E_F,p)\Omega_{E_{2g}}^2(p)} \quad (19)$$

and $\frac{\partial N_N^{\sigma}(E_F,p)}{\partial p}|_{p=0} = -0.0007$ (eV GPa)$^{-1}$. As in the previous cases the result is in very poor agreement with experimental data (see short dashed line in Fig. 4). Now I can see that my simple model is the only one that explains the experimental critical temperatures because other possible models for electron-phonon coupling constant $\lambda_{\sigma\sigma}$ are incompatible with experimental data. I obtain the best fit of experimental data (solid line in Fig. 4) with $\frac{\partial N_N^{\sigma}(E_F,p)}{\partial p}|_{p=0} = 0.00584$ (eV GPa)$^{-1}$. The fact that $N_N^{\sigma}(E_F)$ increases with the pressure is in agreement with theoretical calculations\cite{24}. The only free parameter of this model is $\frac{\partial N_N^{\sigma}(E_F,p)}{\partial p}|_{p=0}$ and so when I have fixed the optimal value from the $T_c$ fit I can calculate, in principle, all other physical quantities. In Fig. 5 the theoretical dependence of the $\sigma$ and $\pi$ gaps from the pressure is shown. Now from the following equality

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bare Fermi velocities are the input parameters with \( \beta \) upper critical field of \( MgB_2 \) for free electron gas, having free parameters I assume that, as in the ref. 26, of \( H_2 \) at \( T = 10 \) K. The fit isn’t so good because, may be, the approximation of the free electron gas is too strong.

Finally I conclude by summarizing the main points of this paper. I have fitted the experimental critical temperatures as a function of pressure in the framework of two bands Eliashberg theory with only a free parameter. The result is very good. After I have calculated other physical quantities can will be compared with future measurement (for example superconducting gaps from tunneling curves) and I can affirm that the \( MgB_2 \) under pressure is, as the same materials in ambient pressure, a moderate coupling two-band phononic systems well described by two-bands Eliashberg theory.

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