The $T_c$ amplification by quantum interference effects in diborides

Annette Bussmann-Holder

*Max-Plamck Institute - fur Festk rperforshung*
*Heisenbergerstrasse 1 D 70759 Stuttgart Germany*

Antonio Bianconi

*Dipartimento di Fisica and Istituto Nazionale per la Fisica della Materia, Universit di Roma "La Sapienza", P. le Aldo Moro 2, 00185 Roma, Italy*

**Abstract**

The model of two ($\sigma$ and $\pi$) channels superconductivity known to be necessary to explain the superconductivity in MgB$_2$ has been applied to the Al$_{1-x}$Mg$_x$B$_2$ diborides by tuning $x$ from MgB$_2$ to AlMgB$_4$. The evolution of the interband coupling parameter (probing the strength of the interchannel pairing due to quantum interference effects) and the two gaps in the $\sigma$ and $\pi$ channel as a function of $x$ have been calculated. While in MgB$_2$ the quantum interference effects gives an amplification of $T_c$ by factor 1.5 in comparison with the dominant intra $\sigma$ band single channel pairing, in AlMgB$_4$ the amplification is about 100, in comparison with the dominant intra $\pi$ band single channel pairing.

For correspondence email addresses:
bianconi@superstripes.com
A.Bussmann-Holder@fkf.mpg.de
The interest in enhancing the superconducting temperature $T_c$ by quantum interference between the pairing in two channels is receiving renewed attention even though its theory has been pointed out in the fifties [1] and extended later by several authors for conventional [2,3] and non-conventional superconductors [4-6] including multi-channel interaction. In fact, the recent experimental results for MgB$_2$ show that the two-band model is needed to explain both the normal and the superconducting properties [7-19]. Here, the key ingredient that allows the physical realization of the process of two channels $T_c$ amplification is the fact that the two gaps referring to two different parts in $k$ space (a large gap in the $\sigma$ Fermi surface and a small gap in the $\pi$ Fermi surface) are well separated in real space, one for the $\sigma$ holes in the boron layers, and the other for $\pi$ electrons in the interstitial space (Mg layers between the boron layers). Therefore, the system can be described as a multi-layer made of alternated layers of metallic and superconducting planes. While in most of the materials (like in conventional isotropic 3D superconductors) the impurity interband scattering suppresses the quantum interference, here it is very low and does not suppress the two-band superconductivity enhancement [19].

It has been found that in the Al$_{1-x}$Mg$_x$B$_2$ alloys [20-31] show a continuous evolution through a complicated mixed phase from MgB$_2$ (at $x=1$) to the end member AlMgB$_4$ (at $x=0.5$) where a well-ordered superlattice structure of boron layers intercalated by alternated layers of Al and Mg is formed [20-24]. In spite of the fact that the alloys with intermediate $x$ are rather disordered, the superconducting transition temperature is still well defined and it drops systematically with decreasing $x$ as it is shown in Fig. 1a [from ref. 25,29,30 in agreement with several independent experiments ref. 21-24]. It shows a a kink around $x=0.7$ where a dimensionality crossover of the Fermi surface takes place.
[31,25-26] and reach 3K at x=0.5 for AlMgB$_4$ and the partial density of states of the $\sigma$ band (Fig.1b) shows a kink. The superconducting phase in the ordered phase AlMgB$_4$ is a highly interesting case since the Fermi level is driven near the top of the $\sigma$ band, the partial density of states (PDOS) in the $\sigma$ band is strongly reduced and the Fermi energy for the $\sigma$ holes $E_f$ is only about 100-200 meV [25-27].

The two-gap scenario has already been invoked for pure MgB$_2$ and electron-phonon interactions together with Coulomb potentials are well known. The interesting question here is whether such an approach can be used for the alloys up to the ordered AlMgB$_4$ phase and how the gap structure and interband couplings develop with doping.

Going from $x=1$ to $x=.5$ a dramatic increase in the $E_{2g}$ phonon mode energy $\omega_{E_{2g}}$ takes place [29-31] going from 70 meV to 115 meV as shown in Fig. 2a (from the data in ref. 30) indicating a strong reduction in the electron-phonon interaction which reflects itself also in a reduction of the phonon damping as shown in Fig. 2b (from the data in ref. 30) while the average phonon frequencies remains nearly constant $\omega_{in}=59-62$ meV. Since the $E_{2g}$ phonon mode strongly couples with the modulation of the top of the $\sigma$ band the electron-phonon coupling [33,37]

$$\lambda_{\sigma} = 2N_\sigma(E_f) \left[ \frac{\hbar}{2M_\sigma \omega_{E_{2g}}} \right] \left| \sum_{j=1,2} \tilde{\bar{\delta}}_j \cdot \tilde{D}_j \right|^2$$

where $D=130$ meV/pm is the deformation potential [33] and $N_\sigma(E_f)$ is the partial density of states at the Fermi level in the $\sigma$ band is such that in MgB$_2$ it reaches
the strong or intermediate coupling regime $\lambda_\sigma = 1$ [33-36]. On the other hand the electron phonon coupling for the $\pi$ electrons remains in the weak coupling regime $\lambda_\pi = 0.44$. While in the early days of the research on superconductivity in MgB$_2$ it was suggested the large value of $\lambda_\sigma$ was enough to explain the high $T_c$ within the standard single band isotropic Migdal-Eliashberg approach is has been recognized recently that this approach fails and it is necessary to consider a two band model [16]. By using the formula (1) to get $\lambda_\sigma(x)$ and $\lambda_\pi(x)$ and considering a Coulomb pseudo potential $\mu_\sigma(x)$ and $\mu_\pi(x)$ that are normalized at $x=1$ at the values given in ref.16 we have calculated using the McMillan or Allen-Dynes formula the ideal superconducting temperature for two ideal different metals made of only of $\sigma$ and $\pi$ electrons respectively that are given in Fig. 3. The screened effective couplings including the Coulomb shielding $\lambda_1(x)$ and $\lambda_2(x)$ respectively that are the inverse of the exponent in the McMillan formula are plotted in Fig. 4. From Fig. 3 we can clearly see that the single band model fails to predict the experimental curve of $T_c(x)$ where it is obvious that a single band approach fails to explain the $T_c$ of 3K for AlMgB$_4$ and is far beyond the experimental data for varying $x$. This motivated us to describe also the alloys within the two-band model in the frame of BCS approximation using the experimental data for the two intraband couplings $\lambda_1(x)$ and $\lambda_2(x)$ in Fig. 4.

Starting form the values of the energies of the phonon modes $\omega_{E2g}(x)$ and $\omega_{tn}(x)$, $T_c(x)$ and $\lambda_1(x)$ and $\lambda_2(x)$ discussed above we have obtained the interband coupling $\lambda_{12}(x)$ and the intra band gaps $\Delta_1(x)$ and $\Delta_2(x)$ for the $\sigma$ and $\pi$ band respectively. The Hamiltonian we used, reads:

$$H = H_0 + H_1 + H_2 + H_{12}$$

(2)
\[ H_0 = \sum_{k_i \sigma} \xi_{k_i} \sigma_{k_i \sigma}^+ \sigma_{k_i \sigma} + \sum_{k_i \sigma} \xi_{k_i} \pi_{k_i \sigma}^+ \pi_{k_i \sigma} \]  
\[ H_1 = - \sum_{k_1 k_1 q} V_1(k_1, k_1') \sigma_{k_1 + q/2}^+ \sigma_{k_1' - q/2} \sigma_{k_1 + q/2} \sigma_{k_1' - q/2} \]  
\[ H_2 = - \sum_{k_2 k_2 q} V_2(k_2, k_2') \pi_{k_2 + q/2}^+ \pi_{k_2' - q/2} \pi_{k_2 + q/2} \pi_{k_2' - q/2} \]  
\[ H_{12} = - \sum_{k_1 k_2 q} V_{12}(k_1, k_2) (\sigma_{k_1 + q/2}^+ \sigma_{k_2 - q/2} \pi_{k_2' + q/2} \pi_{k_2' - q/2} + h.c.), \]  

where \( H_0 \) is the kinetic energy of the bands \( i = 1, 2 \) with \( \xi_{k_i} = \varepsilon_i + \varepsilon_{k_i} - \mu \). Here \( \varepsilon_i \) denotes the position of the \( \sigma \)-band and \( \pi \)-band with creation and annihilation operators \( \sigma^+, \sigma, \pi^+, \pi \), respectively, and \( \mu \) is the chemical potential.

The pairing potentials \( V_i(k_1, k_1') \) are the intraband and, \( V_{12}(k_1, k_2) \) is the interband interaction which is dominated by multiphonon processes. By performing a BCS mean field analysis of Equs. 2 and applying standard techniques, we obtain:

\[ < \sigma_{k_1}^+ \sigma_{k_1}^- > = \frac{\Delta k_1}{2 E_{k_1}} \tanh[\frac{\beta E_{k_1}}{2}] = \Delta_{k_1} \Phi_{k_1} \]  
\[ < \pi_{k_2}^+ \pi_{k_2}^- > = \frac{\Delta k_2}{2 E_{k_2}} \tanh[\frac{\beta E_{k_2}}{2}] = \Delta_{k_2} \Phi_{k_2} \]

with \( E_{k_i}^2 = \xi_{k_i}^2 + |\Delta_{k_i}|^2, \Delta_{k_i} = \Delta_{k_i} + A_{k_i} \) and \( E_{k_2}^2 = \xi_{k_2}^2 + |\Delta_{k_2}|^2, \Delta_{k_2} = \Delta_{k_2} + B_{k_2} \). From this we obtain the selfconsistent set of equations:

\[ \Delta_{k_1} = \sum_{k_1} V_1(k_1, k_1') \Delta_{k_1'} \Phi_{k_1'} + \sum_{k_2} V_{1,2}(k_1, k_2) \Delta_{k_2} \Phi_{k_2} \]  
\[ \Delta_{k_2} = \sum_{k_2} V_2(k_2, k_2') \Delta_{k_2'} \Phi_{k_2'} + \sum_{k_1} V_{1,2}(k_1, k_2) \Delta_{k_1} \Phi_{k_1} \]

which have to be solved simultaneously for each temperature and gap value.

Starting from experimental values of the doping dependence of the phonon
frequencies together with the effective electron-phonon interactions 
\[ \lambda_{ii} = N_{ii}(0)V_i(k_i, k'_i) \] (i=1,2) for the intraband pairing processes, the values of the interband couplings are adjusted to fit the experimental values of \( T_c \) as already outlined above. The results are shown in Fig. 4 where the effective electron-phonon couplings are presented. The corresponding energy gaps at \( T=0 \) K are shown in Fig.5a and the gap to \( T_c \) ratios are depicted in Fig. 5b. As it is well known for the two-band model, both gap to \( T_c \) ratios deviate substantially from BCS predictions – one being strongly enhanced, while the other is far below BCS theory. The obtained value of \( \lambda_{12}(x=1) \) is consistent with the average value of the screened coupling constants \( \lambda_{\sigma\pi} \) and \( \lambda_{\pi\sigma} \) derived form the two band model of MgB\(_2\) [16] using the corresponding values of the pseudopotentials \( \mu_{\sigma\pi} \) and \( \mu_{\pi\sigma} \). The obtained values of \( \Delta_1(x=1) \) and \( \Delta_2(x=1) \) are in very good agreement with the superconducting gaps measured by Ivarrone et al. for MgB\(_2\) [8].

We observe that the interband coupling parameter \( \lambda_{12}(x) \), in Fig. 4 increases by decreasing \( x \) from the value of MgB\(_2\), up to reach a maximum for the values of \( x \) near 0.6-0.7 where the strength of the interchannel pairing due to quantum interference effects is maximum. In the range \( x=0.6-0.7 \) the \( T_c(x) \) curve shows a kink that is the signature that the Fermi level has been tuned at the cross-over of the Fermi surface of the \( \sigma \)-band from 2D to 3D dimensionality. This is the expected position of the “shape resonance” [33]. The two gaps in the \( \sigma \) and \( \pi \) channel as a function of \( x \) plotted in Fig.5 show a very interesting case of interchange of their dominance and a gap crossing takes place at \( x=0.6 \) where the \( \sigma \)-band related gap becomes smaller than the \( \pi \) related gap. For AlMgB\(_2\) we have therefore a different physical situation for the two gap scenario. In fact in MgB\(_2\) the
interchannel interference effects push up $T_c$ in the strong coupling regime 
($2\Delta_1/T_c=4.2$) with an effective amplification of $T_c$ of the order of 1.5-2 increasing 
the strong-intermediate coupling regime of the dominant 2D $\sigma$ band. In AlMgB2 
is the 3D $\pi$ band with the dominant gap D2 that is helped by the 3D $\sigma$ band with a 
lower intraband coupling constant $l_1$ and while for the intraband pairing processes 
will gibe $T_c$ in the range of 1-10 milliK the actual $T_c$ is 3K, i.e. an amplification 
of a factor 100-1000 is realised in this scenario.

As a consequence of the interchange of the driving band going through the 
“shape resonance” at $x=0.6-0.7$ the gap separation is strongly doping dependent, 
being very large for MgB$_2$, intermediate for $x=0.75$ and reversed at $x=0.5$. The 
temperature dependence of the gaps for the above mentioned three cases is shown 
in Fig. 6 where substantial differences predicted for the three cases are very large 
and can be tested by further experiments.

One of A.B. would like to thank the Max Planck Institute for hospitality that allowed us to write this 
paper. This work is supported by “progetto cofinanziamento Leghe e composti intermetallici: stabilità 
termodinamica, proprietà fisiche e reattività” of MIUR, and by “Progetto 5% Superconduttività” of 
Consiglio Nazionale delle Ricerche (CNR).
REFERENCES

Fig. 1 (panel a) The superconducting transition temperature for Al$_{1-x}$Mg$_x$B$_2$ from $x=0.5$ (AlMgB$_4$) to $x=1$ (MgB$_2$) from ref. 25, 29, 30. (panel b) The partial density of states (PDOS) of the $\sigma$ band $N_\sigma$ and of the $\pi$ band $N_\pi$ as function of $x$. 
Fig. 2 (panel a) The variation of the energy $\omega_{E2g}$ of the E$_{2g}$ phonon mode as function of $x$ from $x=1$ to $x=.5$ while the average phonon frequencies remains nearly constant $\omega_{1n}=62$ meV. (panel b) The E$_{2g}$ phonon damping, defined as the ratio of the total width on the average energy of the Raman line as a function of $x$ (from the data in ref. 30).
Fig. 3 The calculated superconducting temperature for two ideal systems made of only of $\sigma$ and $\pi$ electrons respectively are compared with the experimental data. The single band isotropic Migdal-Eliasberg approach has been considered and $T_c$ gave been calculated by the McMillan or Allen-Dynes formula considering a Coulomb pseudo potential $\mu_{\sigma}(x)$ and $\mu_{\pi}(x)$ and electron phonon interactions normalized at $x=1$ at the values given in ref.16.
Fig. 4 The screened effective couplings $\lambda_1(x)$ and $\lambda_2(x)$ for the $\sigma$ and $\pi$ electrons respectively that are the inverse of the exponent in the McMillan formula. The interband coupling $\lambda_{12}$ has been found using the two band interference model in such a way as to reproduce the experimental $T_c$ at each value of $x$. 
Fig. 5 (panel a) The energy gaps, at T=0 K, $\Delta_1(x)$ and $\Delta_2(x)$ for the $\sigma$ and $\pi$ electrons respectively obtained by equations 3 and 4 and (panel b) the gap to $T_c$ ratios as a function of $x$. 
Fig. 6 The predicted temperature dependence of the gaps for three different systems MgB$_2$, Al$_{0.25}$Mg$_{0.75}$B$_2$ and AlMgB$_4$. 