Raising the diboride superconductor transition temperature using quantum interference effects

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The model of two (σ and π) channel superconductivity known to be necessary to explain the superconductivity in MgB_2 has been applied to the $Al_{1-x}Mg_xB_2$ diborides by tuning x from MgB_2 to $AlMgB_4$. The interband coupling parameter (probing the strength of the interchannel pairing due to quantum interference effects) and the two gaps in the σ and π channel have been calculated as a function of x by using experimental data for the two phonon mode energies which are most relevant for the pairing interaction. It is found that the two gaps reverse in leading order around $x=0.6$ and that in comparison with the dominant intra-σ-band single channel pairing an increase in T_c of 1.5 occurs for MgB_2 while in $AlMgB_4$ the dominant π band single channel pairing leads to enhancement of T_c of 100.

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The interest in enhancing the superconducting transition temperature T_c by quantum interference between the pairing in two channels is receiving renewed attention even though its theory was established in the fifties (Ref. 1) and extended later for conventional[2,3] and nonconventional superconductors.[4–6] In fact the recent experimental results for MgB_2 show that a two-band model (TBM) is needed to explain both the normal and the superconducting properties[7–19] especially in view of the fact that two superconducting gaps have been observed by different techniques. Most interestingly the two gaps refer to two different parts in k space (a large gap on the σ Fermi surface and a small gap on the π Fermi surface) and are well separated in real space, one for the σ holes in the boron layers, and the other for π electrons in the interstitial Mg layers. Consequently the system can be viewed as a multilayer structure of alternating metallic and superconducting planes. While in many materials [e.g., conventional isotropic three-dimensional (3D) superconductors] the impurity interband scattering suppresses interference processes between the two bands, here it is very low and admits high-temperature superconductivity due to interband interaction enhancement.[19]

The $Al_{1-x}Mg_xB_2$ alloys[20–31] show a continuous evolution through a complicated mixed phase from MgB_2 ($x=1$) to the end member $AlMgB_4$ ($x=0.5$) where an ordered superlattice structure of boron layers intercalated by alternating layers of Al and Mg is formed.[20–24] Even though the alloys with intermediate x are rather disordered, their T_c is well defined and drops with decreasing x.[21–25,29,30] Around $x=0.7$ T_c shows a kink which is attributed to a dimensionality crossover of the Fermi surface[31,25–26] and at $x=0.5$, $T_c=3$ K. At $x=0.7$ the partial density of states (PDOS) of the σ band also shows a kink. The superconducting phase in the ordered phase $AlMgB_4$ ($x=0.5$) is highly interesting since the Fermi level is driven to the top of the σ band, the PDOS in the σ band is strongly reduced and the Fermi energy E_F for the σ holes is only 100–200 meV.[25–27]

Since the two-gap scenario has already been used for MgB_2 electron-phonon interactions together with Coulomb potentials are well known.[14,16,17] The interesting question here is whether this model can be used for the alloys and how the gaps and interband couplings develop with doping.

Going from $x=1$ to $x=0.5$ a dramatic increase in the E_{2g} phonon mode energy ω_{E2g} takes place[29–31] increasing from 70 to 115 meV (Ref. 30) indicating a strong decrease in the electron-phonon interaction which reflects itself also in a reduction of the phonon damping[30] while the average phonon frequencies remain nearly constant $\omega_{\ln}=59-62$ meV. The E_{2g} phonon mode is known to couple strongly to the σ band and defining the electron-phonon coupling[32,33,37] as $\lambda_\sigma = 2N_\sigma(E_F)[\hbar/(2M_B\omega^2_{E_{2g}})]|\Sigma_{j=1,2}\hat{\varepsilon}_j\cdot\mathbf{D}_j|^2$ where $D=130$ meV/pm is the deformation potential,[33] $N_\sigma(E_F)$ is the PDOS at the Fermi level in the σ band, and M_B the B ion mass. λ_σ in MgB_2 reaches the strong-intermediate coupling regime $\lambda_\sigma=1$,[33–36] while the π band electron-phonon coupling is in the weak coupling limit $\lambda_\pi=0.44$. Although it was suggested that the large value of λ_σ is sufficient to explain the high T_c within the single band approach, it has been recognized that it will soon be necessary to consider the TBM.[16] By using the above definition of the electron-phonon coupling to obtain $\lambda_\sigma(x)$ and $\lambda_\pi(x)$ and considering Coulomb pseudopotentials $\mu_\sigma(x)$ and $\mu_\pi(x)$ that are normalized at $x=1$ to the values of Ref. 16 we have calculated T_c within the Allen-Dynes approach. The variations in λ with Al doping have been included by relating the deformation potentials to the observed doping dependent changes in the phonon linewidth within the scheme of Ref. 37. The corresponding changes in the Coulomb potentials have been derived from the changes in the density of states at E_f together with the modifications of the frequencies.[25] The optimum superconducting transition temperatures for two ideal different metals made of σ and π electrons only, without interband interactions are shown in Fig. 1. The corresponding screened effective couplings are plotted in Fig. 2. From Fig. 1 we can clearly see that the single band model fails to predict the experimental $T_c(x)$ dependence, to explain the T_c of 3 K observed in $AlMgB_4$ and is incapable of reproducing experi-

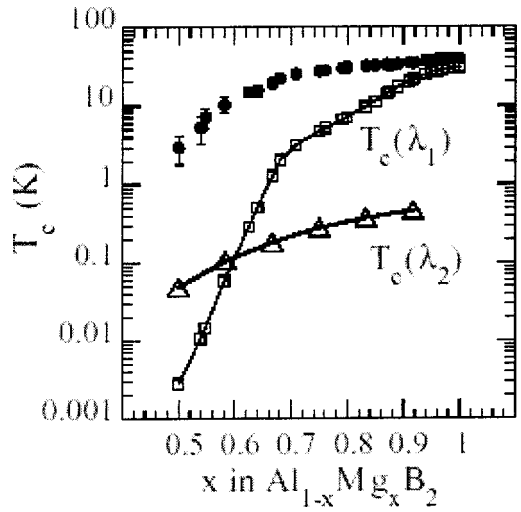

FIG. 1. The calculated superconducting transition temperature T_c for two ideal systems made of σ and π electrons only are compared with the experimental data. The single band isotropic Migdal-Eliashberg approach has been considered and T_c has been calculated using the McMillan or Allen-Dynes formula considering Coulomb pseudopotentials $\mu_\sigma(x)$ and $\mu_\pi(x)$ and electron phonon interactions normalized at $x=1$ to the values given in Ref. 16.

mental data for varying x. This finding motivated us to also model the alloys within the two-band scenario using the BCS approximation and the experimental data for the two intraband couplings $\lambda_1(x)$ and $\lambda_2(x)$ (Fig. 2).

Taking as input the experimental values of the phonon mode energies $\omega_{E2g}(x)$ and $\omega_{\ln}(x)$, $T_c(x)$, $\lambda_1(x)$, and $\lambda_2(x)$, the interband coupling $\lambda_{12}(x)$ and the intraband gaps $\Delta_1(x)$ and $\Delta_2(x)$ for the σ and π band, respectively, are obtained. Our Hamiltonian reads

$$H=H_0+H_1+H_2+H_{12}, \tag{1a}$$

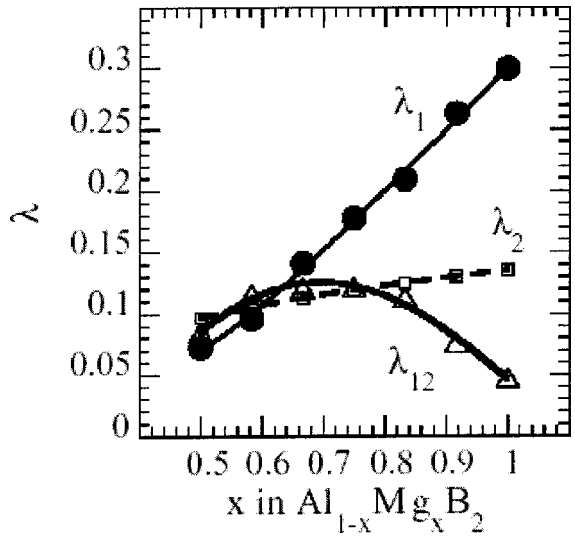

FIG. 2. The screened effective couplings $\lambda_1(x)$ and $\lambda_2(x)$ for the σ and π electrons, respectively, which are the inverse of the exponent in the McMillan equation. The interband coupling λ_{12} has been calculated by using the two band interference model in such a way as to reproduce the experimental values of T_c for each value of x.

$$H_0=\sum_{k_1\sigma}\xi_{k_1}\sigma^+_{k_1\sigma}\sigma_{k_1\sigma}+\sum_{k_2\sigma}\xi_{k_2}\pi^+_{k_2\sigma}\pi_{k_2\sigma}, \tag{1b}$$

$$H_1=-\sum_{k_1k_1'q}V_1(k_1,k_1')\times\sigma^+_{k_1+q/2\uparrow}\sigma^+_{-k_1+q/2\downarrow}\sigma_{-k_1'+q/2\downarrow}\sigma_{k_1'+q/2\uparrow}, \tag{1c}$$

$$H_2=-\sum_{k_2k_2'q}V_2(k_2,k_2')\times\pi^+_{k_2+q/2\uparrow}\pi^+_{-k_2+q/2\downarrow}\pi_{-k_2'+q/2\downarrow}\pi_{k_2'+q/2\uparrow}, \tag{1d}$$

$$H_{12}=-\sum_{k_1k_2q}V_{12}(k_1,k_2)\times\{\sigma^+_{k_1+q/2\uparrow}\sigma^+_{-k_1+q/2\downarrow}\pi_{-k_2+q/2\downarrow}\pi_{k_2+q/2\uparrow}+\text{H.c.}\}, \tag{1e}$$

where H_0 is the kinetic energy of bands $i=1$, 2 with $\xi_{k_i}=\varepsilon_i+\varepsilon_{k_i}-\mu$. ε_i denotes the position of the σ and π bands with creation and annihilation operators σ^+, σ, π^+, π, respectively, and μ is the chemical potential. The pairing potentials $V_i(k_i,k_i')$ act intraband and $V_{12}(k_1,k_2)$ is the interband interaction dominated by multiphonon processes. By applying standard techniques, we obtain

$$\langle\sigma^+_{k_1\uparrow}\sigma^+_{-k_1\downarrow}\rangle=\frac{\overline{\Delta}_{k_1}}{2E_{k_1}}\tanh\left[\frac{\beta E_{k_1}}{2}\right]=\overline{\Delta}_{k_1}\Phi_{k_1}, \tag{2a}$$

$$\langle\pi^+_{k_2\uparrow}\pi^+_{-k_2\downarrow}\rangle=\frac{\overline{\Delta}_{k_2}}{2E_{k_2}}\tanh\left[\frac{\beta E_{k_2}}{2}\right]=\overline{\Delta}_{k_2}\Phi_{k_2} \tag{2b}$$

with $E^2_{k_1}=\xi^2_{k_1}+|\overline{\Delta}_{k_1}|^2$, $\overline{\Delta}_{k_1}=\Delta_{k_1}+A_{k_1}$ and $E^2_{k_2}=\xi^2_{k_2}+|\overline{\Delta}_{k_2}|^2$, $\overline{\Delta}_{k_2}=\Delta_{k_2}+B_{k_2}$. In addition the following definitions are introduced: $\Delta_{k_i'}=\Sigma_{k_i}V_i(k_i,k_i')\langle c^+_{k_i\uparrow}c^+_{-k_i\downarrow}\rangle$ ($c=\sigma$, $i=1;c=\pi,i=2$) together with $A_{k_1}=\Sigma_{k_2}V_{12}(k_1,k_2)\times\langle\pi^+_{k_2\uparrow}\pi^+_{-k_2\downarrow}\rangle$, $B_{k_1}=\Sigma_{k_2}V_{12}(k_1,k_2)\langle\sigma^+_{k_2\uparrow}\sigma^+_{-k_2\downarrow}\rangle$, and $V^*_{12}=V_{12}$. From this the coupled gap equations are given by

$$\overline{\Delta}_{k_1}=\sum_{k_1'}V_1(k_1,k_1')\overline{\Delta}_{k_1'}\Phi_{k_1'}+\sum_{k_2}V_{1,2}(k_1,k_2)\overline{\Delta}_{k_2}\Phi_{k_2}, \tag{3a}$$

$$\overline{\Delta}_{k_2}=\sum_{k_2'}V_2(k_2,k_2')\overline{\Delta}_{k_2'}\Phi_{k_2'}+\sum_{k_1}V_{1,2}(k_1,k_2)\overline{\Delta}_{k_1}\Phi_{k_1} \tag{3b}$$

which have to be solved simultaneously and selfconsistently for each temperature and $\overline{\Delta}_{k_i}$. The results for the interband coupling parameters are shown in Fig. 2 together with the effective electron-phonon couplings for intraband interactions. The corresponding energy gaps at $T=0$ K are shown in Fig. 3(a) and the gap to T_c ratios are depicted in Fig. 3(b). As is well known for the two-band model, both gap to T_c ratios deviate substantially from BCS predictions—one being

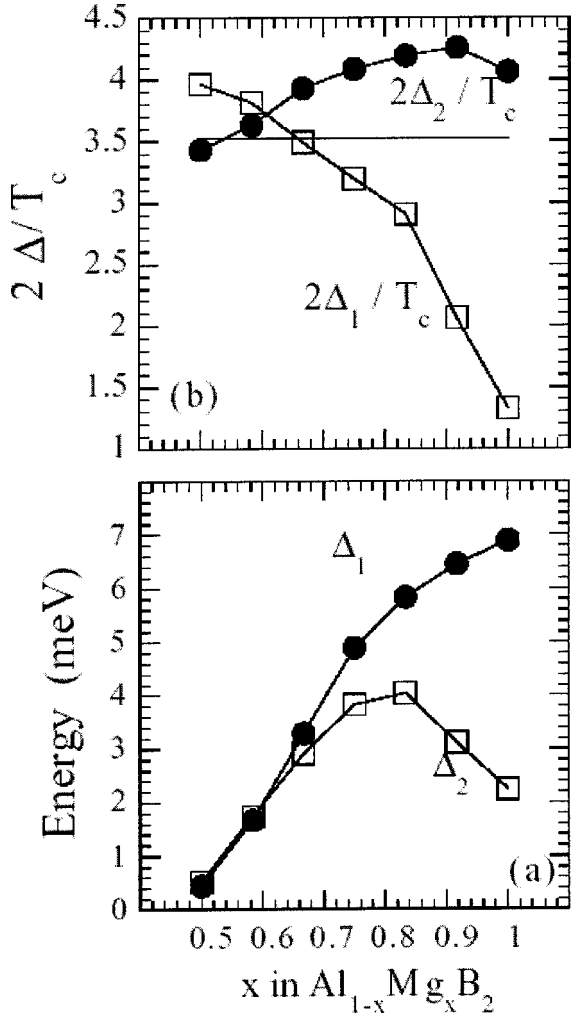

FIG. 3. (a) The energy gaps at $T=0$ K, $\Delta_1(x)$ and $\Delta_2(x)$ for the σ and π electrons, respectively, as obtained by solving Eqs. (3) and (4) simultaneously and self-consistently and (b) the corresponding gap to T_c ratios as a function of x.

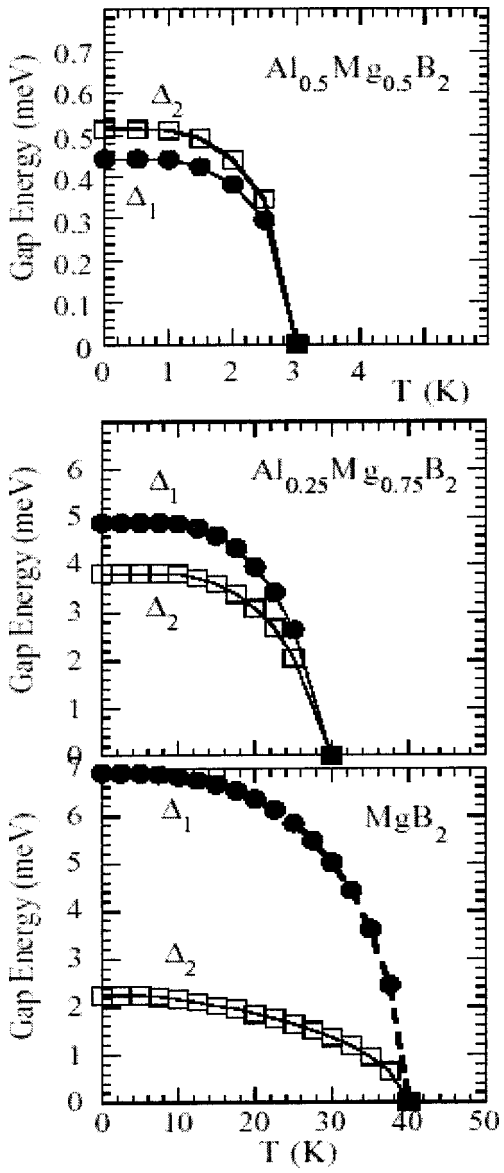

FIG. 4. The predicted temperature dependence of the gaps for three different systems MgB_2 (top panel), $Al_{0.25}Mg_{0.75}B_2$ (middle panel), and $AlMgB_4$ (lower panel).

strongly enhanced, while the other is far below the predicted value. The calculated 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 from the TBM (Ref. 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 experimental ones.[8]

Interestingly the interband coupling $\lambda_{12}(x)$ (Fig. 2) increases with decreasing x to reach a maximum around $x \sim 0.6-0.7$ where the strength of the interchannel pairing due to quantum interference effects is optimum. Here the $T_c(x)$ curve also shows a kink signaling that the Fermi level has been tuned at the cross-over of the Fermi surface of the σ band from 2D to 3D dimensionality. This is the expected position of the "shape resonance."[33] The related σ and π gaps as a function of x (Fig. 3) show the very interesting case of interchange of their dominance and a gap crossing takes place at $x=0.6$ where the σ-band related gap becomes smaller than the π related one. For $AlMgB_4$ we have therefore a different physical situation for the two gap scenario. In fact, in MgB_2 the interchannel interference effects push T_c up to 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 σ band. In $AlMgB_2$ the π band is the dominant one which is supported by the 3D σ band with small intraband coupling λ_1. While the intraband pairing alone yields a T_c of 1–10 mK, the actual T_c is 3 K, corresponding to an amplification of 100–1000. The consequence of the interchange of the driving band going through the "shape resonance" at $x=0.6-0.7$ is that the gap separation is strongly doping dependent, being large for MgB_2, intermediate for $x=0.75$ and reversed at $x=0.5$. The temperature dependence of the gaps for these three cases is shown in Fig. 4 where substantial differences are predicted which can be tested by further experiments.

In conclusion, we have shown that in Al doped MgB_2 superconductivity persists up to the ordered structure

$AlMgB_4$. The dependence of the superconducting transition temperature on doping cannot be described within a single band BCS scenario when using the experimental values for the phonon energies and dampings since T_c is found to be strongly underestimated within such an approach. Opposite to this result we find that the two-band two-gap model yields very good agreement with experiments. Most interestingly we find that a reversal in the leading gap takes place around $x=0.6$ which should be tested experimentally. The kinklike behavior in the $T_c(x)$ around $x=0.7$ is attributed to a maximum in the interband interaction which does not drop systematically with decreasing T_c.

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