The isostructural AlB2

The low-frequency mode interacting with the $\pi$-(states) to the E$_{2g}$-vibrations respectively. Using two-band Eliashberg theory, $\lambda_\pi = 1.4$ and $\lambda_\sigma = 0.7$, we calculate the gap functions $\Delta_i(\omega, 0) (i = \pi, \sigma)$. Our results provide an explanation of recent tunneling experiments. We get $H^{\text{sh}}_{c2}/H^{\text{c2}}_{c2} \approx 3.9$.

74.70.-b, 74.20.-z, 74.25.Kc

We analyze superconductivity in MgB$_2$ observed below $T_c = 39$ K resulting from electron-phonon coupling involving a mode at $\hbar \omega_1 = 24$ meV and most importantly the in-plane B-B $E_{2g}$ vibration at $\hbar \omega_2 = 67$ meV. The quasiparticles originating from $\pi$- and $\sigma$-states couple strongly to the low-frequency mode and the $E_{2g}$-vibrations respectively. Using two-band Eliashberg theory, $\lambda_\pi = 1.4$ and $\lambda_\sigma = 0.7$, we calculate the gap functions $\Delta_i(\omega, 0) (i = \pi, \sigma)$. Our results provide an explanation of recent tunneling experiments. We get $H^{\text{sh}}_{c2}/H^{\text{c2}}_{c2} \approx 3.9$.

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In recent Raman [6], tunneling [7,8], photoemission [9], and transport [11] studies it was noted that the experimental data are compatible with a multi-component superconducting gap. This is consistent with the large observed anisotropy of $H_{c2}$. Inelastic neutron scattering(INS) experiments [12] and point-contact spectroscopy studies [13] reveal a peak at approximately 24 meV in the phonon density of states in contrast to first principles calculations [15]. Recently, this peak was also indirectly confirmed by the analysis of the temperature dependence of the upper critical field $H_{c2}(T)$ [15]. The isostuctural AlB$_2$ is not superconducting.

In this paper we analyze superconductivity in MgB$_2$ using Eliashberg theory assuming that it arises due to electron-phonon coupling of the holes in the Boron planes (\(\sigma\)-states) to the $E_{2g}$-mode of B-B vibrations and due to the low-frequency mode interacting with the $\pi$-states.

In Fig. 1 we illustrate the simple physical picture for superconductivity and the structure of MgB$_2$. Similar to graphite, it has a quasi 2D-like structure, but with strong covalent bonds. According to previous studies [4][14], superconductivity occurs mainly in the B-planes involving two-dimensional $\sigma$- and and three-dimensional $\pi$-states. In the first case the electron-phonon coupling can be estimated from $g_{\sigma-\pi} < \sigma_B V | | \sigma_B \rangle \cdot \epsilon$, where the polarization vector $\epsilon$ refers to the $E_{2g}$-mode [13] and $\sigma_B$ refers essentially to the in-plane wave function of Boron bonds. Note, we obtain $g_{\sigma-\pi} \sim \nabla \epsilon \cdot \epsilon$ (denotes the corresponding hopping matrix element) and expect a resulting moderate electron-phonon coupling like in transition metals.

It is known from first principle calculations that MgB$_2$ consists of four important phonon modes [13]. Two modes involve vibrations of the Mg-B planes: the $E_{1u}$ mode (49meV) corresponds to a sliding mode in $xy$-direction, and the $A_{2u}$ mode (49meV) corresponds to a vibration in $z$-direction. On the other hand, the other two modes involve the B-B bonds: the $E_{2g}$ mode (67meV) mentioned earlier corresponds to an in-plane breathing mode, and the $B_{3g}$ mode (87meV) refers to an out-of-plane tilting mode of Boron atoms. First-principle calculations of the electron-phonon coupling $\alpha^2 F(\omega)$ in Ref. [15] obtain that the dominating part of the pairing interaction stems from the $E_{2g}$ mode. In the non-superconducting AlB$_2$, this $E_{2g}$-mode lies at $\hbar \omega = 120$ meV. Recent INS and Raman experiments in MgB$_2$ reveal an additional peak in the phonon density of states at approximately 17-25meV [16] and, most importantly, its softening in the superconducting state. It was noted [4] that this mode very likely is involving Mg vibrations. Thus, one expects the coupling of this mode mainly to the $p_z$ ($\pi$) band due to its dispersion along the $z$-axis. Therefore, we conclude that superconductivity in MgB$_2$ is mainly induced by Boron $\pi$- and $\sigma$-states coupled to low-frequency mode at 24meV and the $E_{2g}$-mode at 67meV respectively. Due to the different character of both states and their coupling to different phonon modes one expects the occurrence of superconducting gaps referring mainly to the $\pi$- and $\sigma$-bands. This is necessary as well for the analysis of the observed anisotropy in the upper critical field.

For our analysis we use a two-band extension of Migdal-Eliashberg theory [20,21]. We approximate the phonon spectral density $F^i(\omega)$ by two Lorentzians centered at $\hbar \omega_1 \approx 24$ meV for the $\pi$-band and $\hbar \omega_2(E_{2g}) = 67$ meV for the $\sigma$-band. Hence, 

$$\alpha^2 F^i(\omega) = \frac{1}{\pi} g^{(i)}_p \frac{\omega \Gamma^3_i}{[(\omega - \omega_i)^2 + \Gamma^2_i]^2} F^i(\omega),$$

(1)

describing the pronounced phonon peaks at the observed frequencies. Here, $g^{(i)}_p$ refers to the strength of the phonon mode $i$, and $\Gamma_i$ corresponds to its damping. For simplicity we neglect the $\mathbf{q}$-dependence of the spectral functions, i.e. $F_i(\mathbf{q}) \equiv 1$. We employ $\Gamma_1 = 5$ meV and $\Gamma_2 = 10$ meV. Thus, the Eliashberg coupling constants (for $\sigma$- and $\pi$-states)
\[ \lambda_i = 2 \int_0^\infty d\omega \omega^{-1} \alpha^2 F^i(\omega) \] (2)

become

\[ \lambda_i = \frac{1}{\pi} \left[ \frac{g_p(i)}{2} + \arctan \left( \frac{\nu}{\omega} \right) \right] \] . (3)

Note, the single T_c is provided by the non-zero value of \( \lambda_{\pi \sigma} \) and \( \lambda_{\pi \pi} \) due to transitions between \( \sigma \)- and \( \pi \)-states [20]. However, their effect at low temperatures on the solution of the Eliashberg equations seems not to be of significant importance. Thus we neglect them for \( T=0 \). Regarding the value of \( \lambda_{\pi} \) we have chosen it 0.7 in quantitative agreement with first principle calculations [4]. The strength of the coupling of the \( \pi \)-electrons to the low-frequency mode is unknown. However, using an Einstein model for the phonon spectrum yielding \( \alpha^2 F(\omega) = g^2/\omega E \), one expects \( \lambda_{\pi} > \lambda_{\sigma} \) [22] (see also [23]). Taking into account also recent experiments indicating that the larger gap shows much smaller coherence peaks in the tunneling density of states [23] one concludes also that \( \lambda_{\pi} > \lambda_{\sigma} \). In the following, we approximate \( \lambda_{\pi} = 1.4 \). Then we use Eliashberg equations referring to the \( \pi \)- and \( \sigma \)-states separately for \( T=0 \) (\( \omega_c \) is a cutoff frequency):

\[ \Delta^i(\omega) = \frac{1}{Z_i^0(\omega)} \int_0^{\omega_c} d\nu \text{Re} \left\{ \frac{\Delta^i(\nu)}{[\nu^2 - (\Delta^i)^2(\nu)]^{1/2}} \right\} \times \{ K^i_+(\nu, \omega) - N_i(\epsilon_F)U^i_{\text{c}} \} \] . (4)

\[ \int_0^{\omega_{\text{max}}} d\nu \text{Re} \left\{ \frac{\nu}{[\nu^2 - (\Delta^i)^2(\nu)]^{1/2}} \right\} K^i_-(\nu, \omega) \] , (5)

with the kernel

\[ K^i_+(\nu, \omega) = \int_0^{\omega_{\text{max}}} d\omega' \alpha^2 F^i(\omega') \times \left[ \frac{1}{\omega + \omega' + \nu + i\delta} + \frac{1}{\omega - \omega' - \nu + i\delta} \right] \] , (6)

where \( i \) refers to \( \pi \)- and \( \sigma \)-electrons. Here \( Z_i^0(\omega) \) denotes the effective mass renormalization function of the \( \sigma \)- and \( \pi \)-bands in the superconducting state and \( U^i_{\text{c}} \) refers to the screened Coulomb (pseudo-)potential calculated within the static Thomas-Fermi approximation for 3D metals. Solving these equations self-consistently for the given phonon spectrum (\( \pi \)-states couple to \( \omega_1 \), while \( \sigma \)-states to \( \omega_2 \)-mode) we obtain \( \Delta^i(\omega, T) \) with structures due to the two pronounced modes in \( \alpha^2 F^i(\omega) \) [23]. Regarding the choice of the values for \( \mu_{\pi}^* \), note that the \( \sigma \)-band is more metallic than the \( \pi \)-band, which is reflected by their different Fermi velocity and density of states at the Fermi level [13]. This leads to \( \mu_{\pi}^* > \mu_{\pi}^* \). Taking \( \mu_{\pi}^* = 0.1 \) and the appropriate values of \( N_i(\epsilon_F) \) and \( \omega_i \), we obtain \( \mu_{\pi}^* = 0.18 \). These values of \( \mu_{\pi}^* \) and \( \lambda_i \) give the observed magnitude of the superconducting gaps, their ratio and the anisotropy of the upper critical field \( H_{c2} \). From this point of view, MgB_2 can therefore be referred to as a conventional electron-phonon mediated superconductor with moderate coupling.

In Fig. 3 we show the results for the superconducting gaps for the \( \sigma \)- and \( \pi \)-bands solving Eqs. (1)-(3). Due to the larger \( \lambda \) and smaller \( \mu^* \) the gap value \( \Delta_{\pi} = 7.5 \text{ meV} \) for the \( \pi \)-band is almost two times larger than superconducting gap \( \Delta_\sigma = 4.2 \text{ meV} \) for the \( \sigma \)-band. The values of the gaps and their ratio are in good agreement with experimental data [6 18]. The curves also reflect the underlying phonon spectrum \( \alpha^2 F^i(\omega) \). Re \( \Delta^i(\omega) \) changes its sign above \( \omega_i \) due to the over-screened pairing potential and Im \( \Delta^i(\omega) \) starts to increase at \( \omega_i \) because of phonon emission processes.

In order to test whether the effective one-band model can be applied, we also have solved the one-band version of the Eliashberg equation for the average \( \lambda = \frac{N_{\sigma}(0)}{N_{\text{tot}}} \lambda_{\sigma} + \frac{N_{\pi}(0)}{N_{\text{tot}}} \lambda_{\pi} \approx 0.87 \) and average \( \mu_{\pi} = 0.5 \left( \mu_{\sigma}^* + \mu_{\pi}^* \right) \). The corresponding phonon density of states includes both low-frequency and \( E_{2g} \) peaks with the coupling to the effective Bloch states. The values of \( g_i \) were chosen in order to have the same relative strength as in the case of the two-band model and also to satisfy the absolute value of \( \lambda \). Then, we find a superconducting gap \( \Delta_0 = 4 \text{ meV} \).

In Fig. 3(a) we present our results for the tunneling density of states for the effective gap. The obtained coherence peaks at 4 meV due to the effective superconducting gap \( \Delta_0 \) agree with the experimentally observed position of the order of 4 meV [3]. However, no further pronounced structure at approximately 7 meV as observed in experiment is obtained. This suggests that an effective one gap approximation is not a good one.

In Fig. 3(b), we show results for the two-band Eliashberg theory. The tunneling density of states resulting from \( \pi \)- and \( \sigma \)-bands is then given by

\[ N_S(\omega)/N_n(\epsilon_F) = \frac{N_{\sigma}(0)}{N_{\text{tot}}} \text{Re} \left[ \frac{\omega}{\sqrt{\omega^2 - (\Delta_{\sigma}^*(\omega))^2}} \right] + \frac{N_{\pi}(0)}{N_{\text{tot}}} \text{Re} \left[ \frac{\omega}{\sqrt{\omega^2 - (\Delta_{\pi}^*(\omega))^2}} \right] . \] (7)

The results depicted in Fig. 3(b) clearly show larger and smaller coherence peaks reflecting the corresponding superconducting gaps in the \( \pi \)- and \( \sigma \)-bands respectively. The position of these peaks(\( \Delta_{\pi}^* = 4.2 \text{ meV} \) and \( \Delta_{\sigma}^* = 7.5 \text{ meV} \)) are in good agreement with experimental results (4.2 meV and 7.5 meV) indicating that these peaks may result from two superconducting gaps. The smaller coherence peak of the larger gap is due to the smaller density of states of the \( \pi \)-band at the Fermi level with respect
to the $\sigma$-states (see Eq. (7)). This is another indication that the larger gap has to be attributed to the $\pi$-states rather than to a $\sigma$-band.

In order to support further the validity of our results, let us now turn to the discussion of the resulting anisotropy of the upper critical field $H_{c2}$. According to the anisotropic Ginzburg-Landau theory equations, the upper critical field along the $c$-axis is given by $H_{c2}^{ab} = \frac{\Phi_0}{\xi_{ab}^c}$, and for the magnetic field applied in the $ab$-plane by $H_{c2}^{ab} = \frac{\Phi_0}{\xi_{c}^{ab}}$. Here, $\Phi_0$ is the superconducting flux quantum, $\xi_{ab}$ and $\xi_c$ are the coherence lengths referring to the $ab$-plane and the $c$-axis in the clean limit, respectively. The coherence length is determined as $\xi \approx \frac{\hbar v_F}{\pi \alpha}$. Thus, one gets the anisotropy ratio

$$\frac{H_{c2}^{ab}}{H_{c2}^c} = \frac{v_F^ab \Delta_0^c}{v_F^c \Phi_0^{ab}}. \quad (8)$$

Since only the $\pi$-band has a substantial dispersion along the $k_z$-axis, we can approximate $v_F^c$ by $v_F^c \approx 4 \times 10^5 \text{cm/s}$ for the $\pi$-band [5]. Similar arguments for the $\sigma$-band lead to $v_F^ab \approx v_F^c \approx 8.5 \times 10^5 \text{cm/s}$ [4]. Substituting our values for the superconducting gaps we obtain $\frac{H_{c2}^{ab}}{H_{c2}^c} \approx 3.9$, which is in good agreement with the experimental observation [11,23]. The recent suggestion [24-27] that the larger gap belongs to the $\sigma$-band and the smaller gap occurs in the $\pi$-band reduces significantly the anisotropy of the upper critical field and also leads to the ratio of the coherence peaks in the tunneling density of states being inconsistent with experiment [7]. However, we get $H_{c2}^{ab} \approx 5.6 \text{Tesla}$ taking into account the renormalization of the Fermi velocities due to electron-phonon interaction, while some experiments give 15 Tesla or even larger values. Note, further correcting the LDA results for $v_F$ by a factor 1.5 for the $\pi$ and $\sigma$-states we get $H_{c2}^{ab} \approx 14.6 \text{Tesla}$. Many-body effects like electron-electron correlations may cause this correction.

In Fig.4 we show the calculated effective mass renormalization functions $Z_1(\omega)$ for the $\sigma$- and $\pi$-quasiparticles reflecting many-body effects due to electron-phonon interaction and which describe the strength of the interaction between the corresponding quasiparticles. Their structures again reflect the underlying phonon spectrum $F(\omega)$ at 24 meV for the $\pi$-states and at 67 meV for the $\sigma$-electrons. Remarkably, the mass renormalization for $\pi$-electrons is larger due the difference in the corresponding $\lambda_i$.

Let us now estimate the high superconducting transition temperature and the corresponding isotope effect. As we already mentioned the single $T_c$ is expected due to non-zero values of $\lambda_{\pi\sigma}$. Moreover, as was shown earlier [23], even in a two-band case one still can use effective parameters for the determination of $T_c$. Thus, we use the McMillan formula $\langle \omega_2 \sim 1/\sqrt{M_B} \rangle$ [23]

$$k_B T_c \approx \frac{\hbar \omega_D}{1.2} \exp \left\{ -\frac{1.04(1 + \bar{\lambda})}{\lambda - \bar{\mu}^* (1 + 0.62 \lambda)} \right\}, \quad (9)$$

with $\omega_D \approx \omega_2$, and an effective $\bar{\lambda} = 0.87$ and $\bar{\mu}^* = 0.14$ resulting in $T_c \approx 32 \text{K}$. We get for isotope coefficient $\alpha = -d \ln T_c / d \ln M_B$ the value 0.43. Assuming that the isotope effect will be mainly determined by the coupling between $\sigma$-states and the $E_{2g}$-mode we should use in Eq. (9) for $\lambda$ and $\mu^*$ the values referring to the $\sigma$-states. Thus, we find the absolute value $\alpha \approx 0.23$ which is in agreement with experiment [2]. We also would like to point out that despite of the larger gap in the $\pi$-band, superconductivity ($n_s$) and $T_c$ are mainly due to the $\sigma$-states. This can be seen from the estimation of the superfluid density $n_s \sim N_i(\epsilon_F)\omega_i/(\text{unit volume})$ which is much larger for the $\sigma$-electrons due to their larger density of states at the Fermi level and the large $\omega_2$.

In summary, we can explain important facts about superconductivity in MgB$_2$ as resulting from electron-phonon coupling of the $\pi$-states and the $\sigma$-states with the corresponding phonon modes. The larger gap results from the $\pi$-band coupled strongly to the low-frequency mode, while the smaller gap is due to the coupling of $\sigma$-bands with the $E_{2g}$-mode. The structure seen by recent tunneling experiments is due to the larger superconducting gap of the $\pi$-band. We also find $H_{c2}^{ab}/H_{c2}^c \approx 3.9$ in good agreement with experiment. We safely conclude that there is no need for invoking other pairing mechanisms besides electron-phonon interaction. Direct calculations of $g_{el-\text{ph}}^i$ and $\lambda_i$ are necessary for a further support of our simple model. In particular, the origin of the 24 meV peak observed by INS and Raman scattering must be clarified. Using our picture for superconductivity in MgB$_2$, one may estimate the absence of superconductivity in AlB$_2$ due to the decrease of $\lambda_\sigma$ ($\lambda \sim |g|^2/\omega_2$) and the shift of $\pi$-states below $\epsilon_F$ [4].

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Fig. 1. Simplified physical picture for superconductivity in MgB$_2$: a) Top view of the elementary unit cell of MgB$_2$ consisting of hexagonal layers of Mg and graphite-like Boron layer. The Boron $\pi$-states ($p_z$) are involved in superconductivity and couple to the $E_2$ mode of B-B vibrations shown by arrows; b) the Boron $\pi$-states ($p_z$) are coupled to the out-of-plane vibrations shown schematically by arrows.

Fig. 2. Results for the gap function $\Delta^i(\omega)$ at $T=0$K using two-band Eliashberg-theory: (a) $\sigma$-band with $\lambda_\sigma=0.7$ and $\mu_\sigma^*=0.18$ yielding $\Delta_0^\sigma=\Delta^\sigma(\omega=0)=4.2$ meV. (b) $\pi$-band with $\lambda_\pi=1.4$ and $\mu_\pi^*=0.1$ yielding $\Delta_0^\pi=7.5$ meV.

Fig. 3. Calculated tunneling density of states: (a) using an effective one-band Eliashberg theory with elastic scattering strength $\gamma=0.3$meV; (b) using two-band Eliashberg theory and the same $\gamma$ as in (a). In the inset, experimental data is displayed.

Fig. 4. Results for the mass renormalization function $Z_\pi^i(\omega)$ at $T=0$K using two-band Eliashberg-theory for (a) the $\sigma$-band and (b) the $\pi$-band.
\[ \Delta^\sigma \text{ (meV)} \]

\[ \mu_\sigma^* = 0.18 \]
\[ \lambda_\sigma = 0.7 \]

\[ \text{Re } \Delta^\sigma \]
\[ \text{Im } \Delta^\sigma \]
\( \Delta_0 = 4 \text{ meV} \)

\( \gamma = 0.3 \text{ meV} \)
\( \frac{N^\sigma}{N^\text{tot}} + \frac{N^\pi}{N^\text{tot}}(E_F) \)

Inset: Exp. data from F. Guibileo

\[ \text{Exp. data from F. Guibileo} \]

\[ \frac{dI}{dV}, \text{normalized} \]

-20 -10 0 10 20

0.0 0.5 1.0 1.5 2.0

\( \Delta^\sigma = 4.2 \text{ meV} \)

\( \Delta^\pi = 7.3 \text{ meV} \)

\( \gamma = 0.3 \text{ meV} \)

\( \omega \) (meV)
