Superconductivity in MgB$_2$
and B-doped diamond

- two gap superconductivity in MgB$_2$
  L. Lyard, C. Marcenat, J. Marcus

- superconductivity in B-doped diamond: proximity of a metal-insulator transition
  E. Bustarret, E. Gheeraert, C. Marcenat, F. Gustafsson, J. Marcus
MgB$_2$: a new “high $T_c$” superconductor

$T_c \sim 40$ K

- Simple elements (Al, Pb, Nb,...)
- Intermetallic alloys (NbN, Nb$_3$Sn,...) - A$_1$A$_2$
- Cuprates
- Borocarbides
- Heavy fermions

hexagonal structure

B planes similar to C planes in graphite
2 kinds of electronic orbitals derived from
- in plane sp$_2$-boron orbitals : $\sigma$ bands
- $p_z$ boron orbitals : $\pi$ bands

“same” electronic structure than in Graphite
in which the $\sigma$ bands are full
(in involved in covalent bounds)

$\rightarrow$ $\pi$ band : small e/hole pockets close to the $K$ point

in MgB$_2$ the “second” $\pi$ band is lowered
by attractive Mg$^{2+}$ potential

charge transfert from $\sigma$ to $\pi$ bands

$\rightarrow$ unfilled $\sigma$ bands
“2” Fermi surface sheets

actually $2 \times \pi (3D)$ and $2 \times \sigma$ (quasi-2D) bands

the quasi 2D characters leads to a “large” DOS $\sim 0.30 \text{ st/ev.cell}$
(close to the 2D value $m^*a^2/\pi \hbar^2 \sim 0.33 \text{ st/ev.cell}$)

despite the small hole doping level $\sim 0.07 \text{ hole/B}$
strong coupling of $\sigma$ electrons with $E_{2g}$ vibration mode
+ large DOS

$\rightarrow$ electron-phonon coupling constant $\lambda \sim 1.8$

despite a larger DOS ($\sim 0.4$st/ev.cell)

the coupling is much worse in the $\pi$ band; $\lambda \sim 0.45$

Mac-Millan expansion
screening coefficient: 0.15
$\omega = 540K$
Two co-existing superconductors????

2 SF sheets $\rightarrow$ 2 gaps

BCS value

Two co-existing superconductors????

2 SF sheets $\rightarrow$ 2 gaps

BCS value
confirmed by specific heat (i.e. bulk) measurements

\[ C_p/T : \gamma \propto e^{-\Delta/kT} \]

2 gaps => 2 \( T_c \) values???
but present different field dependences

both gaps are closing at the same $T_c$ => weakly coupled bands

zero coupling => $2T_c$'s

strong coupling => FS averaged $\lambda$ value (~0.7) => $T_c \sim 20K$

the small gap is very sensitive to $H$ i.e. “disappears” around 1T
and the vortex lattice rotates by 30°

SANS measurements R. Cubitt et al. PRL 03

\[ \gamma / \gamma_0 \]

\[ \mu_0 H_a (T) \]

+ anomalous field dependence of \( \gamma \)

\[ \xi \text{ and } \lambda \text{ values (associated with each band)} \]

Should the system be described by two \( \xi \) and two \( \lambda \) values (associated with each band) or only one field dependent value (as we believe)?

In any case the "properties" of the superconducting state are going to be strongly field dependent: 

exemple of the anisotropy
\[ \Gamma = \frac{\langle m_{ab}^* \rangle_{FS}}{\langle m_c^* \rangle_{FS}} = \sqrt{\frac{\langle v_{F,c}^2 \rangle_{FS}}{\langle v_{F,ab}^2 \rangle_{FS}}} = \frac{\lambda_c}{\lambda_{ab}} = \frac{\xi_{ab}}{\xi_c} \]

Which Fermi Surface should we take into account???

How can we get \( \Gamma \)???

High field:
\[ \Gamma = \Gamma_{H_{c2}} = \frac{H_{c2,ab}}{H_{c2,c}} \]

Low field:
\[ \Gamma \sim \Gamma_{H_{c1}} = \frac{H_{c1,c}}{H_{c1,ab}} \]

from \( C_p \) and magnetotransport, Lyard et al. PRB 02

from \( C_p \) and Hall probe magnetometry, Lyard et al. PRL 04
what about Graphite.....

doping by intercalation (Na,...) leads to superconductivity: $T_c \approx 5K$

but superconductivity remains in the “soft” $\pi$ band (similar to alkali doped fullerides)

DIAMOND
very “strong” $\sigma$ bounds

but 3D (sp3)....

Superconductivity ($T_c \approx 7K$) has been observed in Ba doped Si-clathrates (cage like structure with sp3 bounds)
all 4e are involved in covalent bounds -> large gap semiconductor
can be either n or p doped by substituting C atoms by P or B atoms, respectively

In B-doped samples, the system becomes metallic when the boron impurity band overlaps the diamond valence band i.e. for boron concentrations > a few $10^{20}$ cm$^{-3}$

what about the e-phonon coupling $\lambda$ ???

$$\lambda = N(E_F) \cdot \frac{I^2}{M\omega^2}$$

<table>
<thead>
<tr>
<th></th>
<th>$N$</th>
<th>$l$ (eV/A)</th>
<th>$\omega$ (cm$^{-1}$)</th>
<th>$I^2/M\omega^2$</th>
<th>$\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MgB$_2$</td>
<td>0.15</td>
<td>12</td>
<td>540</td>
<td>6.7</td>
<td>1.0</td>
</tr>
<tr>
<td>C-B3%</td>
<td>0.06±0.01</td>
<td>24±3</td>
<td>1080</td>
<td>7.5±0.8</td>
<td>0.45±0.1</td>
</tr>
</tbody>
</table>

2x the already large MgB$_2$ value
1/2 of MgB$_2$ value to smaller DOS (3D)
<table>
<thead>
<tr>
<th>Method</th>
<th>Model</th>
<th>( E/C ) at.%</th>
<th>( n_B ) 10(^{20}) cm(^{-3})</th>
<th>( \lambda )</th>
<th>( T_c ) (K)</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boeri et al</td>
<td>First Principles LMTO</td>
<td>VCA Virtual crystal</td>
<td>3</td>
<td>50</td>
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<tr>
<td>Lee et al</td>
<td>First principles APW-CPA</td>
<td>VCA Virtual crystal</td>
<td>2.5</td>
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<td>0.53</td>
<td>9</td>
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<tr>
<td>Xiang et al</td>
<td>First principles supercell DFT-LDA</td>
<td>C(_{50})B</td>
<td>2.8</td>
<td>49</td>
<td>0.39</td>
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<tr>
<td>Blase et al</td>
<td>Ab initio Supercell DFT-LDA</td>
<td>C(_{53})B</td>
<td>1.85</td>
<td>33</td>
<td>0.43</td>
<td>4</td>
</tr>
</tbody>
</table>

**Remark:** Phonon modes involved in \( e/\lambda \) coupling not clearly identified.
Polycrystalline diamond (HPHT bulk)
Doping level: $10^{21} \text{B/cm}^3$ : $T_c \sim 3K$

confirmed on homoepitaxial films
E.Bustarret 04

Ekimov et al. Nature 04

MIT

$n_B (10^{20} \text{cm}^{-3})$

$T_c (K)$

$R(\Omega)$

$a$
is there any relation between this metal-insulator transition and superconductivity???

\[ T_c \sim \sigma(0) \] ???

enhanced superconductivity due to reduced screening close to the MIT???
Soulen - Osofsky et al.

normal state conductivity extrapolated to zero
Hole doping of the \( \sigma \) bands leads to very efficient electron-phonon interaction potential.

+ large DOS due to 2D character (sp2) in MgB\(_2\) => \( T_c \approx 40K \)

superconducting is also "induced" in the \( \pi \) band => two gap superconductivity

anomalous field and temperature dependence of the superconducting properties

\[ \lambda \approx 1.4 \ \xi \ \omega \approx 1500K \]
\[ => T_c \] between 50 and ...150K !!!

(\( T_c \) values predicted in C clathrates (X\( _8 \)@C\( _{46} \))

\[ => T_c \] between 50 and ...150K !!!

(superconductivity appears in the vicinity of a MIT)

\( \text{(depending on screening coefficient)} \)

Connatble et al. 2003