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Origin of superconductivity in B-doped Diamond

Kwan-Woo Lee
Warren E. Pickett

UC Davis

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Outline

- Experimental data
- Approach & Comparison with MgB₂
- Theoretical background
- Results
  - el.-ph. coupling constant obtained from two methods
- Other theoretical works
- Conclusion
B-doped diamond superconductor

- synthesized at high P (100,000 atm) and T (2500-2800K)
- \( c_{SC} = 5 \times 10^{21} \text{ cm}^{-3} = 25c_{MI} \)
  \[ c_{MI} = 2 \times 10^{20} \text{ cm}^{-3} \]
- \( T_c \approx 4 \text{K} \)
- grown by microwave plasma-assisted chemical vapor deposition (MPCVP)
- \( T_c \approx 7.4 \text{K} \)

(Russian AS, LANL)

Takano et al., APL 85, 2851 (2004).  
(NIMS, Waseda U in Japan)
By Fontaine, the activation energy depends on $c_B$.

- 0.37 eV for low concentration
- 0 eV for above $c_{sc}/6$

⇒ a degenerate metal for a larger concentration

.: Our viewpoint: The majority fraction of the hole carriers reside in states overlapping the diamond VB, and behave as degenerate valence band holes.

Virtual crystal approximation (VCA)

[nuclear charge $Z=(1-x)Z_C + xZ_B$ for the B-doped diamond]


R_{mtK_{max}}=7.0 with a sphere radius 1.2, 1156 irreducible k-point

2.5% B-doped diamond

- $E_F = -0.61$ eV from the VBM (calculated)
- The Fermi surfaces consist of 3 zone-centered spheroids.

<table>
<thead>
<tr>
<th>Analogy</th>
<th>carrier states</th>
<th>MgB$_2$</th>
<th>B-doped diamond</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>the very strongly covalent bonding states</td>
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<td></td>
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<td>These states should be sensitively coupled to the bond-stretching mode.</td>
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<td>($\Omega_0 = 1332 \text{ cm}^{-1} \approx 0.16$ eV in diamond)</td>
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<tr>
<td>DOS</td>
<td>2D</td>
<td>3D</td>
<td></td>
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<tr>
<td>Bond-stretching mode</td>
<td>2 of the 9 phonon modes</td>
<td>3 of the 6 phonon modes</td>
<td></td>
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</table>
Electron-Phonon coupling constant $\lambda$

- Rigorously,
  \[
  \lambda = \frac{\sum_b N_b (0) \langle I_b^2 \rangle}{M \langle \omega^2 \rangle} = \frac{N (0) I_{rms}^2}{M \omega_0^2}
  \]
  - $M$: carbon mass
  - $I_b^2 \equiv \left\langle \left| I_b(k,k') \right|^2 \right\rangle_{FS}$
    - FS averaged el.-ph. matrix element squared for band $b$
  - $\langle \omega^2 \rangle \sim \omega_0^2$: renormalized bond-stretch freq.
  - $N(0)=0.06$ states/eV/cell/spin

Obtaining $\lambda$

1. Calculate the $Q=0$ deformation potentials

2. Calculate the phonon softening and use the lattice dynamical result

\[
\omega_Q^2 = \Omega_Q^2 + 2\Omega_Q \text{Re} \Pi(Q,0)
\]

\[
\omega_0^2 = \omega_{Q \rightarrow 0}^2 \Rightarrow \Omega_0^2 - 2\Omega_0 N(0)|M|^2
\]

$M$: el.-ph. matrix element determined by $I_{rms}$
Deformation Energy ($D$)

By Khan and Allen, $D$ is the shift in the VB edge w.r.t the bond-stretching motion of scale

$$u_0 = \sqrt{\hbar / 2M \Omega_0} = 0.034 \ \text{Å}$$

$$\left(\varepsilon_{\text{upper}}-\varepsilon_{\text{lower}}\right)_{k=0}/\Delta d_{\text{bond}}=21\text{eV/Å}$$

\[
\begin{align*}
D_1 &= 14 \ \text{eV/Å} \ (\text{single band}) \\
D_2 &= 7 \ \text{eV/Å} \ (\text{2-fold band}) \\
\therefore \ I_{rms} &= 10 \ \text{eV/Å}
\end{align*}
\]

$\text{rms el.-ph. Matrix element}$

$$M = \sqrt{\frac{\omega_0}{\Omega_0}} u_0 I_{rms} = 0.70 \ \text{eV}$$

( where $\omega_0^2 = 0.68\Omega_0^2$ )
el.-ph. coupling constant $\lambda = 0.55$

neglecting very minor strong-coupling corrections,

$$ T_c = \frac{\omega_0}{1.2} \exp \left[ -1/\left( \frac{\lambda}{1 + \lambda} - \mu^* \right) \right] $$

Using the conventional value $\mu^* = 0.15$ with $\omega_0 = 0.128$ eV, $T_c = 9$K (good agreement with the observed 4~7K)

$T_c = 4$K would require $\lambda = 0.48$ or $\mu^* \approx 0.20$. (relatively small changes)
Phonon Softening

For the doped case, much more complex due to disappearing some piece of FS.

From the coefficient of the 2nd order terms,

\[
\begin{align*}
\Omega_{\text{harm}} &= 1308 \text{ cm}^{-1} \\
\omega_0 &= 1070 \text{ cm}^{-1}
\end{align*}
\]

\[
M = 0.67 \text{ eV}
\]

\[\Rightarrow \lambda = 0.53 \pm 0.03\]
Other theoretical works

L. Boeri et al. (Stuttgart, Germany), PRL 93, 237002 (2004).
From the same viewpoint as ours (VCA)

H.J. Xiang et al. (Hefei, China), PRB 70, 212504 (2004).
2x2x2 and 3x3x2 diamond supercell

X. Blase et al. (LPMCN, France), PRL 93, 237004 (2004).
3x3x3 (54 atom) supercell
⇒ a half of $\lambda$ originates in strongly localized defect-related vibrational modes.
Our treatment neglects some complicating features.

- **Jahn-Teller splitting**: just $0.8 \text{ cm}^{-1}$ for the isolated B substitutional impurity
- **Anharmonicity**: The correction need not change the effective $\omega_{\text{ph}}$ largely, as shown in MgB$_2$.
- **Nonadiabatic effect**: $\omega_{\text{ph}}/E_F = 0.25$
  (a new system to investigate the effects)
Conclusion

- Analogy to MgB$_2$: deformation potentials due to bond-stretching are extremely large.
- The electron-phonon coupling strength $\lambda \sim 0.55$
- A renormalization of the optic mode frequency by -20%
- $T_c \sim 5-10K$ (consistent with the experiments)
- CPA shows a band like VCA, except small disorder broadening.
- Phonon coupling is the likely candidate for the pairing mechanism.