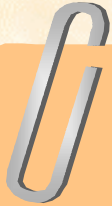


2005 APS March Meeting

Los Angeles



**Origin of superconductivity
in B-doped Diamond**



UC Davis

**Kwan-Woo Lee
Warren E. Pickett**

PRL 93, 237003 (2004)

Acknowledgements to: Z. Fisk, J. Kunes, K. Koepernik

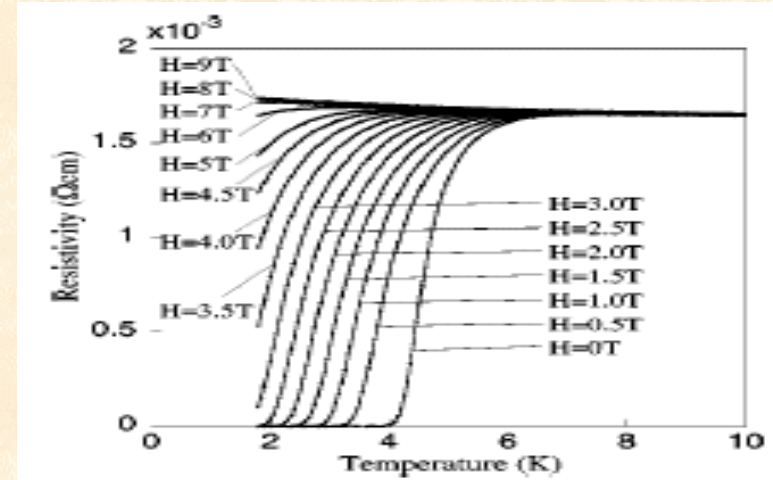
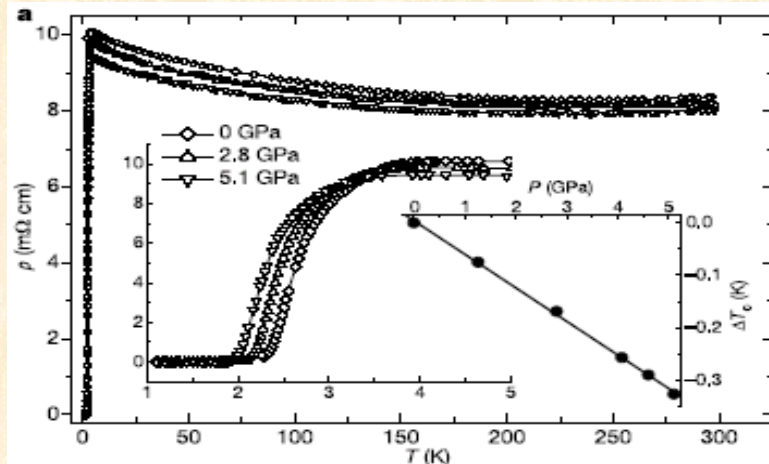


Outline

- ✦ Experimental data
- ✦ Approach & Comparison with MgB_2
- ✦ 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)

- $T_c \approx 7.4\text{K}$

Ekimov et al., Nature 428, 542 (2004)

(Russian AS, LANL)

Takano et al., APL 85, 2851 (2004).

(NIMS, Waseda U in Japan)



Approach

- ✦ By Fontaine, the activation energy depends on c_B .

$$\begin{cases} 0.37 \text{ eV for low concentration} \\ 0 \text{ eV for above } c_{sc}/6 \end{cases}$$

⇒ 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]

- ✦ **LAPW (Wien 2K)** (P. Blaha et al., Comput. Phys. Commun. 59, 399 (1990))
RmtK_{max}=7.0 with a sphere radius 1.2, 1156 irreducible k-point

- ✦ **FPLO** (K. Koepernik and H. Eschrig, Phys. Rev. B 59, 1743 (1999))



2.5% B-doped diamond

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

		MgB ₂	B-doped diamond
Anal-ogy	carrier states	<ul style="list-style-type: none">✦ the very strongly covalent bonding states✦ These states should be sensitively coupled to the bond-stretching mode. <p>($\Omega_0 = 1332 \text{ cm}^{-1} \approx 0.16 \text{ eV}$ in diamond)</p>	
Differ-ence	DOS	2D	3D
	Bond-stretching mode	2 of the 9 phonon modes	3 of the 6 phonon modes



Electron-Phonon coupling constant λ

✦ 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

• $I_b^2 \equiv \left\langle \left\langle |I_b(k, k')|^2 \right\rangle \right\rangle_{FS}$

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 λ

1. Calculate the $Q=0$ deformation potentials
2. Calculate the phonon softening and use the lattice dynamical result

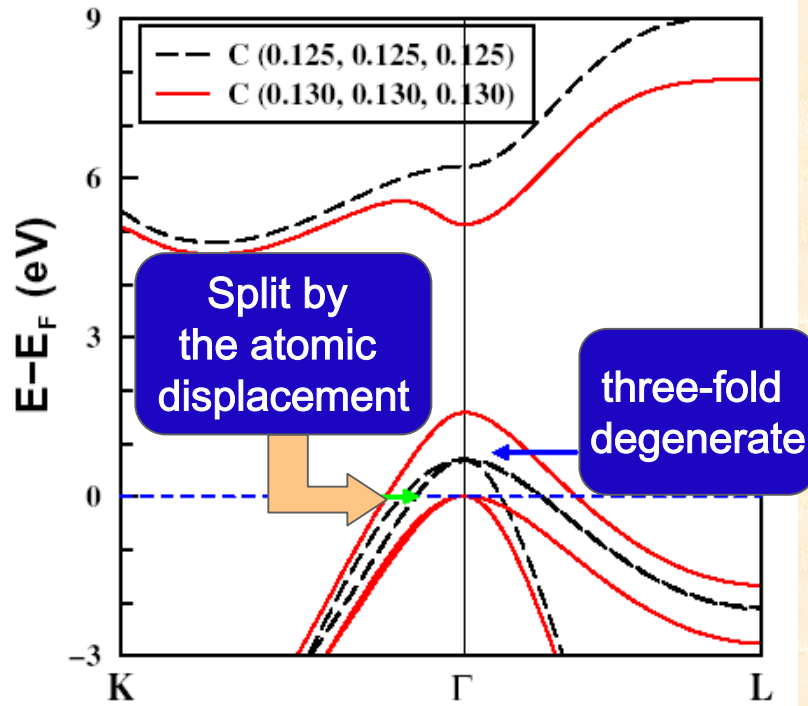
$$\omega_Q^2 = \Omega_Q^2 + 2\Omega_Q \text{Re}\Pi(Q, 0)$$

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

M : el.-ph. matrix element detemind by I_{rms}



Deformation Energy (D)



Blowup VCA band of 2.5% B-doped diamond without and with stretched C-C bonds

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

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

- $(\epsilon_{\text{upper}} - \epsilon_{\text{lower}})_{k=0} / \Delta d_{\text{bond}} = 21 \text{ eV/\AA}$

$$\left(\begin{array}{l} D_1 = 14 \text{ eV/\AA (single band)} \\ D_2 = 7 \text{ eV/\AA (2-fold band)} \end{array} \right)$$

$$\therefore I_{rms} = 10 \text{ eV/\AA}$$

- rms el.-ph. Matrix element

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

$$\left(\text{where } \omega_0^2 = 0.68 \Omega_0^2 \right)$$



continued

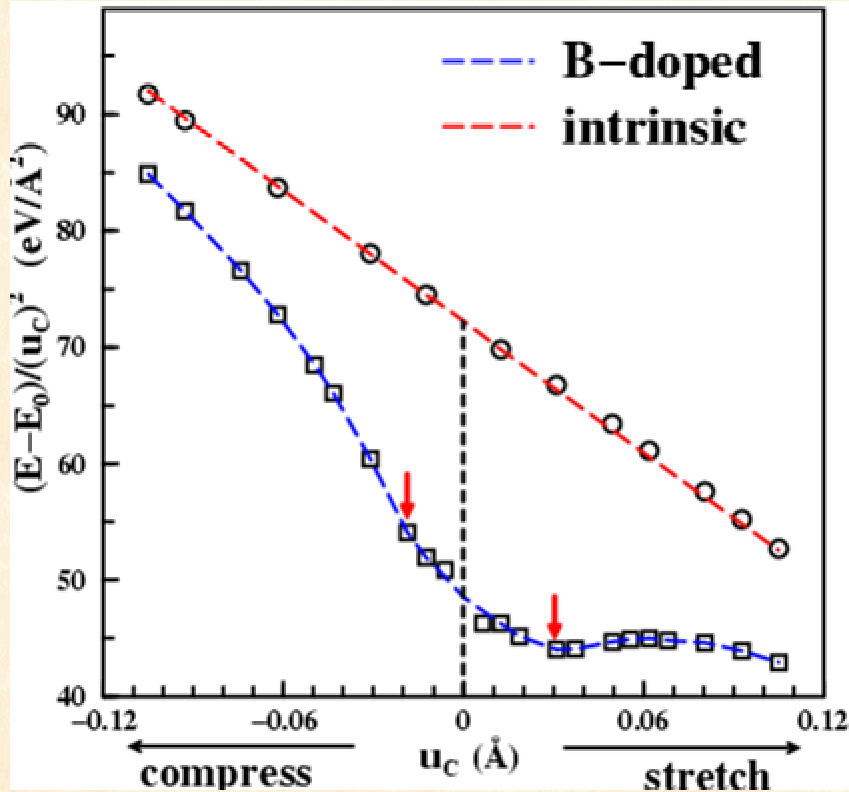
- el.-ph. coupling constant $\lambda = 0.55$
- neglecting very minor strong-coupling corrections,

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

- 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



Energy of distortion for the frozen-in bond-stretch mode for intrinsic and 2.5% B-doped diamond

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

From the coefficient of the 2nd order terms,

$$\left[\begin{array}{l} \Omega_{\text{harm}} = 1308 \quad \text{cm}^{-1} \\ \omega_0 = 1070 \quad \text{cm}^{-1} \end{array} \right]$$

$M = 0.67 \text{ eV}$

$$\Rightarrow \lambda = 0.53 \pm 0.03$$



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 λ originates in strongly localized defect-related vibrational modes.



Discussion

Our treatment neglects some complicating features.

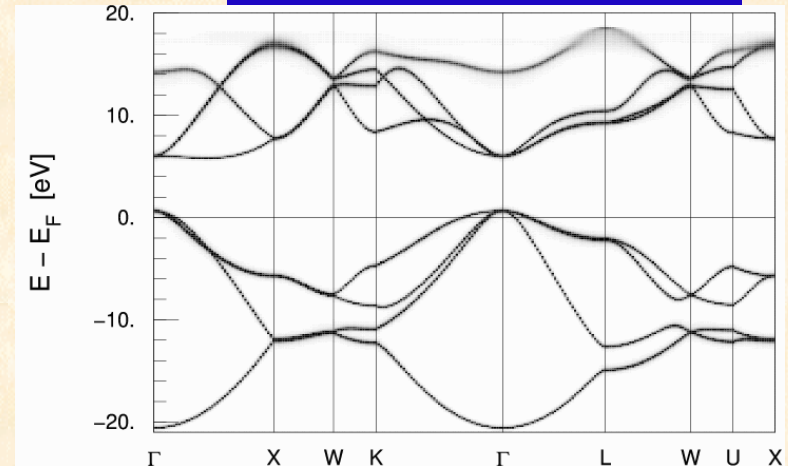
- ✦ **Jahn-Teller splitting:** just 0.8 cm^{-1} for the isolated B substitutional impurity
- ✦ **Anharmonicity:** The correction need **not** change the effective ω_{ph} largely, as shown in MgB_2 .

- ✦ **Nonadiabatic effect:**

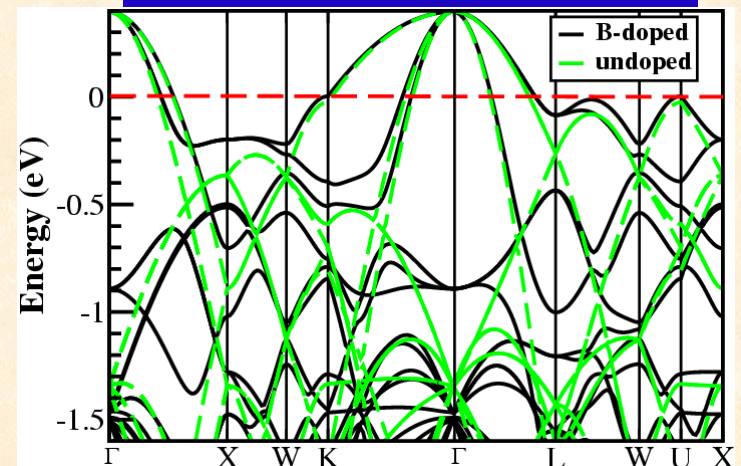
$$\omega_{\text{ph}}/E_{\text{F}} = 0.25$$

(a new system to investigate the effects)

CPA (2.5% B-doped)



4 x 4 x 4 fcc (128 atom)





Conclusion

- ✦ Analogy to MgB₂: 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.**