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Origin of superconductivity in B-doped Diamond

UC Davis

Kwan-Woo Lee

Warren E. Pickett

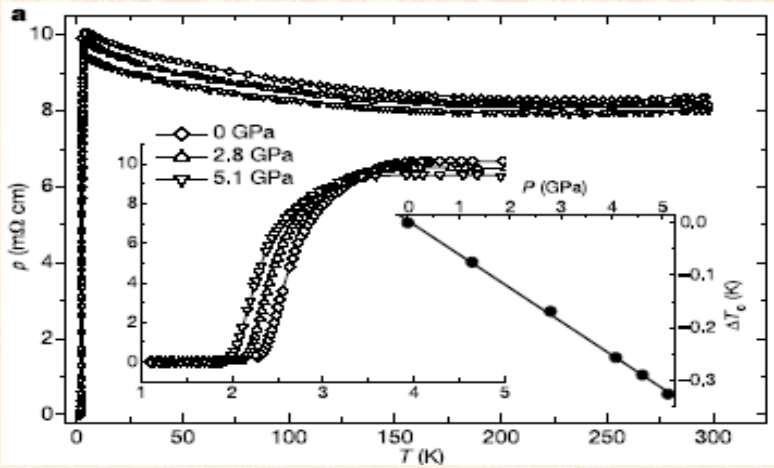
PRL 93, 237003 (2004)

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

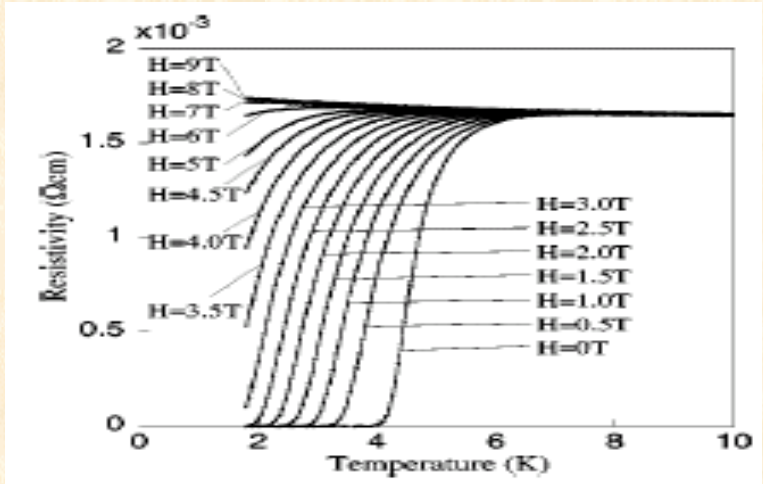


- synthesized at high P (100,000 atm) and T (2500-2800K)
- $c_{SC} = 5 \times 10^{21} cm^{-3} = 25 c_{MI}$

  $\left(c_{MI} = 2 \times 10^{20} cm^{-3} \right)$
- Tc ≈ 4K

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

(Russian AS, LANL)



- grown by microwave plasma-assisted chemical vapor deposition (MPCVP)
- Tc ≈ 7.4K

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

(NIMS, Waseda U in Japan)

Approach

- 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]

- LAPW (Wien 2K) (P. Blaha et al., Comput. Phys. Commun. 59, 399 (1990))

$R_{mt}K_{max}$=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	the very strongly covalent bonding states These states should be sensitively coupled to the bond-stretching mode. (Ω_o =1332 cm^{-1} ≈ 0.16 eV in diamond)	
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,

$$\lambda = \frac{\sum_b N_b(0)\left\langle I_b^2 \right\rangle}{M\left\langle \omega^2 \right\rangle} = \frac{N(0) I_{rms}^2}{M\omega_0^2}$$

- M: carbon mass
- $I_b^2 \equiv \left\langle\left\langle \left| I_b(k,k') \right|^2 \right\rangle\right\rangle_{FS}$

  FS averaged el.-ph. matrix element squared for band b

- $\left\langle \omega^2 \right\rangle \sim \omega_0^2$: renormalized bond-stretch freq.
- N(0)=0.06 states/eV/cell/spin

Obtaining λ

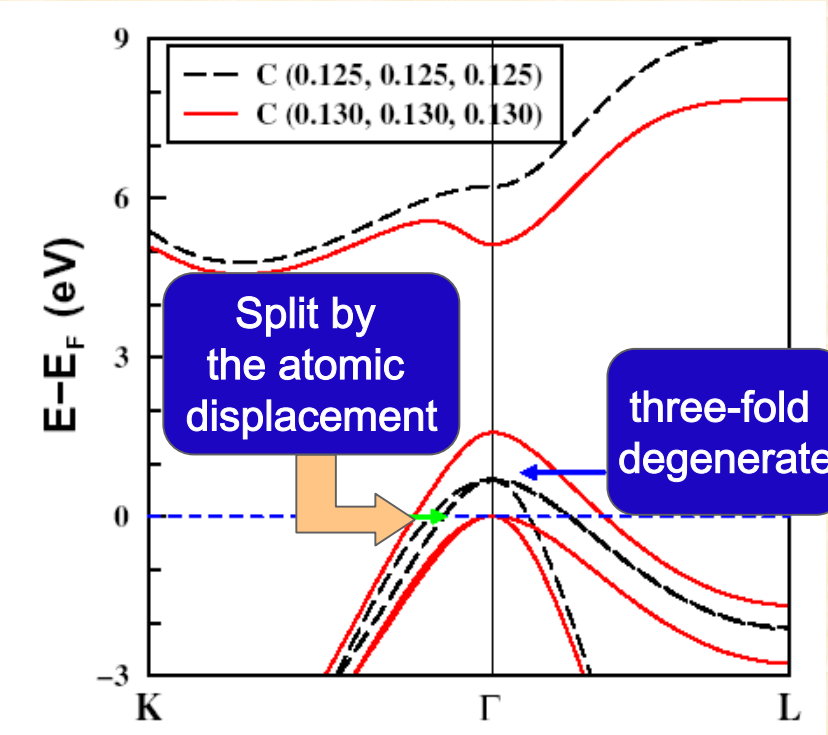
1. Calculate the Q=0 deformation potentials
2. Calculate the phonon softening and use the lattice dynamical result

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

$$\omega_0^2 = \omega_{Q\to 0}^2 \Rightarrow \Omega_0^2 - 2\Omega_0 N(0)\left|\mathrm{M}\right|^2$$

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

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

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

  D_1 = 14 eV/Å (single band)

  D_2 = 7 eV/Å (2-fold band)

  ∴ I_{rms} = 10 eV/Å

- rms el.-ph. Matrix element

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

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

continued

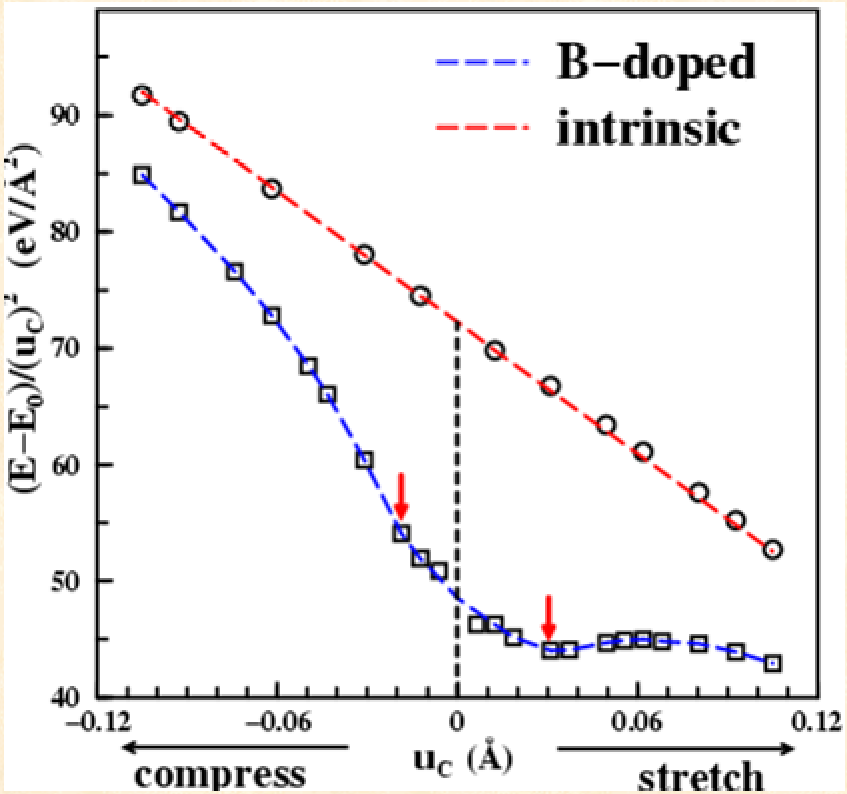
- el.-ph. coupling constant λ = 0.55
- neglecting very minor strong-coupling corrections,

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

- Using the conventional value μ^* = 0.15 with ω_0 = 0.128 eV, T_c = 9K (good agreement with the observed 4~7K)

- T_c = 4K would require λ = 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,

$$\begin{pmatrix} \Omega_{harm} = 1308 & cm^{-1} \\ \omega_0 = 1070 & cm^{-1} \end{pmatrix}$$

- M = 0.67 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

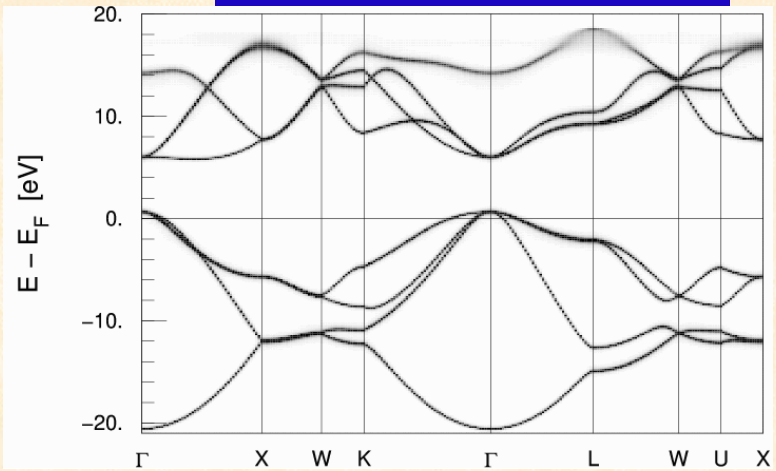
Our treatment neglects some complicating features.

- 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:

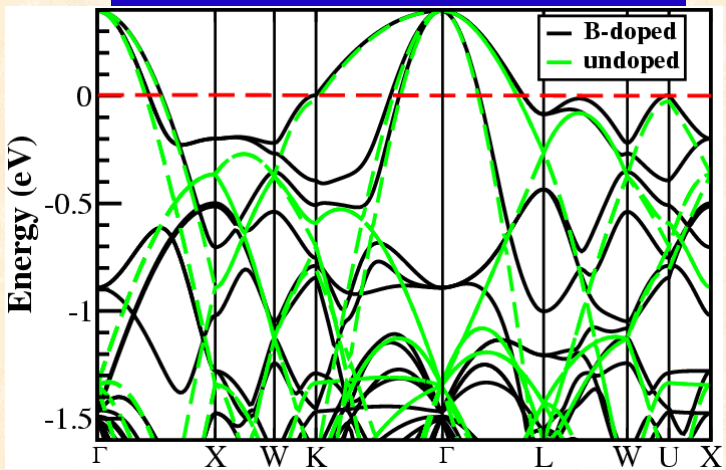
  $\omega_{ph}/E_F = 0.25$

  (a new system to investigate the effects)

CPA (2.5% B-doped)



4 x 4 x 4 fcc (128 atom)



Conclusion

- Analogy to 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.