

Hole-doped Diamond, a 3D version of MgB₂?

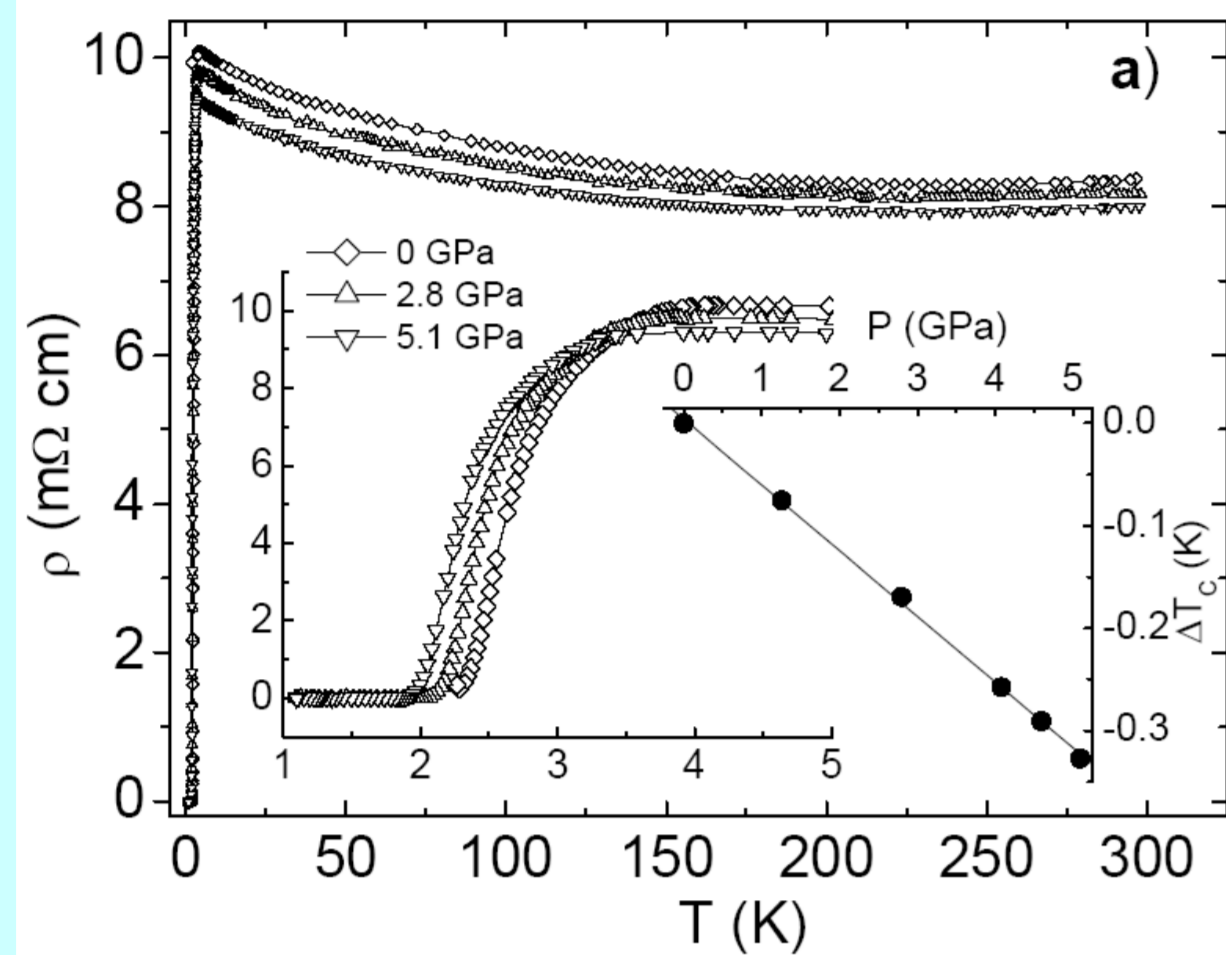


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April 2004: Superconductivity below $T_c = 4\text{K}$ is observed in heavily boron-doped diamond ($\chi=3\%$) [1].

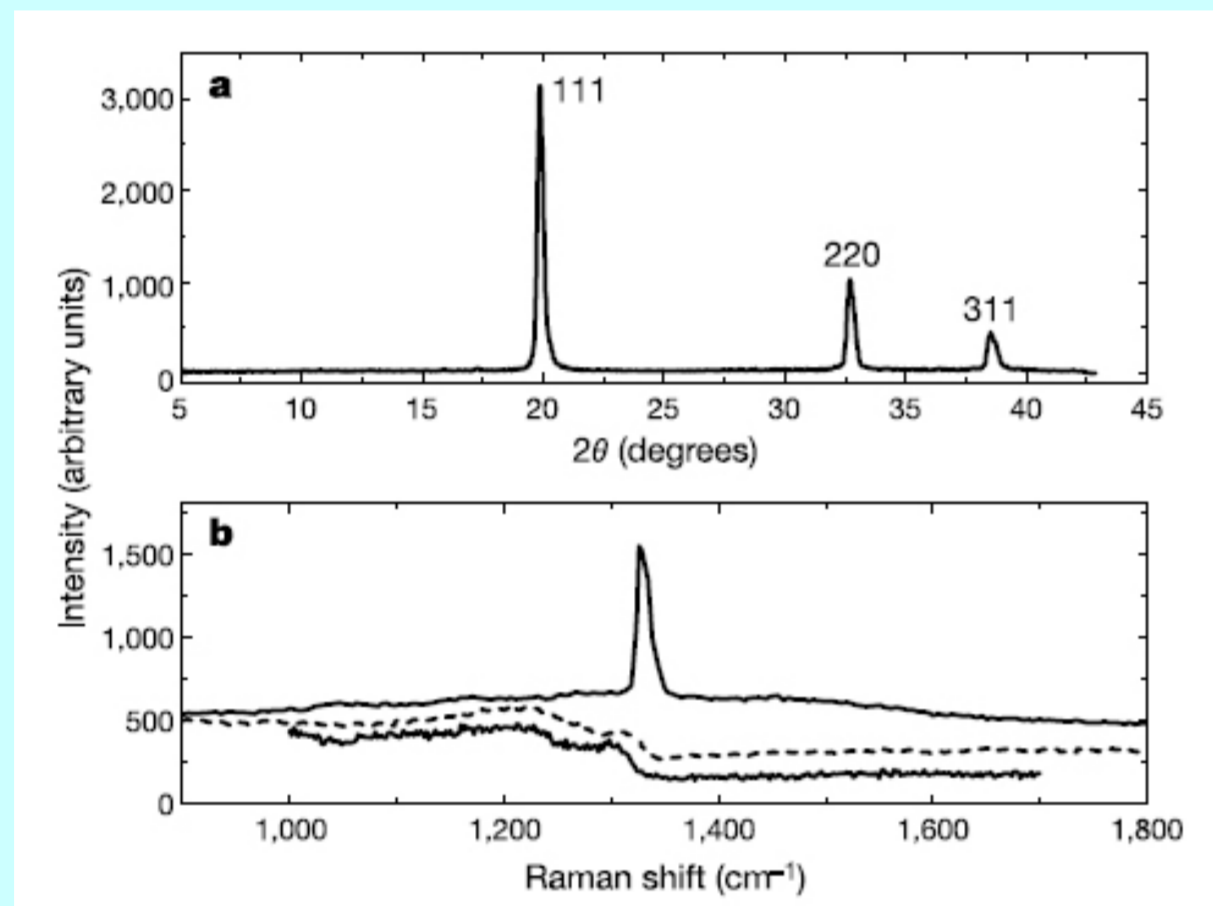


Ekimov et al., Nature 428, 524 (2004)

Boron in diamond is a hole dopant.

Boron-doped diamond is a type-II bulk superconductor.

Superconducting Mechanism?



X-Ray spectrum (top): The crystal structure is the same as the one of pure diamond, with a slightly expanded lattice parameter.

Raman spectrum (bottom): With doping the Raman peak is broadened and shifted to lower frequencies. The same behaviour is observed in MgB₂.

Our Proposal: The observed SC can be understood by the electron-phonon interaction!

Electronic Properties: Full Potential LMTO

Phonons and e-ph interaction: Linear Response (FP-LMTO) [2].

Doping:

- Pure diamond is a band insulator.
- Boron impurity states are $E_B=0.37\text{ eV}$ above the top of the valence band.
- Insulator-metal transition at $\chi=\chi_{cr}\sim 0.1\%$.
- Boron-doped diamond at $\chi=3\%$ is metallic.

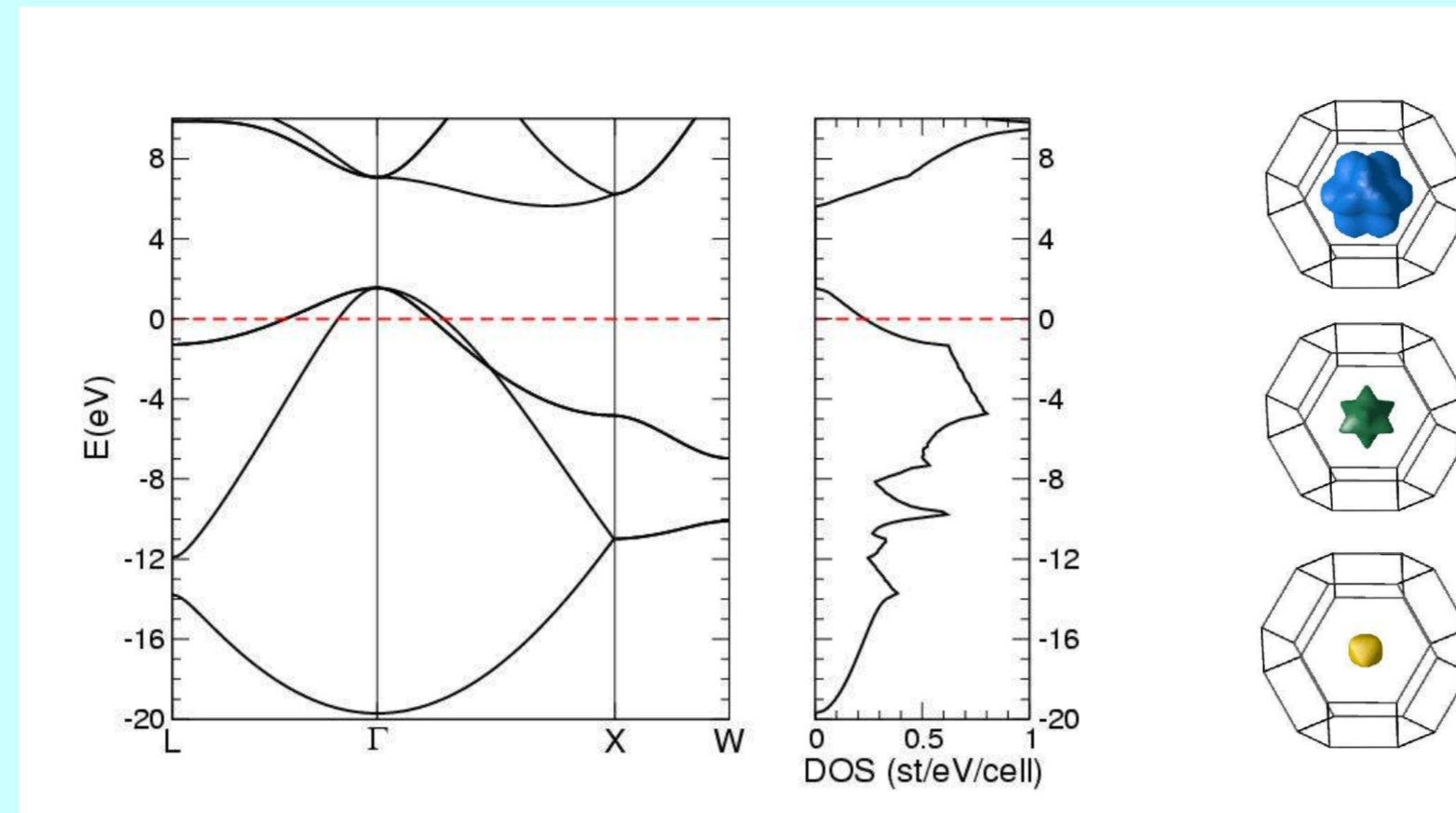
Virtual Crystal Approximation:

To model the effect of $\chi\%$ B doping, the real B and C atoms are replaced by a virtual atom with charge Z^{virt} :

$$Z^{virt} = \chi Z^B + (1-\chi) Z^C$$

- No superstructures or distortions (XRay).
- χ can be varied continuously ($\chi=0.01-0.1$).
- Slight lattice expansion with χ , in agreement with the experiment.

Electronic Structure:

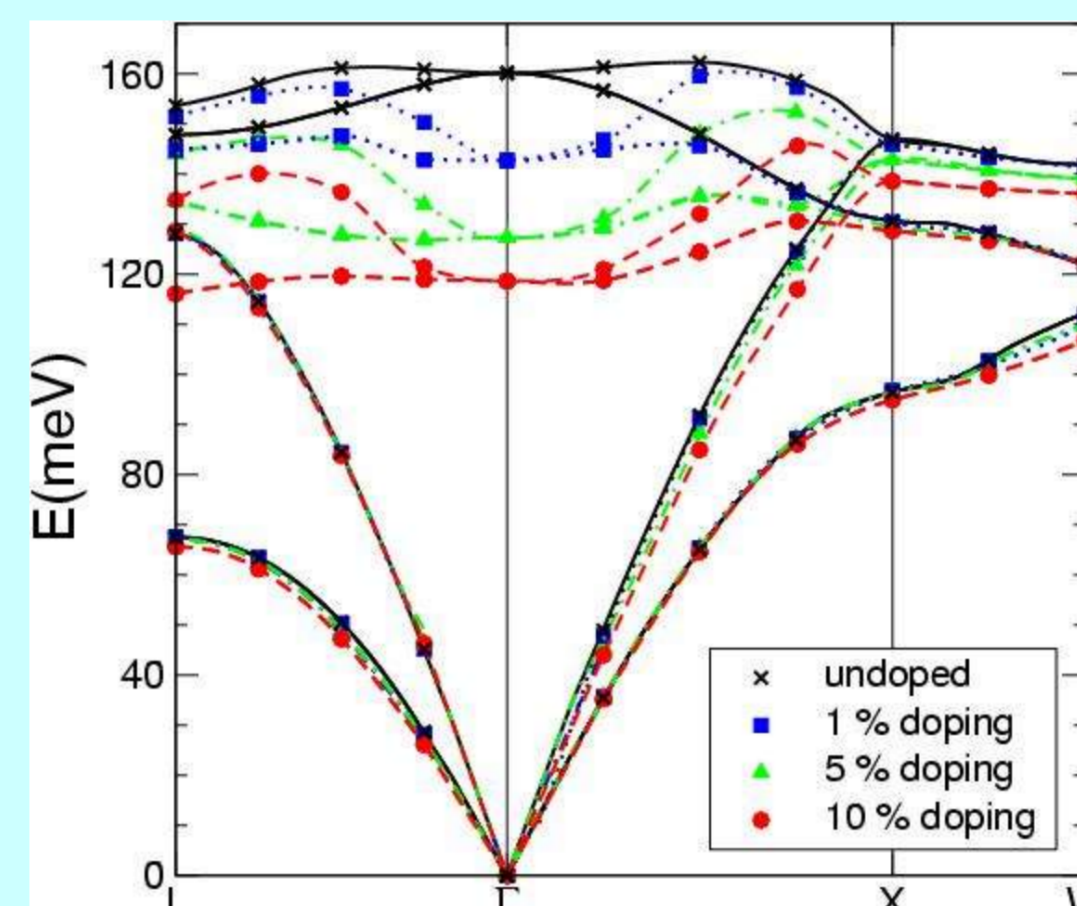


Pure diamond: Four sp^3 hybrids/C atom form 4 bonding (valence) and 4 antibonding (conduction) bands with a 5.5 eV band gap.

The top of the valence band at Γ is a triply degenerate σ band.

Hole doping (VCA): The overall shape is unchanged; E_g is driven into the valence band; the charge carriers are σ holes (MgB₂).

Phonon Dispersions:



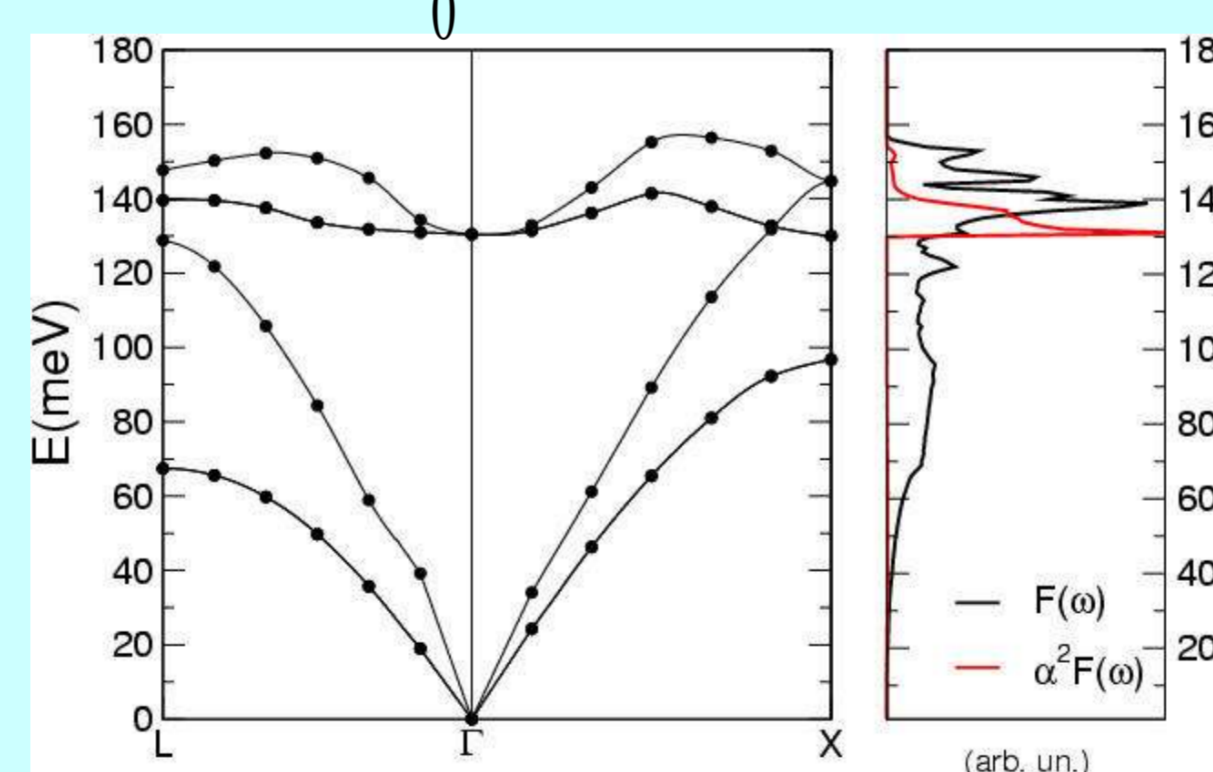
Pure diamond: 6 branches; high optical frequencies $\sim 160\text{ meV}$; stiff σ bonds!

Hole doping (VCA): The triply-degenerate zone-center phonon is softened (MgB₂) [3]. The amount of softening increases with doping:

Strong e-ph Coupling.

Electron-Phonon Coupling:

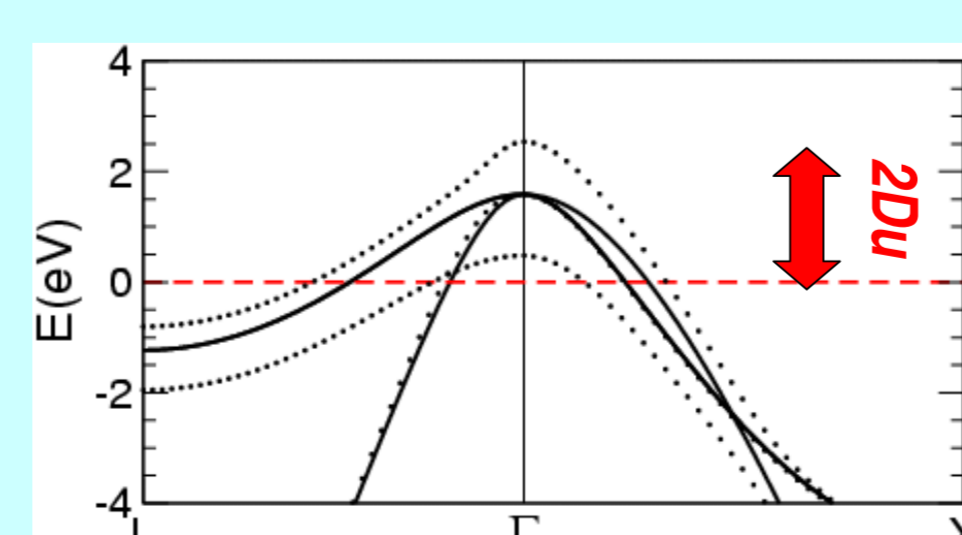
$$\lambda = 2 \int_0^{\infty} d\omega \alpha^2 F(\omega) / \omega$$



$$\alpha^2 F(\omega) = \frac{1}{N(E_F)} \sum_{k,k',ij,\nu} |g_{k,k'}^{ij,\nu}|^2 \delta(\epsilon_k^i) \delta(\epsilon_{k'}^j) \delta(\omega - \omega_{k-k'}^\nu)$$

$\alpha^2 F(\omega)$ does not follow $F(\omega)$: the coupling is concentrated in the zone-center optical bond-stretching modes (MgB₂).

Deformation Potential: The holes at the top of the σ bands couple strongly to the optical bond-stretching mode: phonon vibrations have a big effect on the Fermi surface... (MgB₂).



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

Softening of the phonon frequencies: Only

two out of the three σ are effective in screening the phonon perturbation...

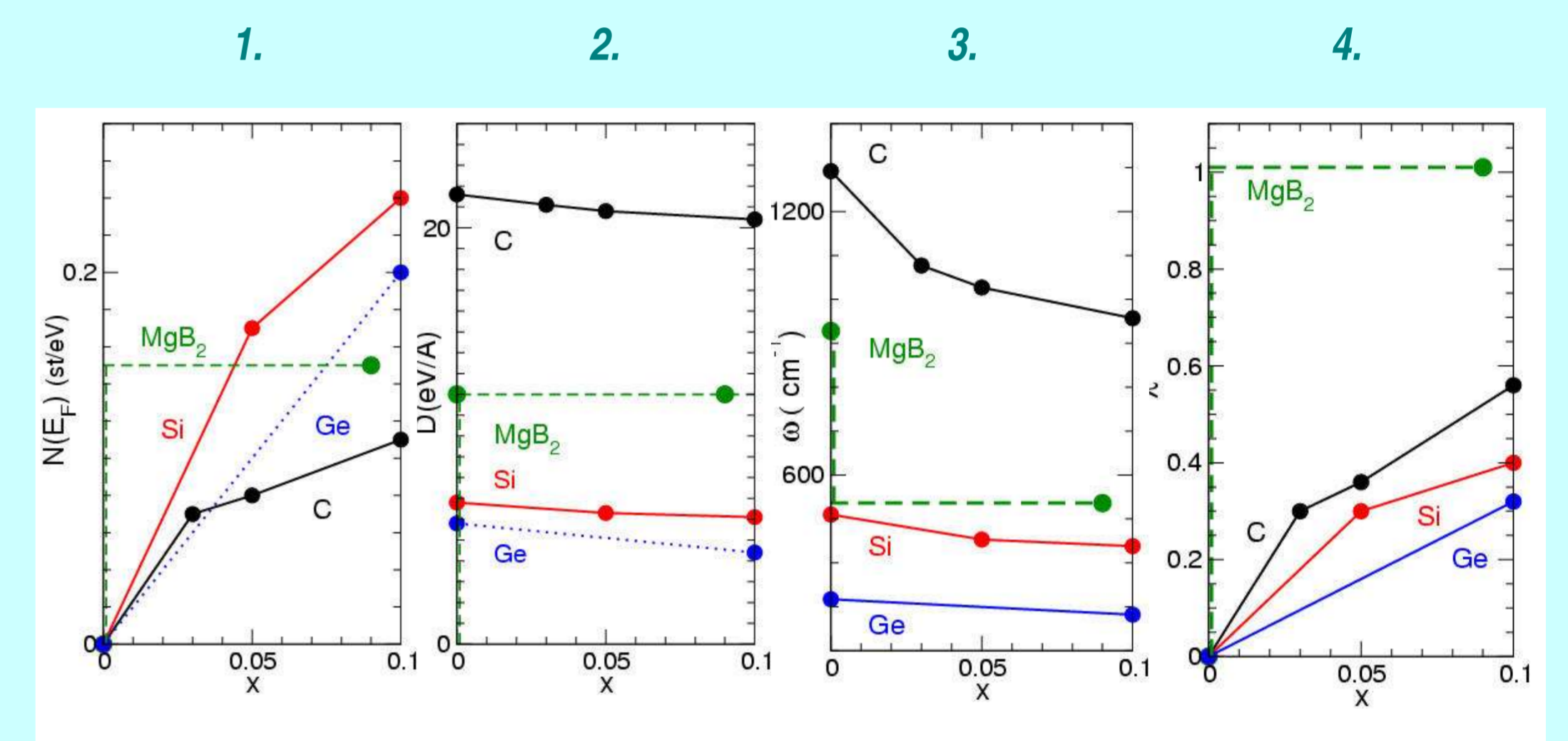
$$\omega^2 = \frac{\omega_0^2}{1 + 2\left(\frac{2}{3}\right)\lambda}$$

What determines the T_c ?

Superconductivity in MgB₂ and hole-doped diamond (and eventually in Si and Ge) is driven by strong e-ph coupling between σ holes and bond-stretching phonons of the same symmetry as the electronic states.

What are the materials dependencies?

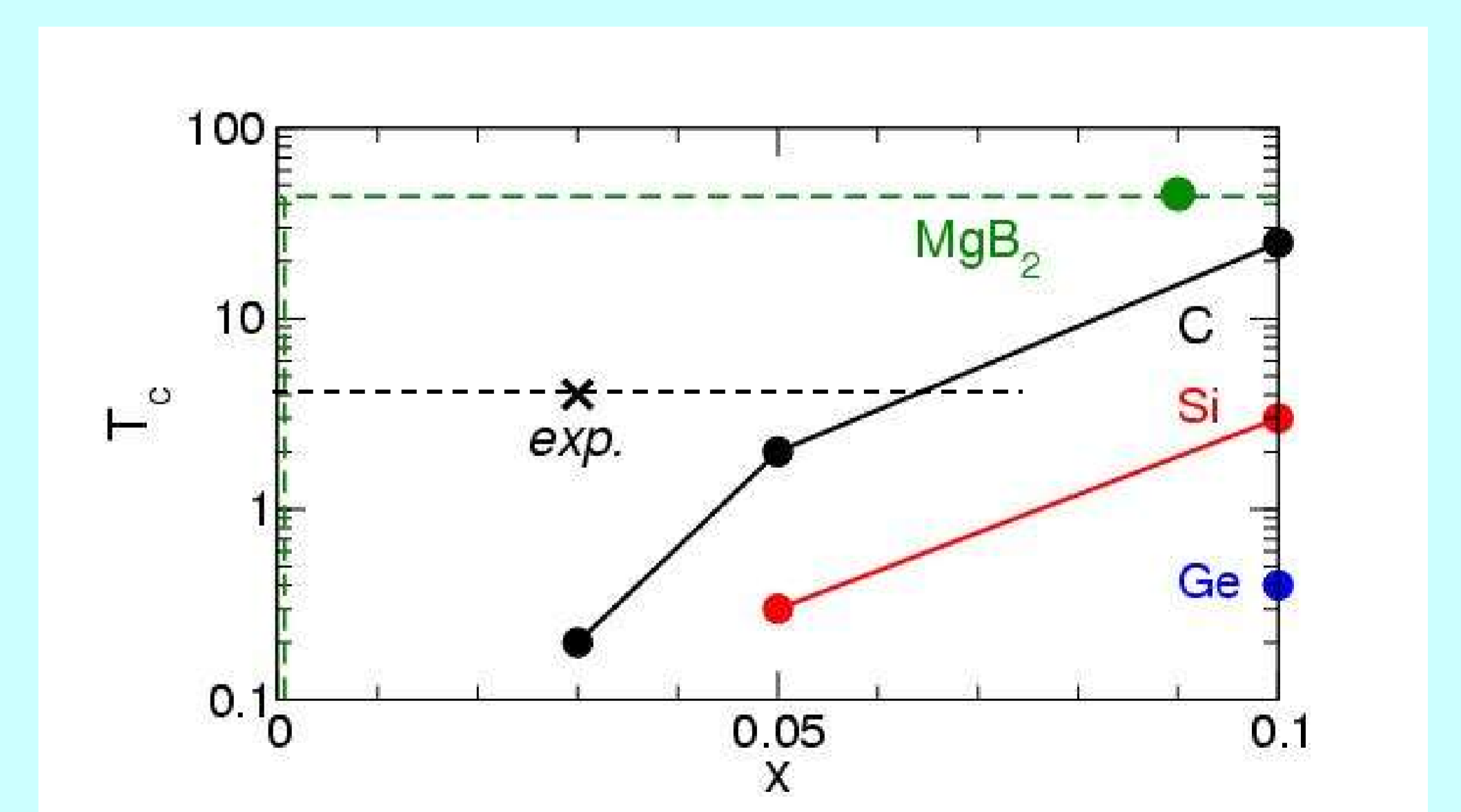
$$\lambda = \frac{N(E_F) D^2}{M\omega^2}$$



1. $N(E_F) \sim \chi^{2/3}$ in 3D (C, Si, Ge); $N(E_F) = \text{const.}$ in 2D (MgB₂).
2. D is much larger in diamond and MgB₂ (stiff bonds) than in Si and Ge.
3. Softening due to e-ph interaction is more pronounced in 2D (MgB₂) than in 3D.
4. The maximum λ in hole-doped diamond ($\chi=0.1$) is half than that of MgB₂.

Critical Temperatures:

$$T_c \propto \omega \exp\left(-\frac{1+\lambda}{\lambda - \mu^*(1+\lambda)}\right)$$



Electron-phonon coupling is the most likely mechanism for superconductivity in hole-doped diamond!

T_c increases with doping [4], however the increase will be limited due to problems related to stability of the material.

L.Boeri, J. Kortus, O.K. Andersen, Cond-Mat 040447, to appear in Phys. Rev. Lett. (2004).

[1] Ekimov et al., Nature 428, 524 (2004).

[2] S. Savrasov, Phys Rev. B 54, 16470 (1996).

[3] S. Sidorov et al., cond-mat 0409624 (2004).

[4] E. Bustarret et al., cond-mat 0408517 (2004).