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

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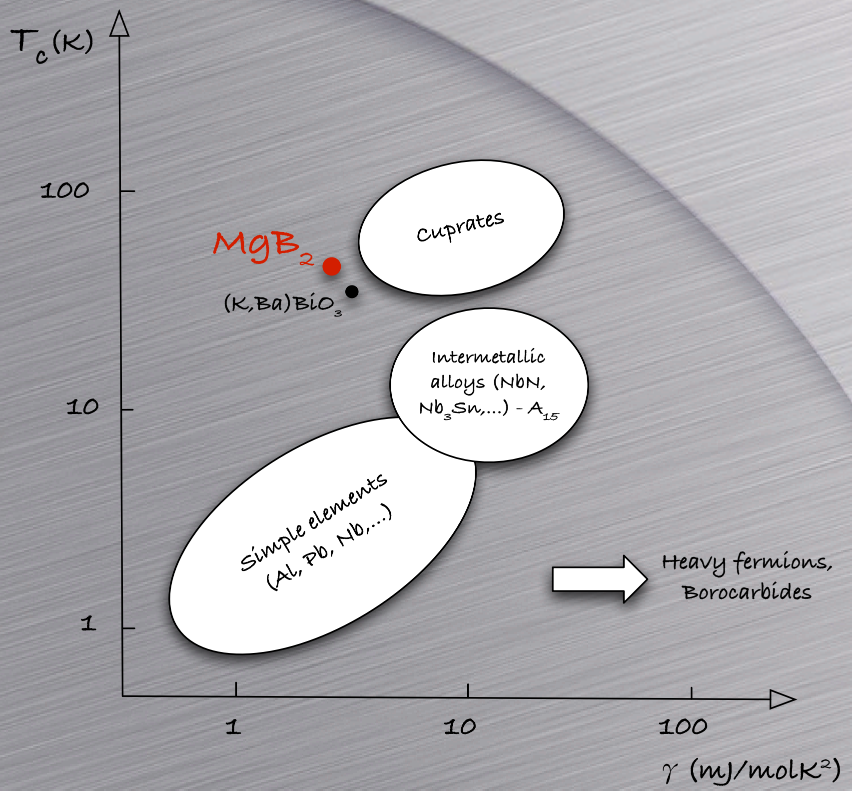
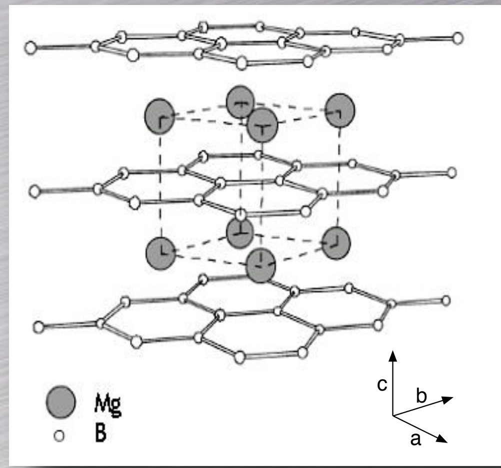
MgB_2 : a new "high T_c" superconductor

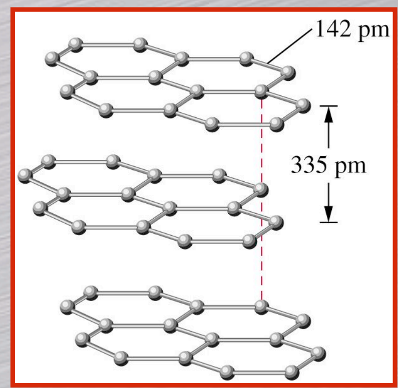
$T_c \sim 40K$





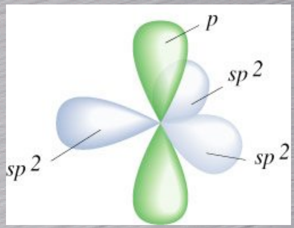
hexagonal structure

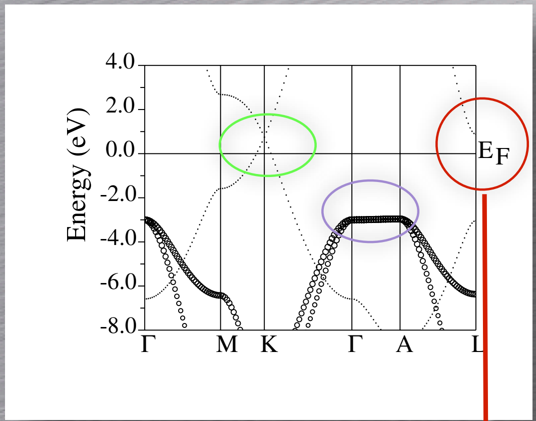
B planes similar to C planes in graphite



2 kinds of electronic orbitals derived from

- in plane sp_2-boron orbitals : σ bands
- p_z boron orbitals : π bands



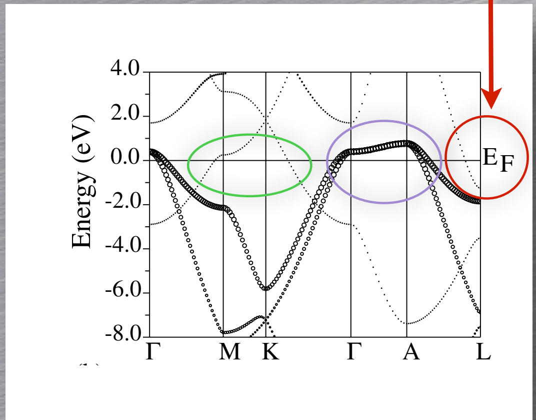


"same" electronic structure than in Graphite

in which the σ bands are full

(involved in covalent bounds)

→ π band : small e/hole pockets close to the K point



in MgB_2 the "second" π band is lowered

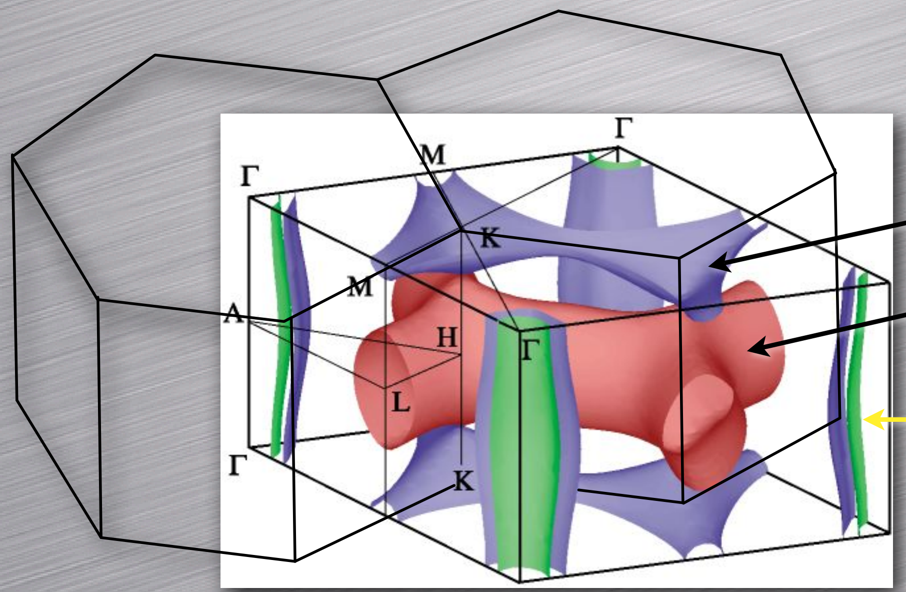
by attractive Mg^{2+} potential

charge transfert from σ to π bands

→ unfilled σ bands

"2" Fermi surface sheets

actually 2x π (3D) and 2x σ (quasi-2D) bands



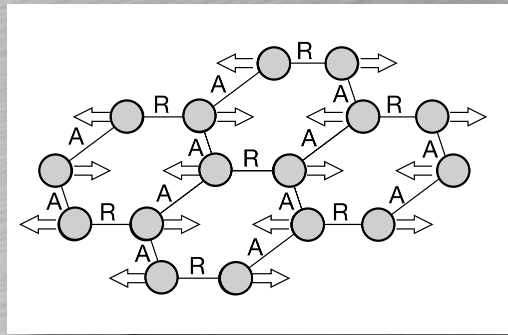
the quasi 2D characters leads to a "large" DOS ~ 0.30 st/eV.cell

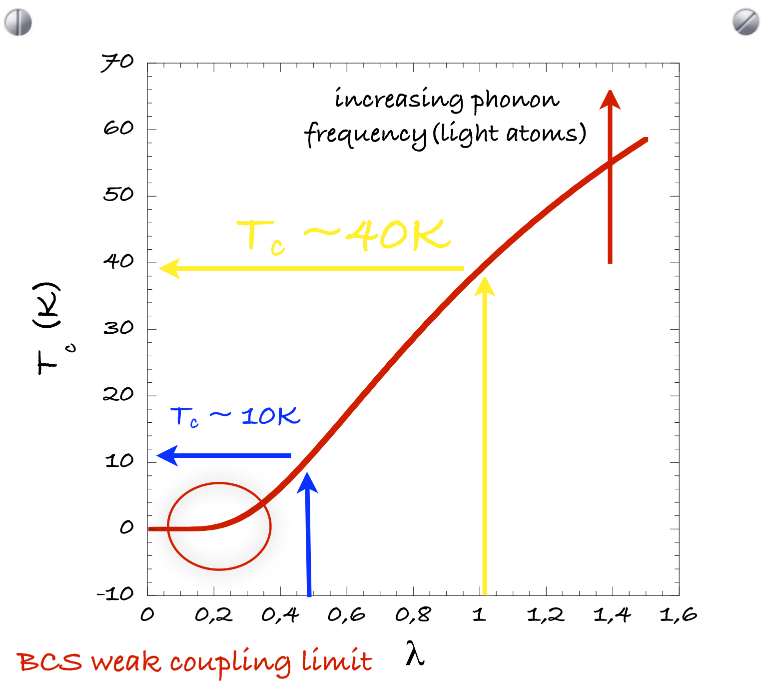
(close to the 2D value $m^* a^2 / \pi \hbar^2 \sim 0.33$ st/eV.Cell)

despite the small hole doping level ~ 0.07 hole/B

strong coupling of σ electrons with E_{2g} vibration mode
+ large DOS
-> electron-phonon coupling constant $\lambda \sim 1.0$

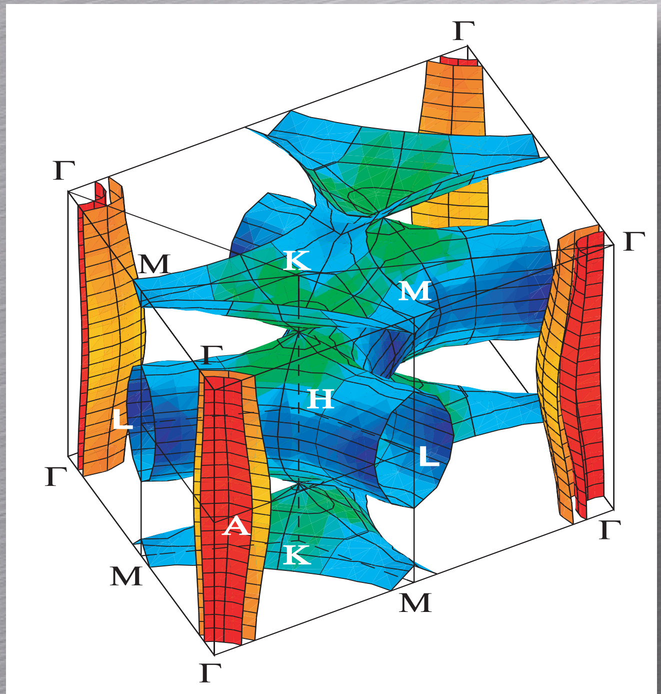
despite a larger DOS (~0.4st/eV.cell)
the coupling is much worse in the π band ; $\lambda \sim 0.45$



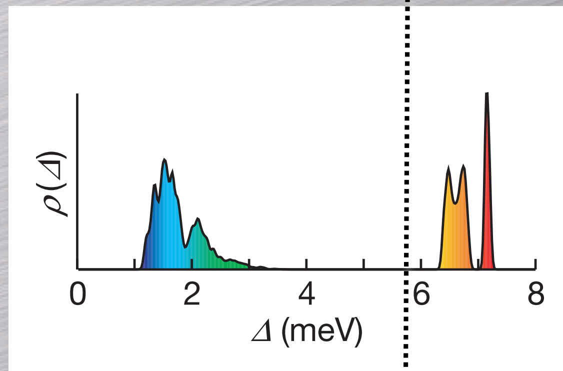


Mac-Millan expansion
screening coefficient : 0.15
ω = 540K

Two co-existing superconductors ????

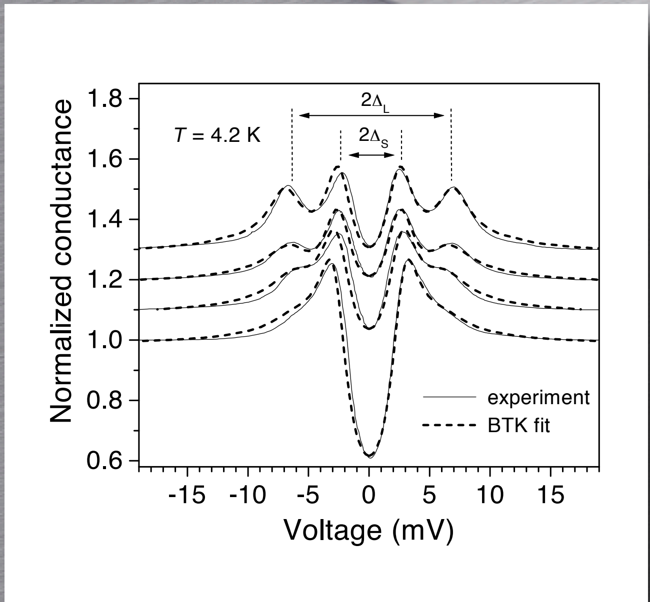


2 SF sheets → 2 gaps



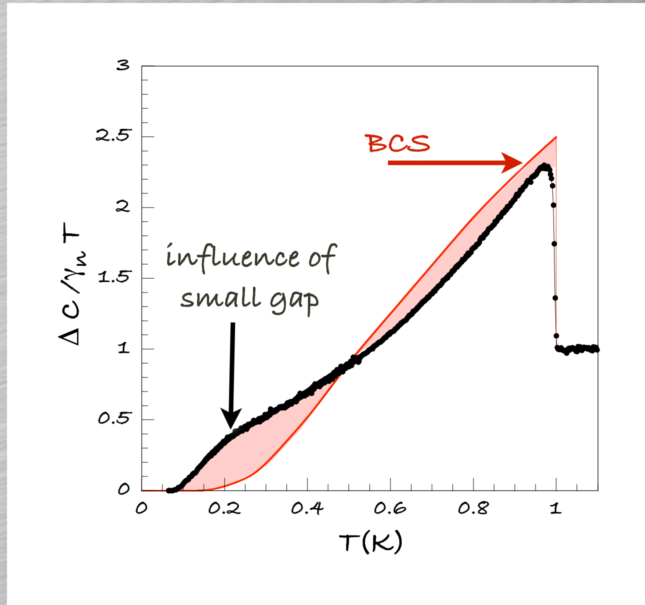
BCS value

point contact spectroscopy



P.Szabo et al. PRL 01

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

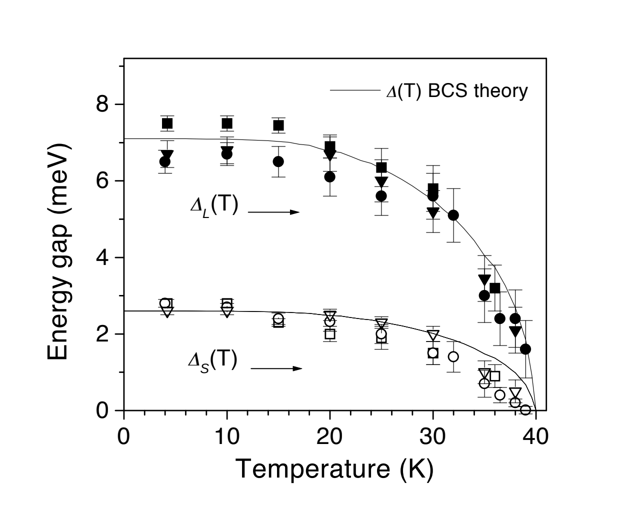


see also F.Bouquet et al. EPL 01

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

2 gaps => 2 T_c values ???

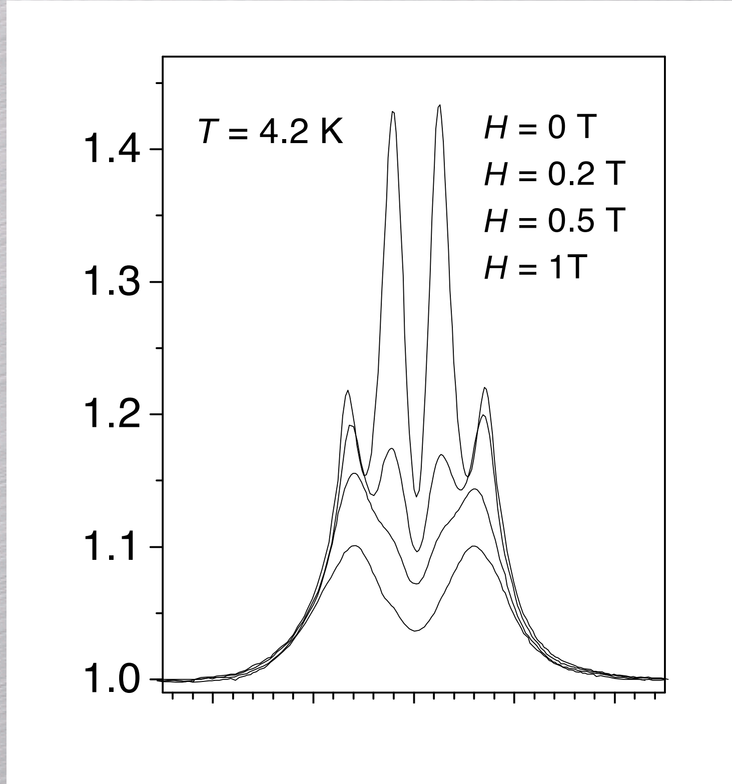
but present different field dependences



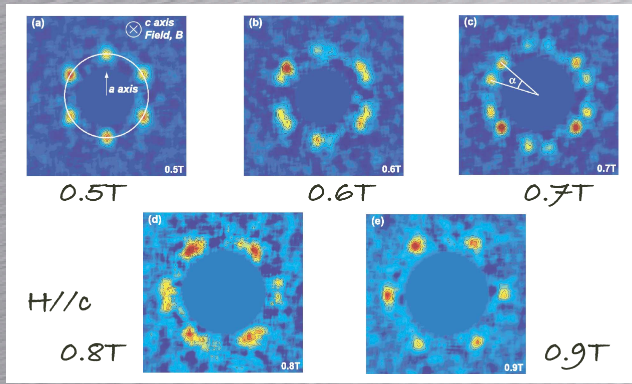
both gaps are closing at the same T_c
=> weakly coupled bands

zero coupling
=> 2 T_c's

strong coupling
=> FS averaged
λ value (~0.7)
=> T_c ~20K

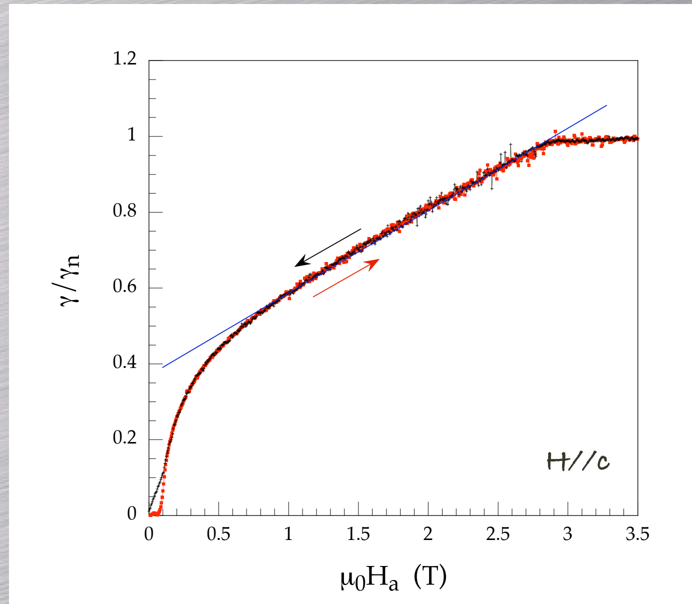


the small gap is very sensitive to H i.e. "disappears" around 1T and the vortex lattice rotates by 30°



SANS measurements R.Cubitt et al. PRL 03

+ anomalous field dependence of γ



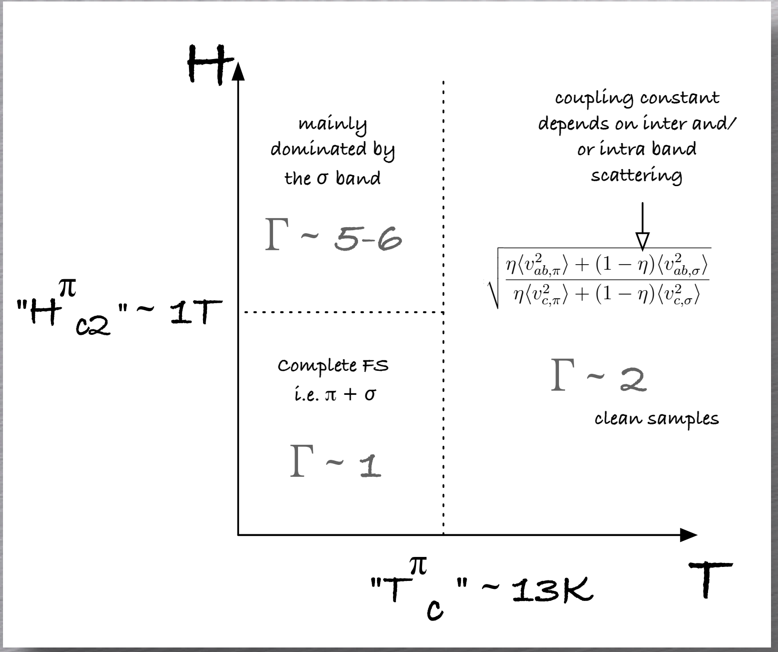
see also F.Bouquet et al. PRL 02

Should the system be described by two ξ and two λ 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

$$\Gamma = \frac{< m^*_{ab} >_{FS}}{< m^*_c >_{FS}} = \sqrt{\frac{< v^2_{F,c} >_{FS}}{< v^2_{F,ab} >_{FS}}} = \frac{\lambda_c}{\lambda_{ab}} = \frac{\xi_{ab}}{\xi_c}$$

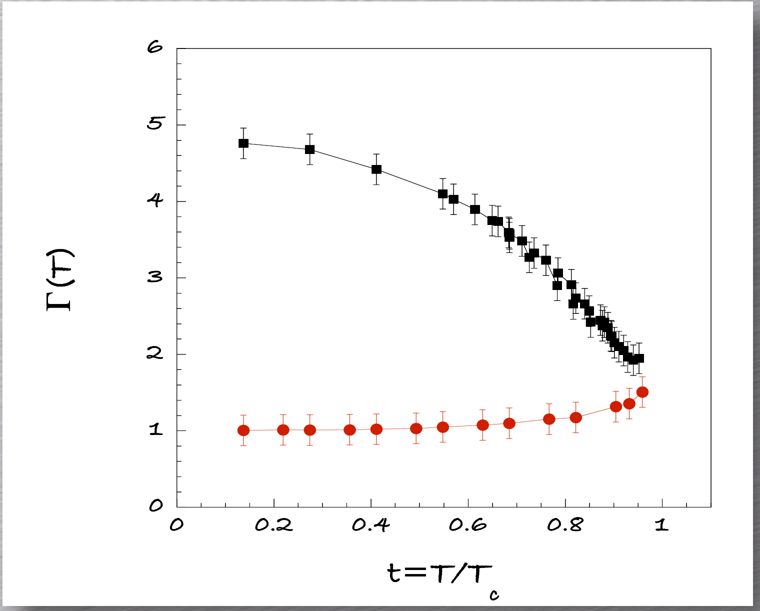
Which Fermi Surface should we take into account ???



How can we get Γ ???

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.....

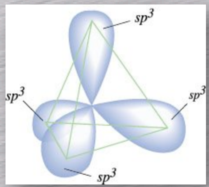
doping by intercalation (Na,...) leads to superconductivity : $T_c \sim 5K$

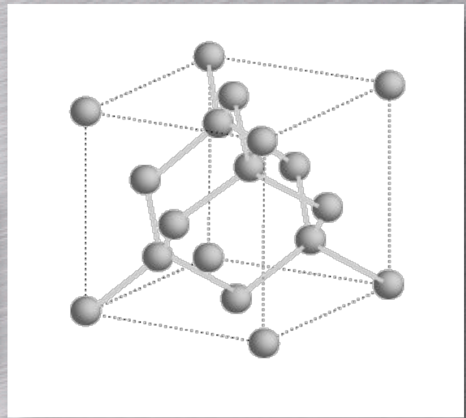
but superconductivity remains in the "soft" π band

(similar to alkali doped fullerides)

DIAMOND

very "strong" σ bounds





but 3D (sp3)....

Superconductivity ($T_c \sim 7K$) 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 λ ???

FS averaged e-ion matrix element

$\pm uI$: splitting of the top of the valence band for the "appropriate" displacement u

DOS st/eV.spin."2 atoms-cell"

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

"appropriately defined" mean square frequency

	N	I (eV/A)	$\omega(cm^{-1})$	$I^2/M\omega^2$	λ
MgB_2	0.15	12	540	6.7	1.0
C-B3%	0.06±0.01	24±3	1080	7.5±0.8	0.45±0.1

2x the already large MgB_2 value

1/2 of MgB_2 value to smaller DOS (3D)

	method	model	B/C at.%	n_B 10^{20} cm^{-3}	e$^-$/ph coupling λ	T_c (K)	Remark
Boeri et al PRL 93, 237002	First Principles LMTO	VCA Virtual crystal	3	50	0.37	0.2	T_c = 25 K for 10 at%
Lee et al PRL 93, 237003	First principles APW-CPA	VCA Virtual crystal	2.5	44	0.53	9	E_F at VBM^u–0.6eV
Xiang et al Cond-mat 0406446	First principles supercell DFT-LDA	$C_{35}B$	2.8	49	0.39	4.4	B modes contribute to e$^-$/ph coupling
Blase et al PRL 93, 237004	Ab initio Supercell DFT-LDA	$C_{53}B$	1.85	33	0.43	4	« Local » C-B modes couple with free carriers E_F at -0.52eV

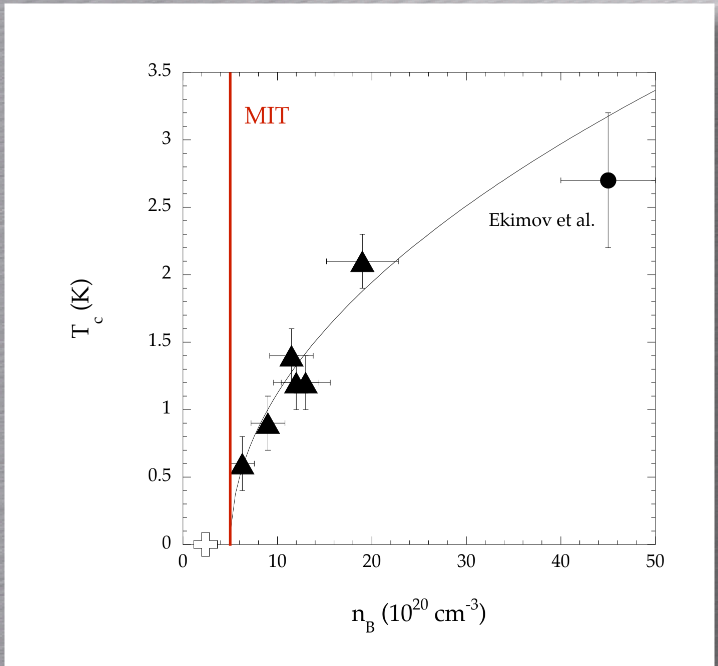
phonon modes involved in e/ph coupling not clearly identified

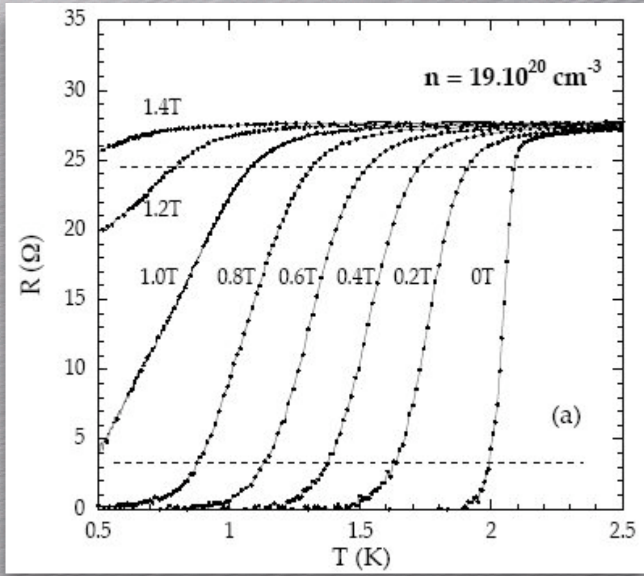
Ekimov et al. Nature 04

- Polycrystalline diamond (HPHT bulk)
- Doping level : 10^{21} B/cm^3 : $T_c \sim 3K$

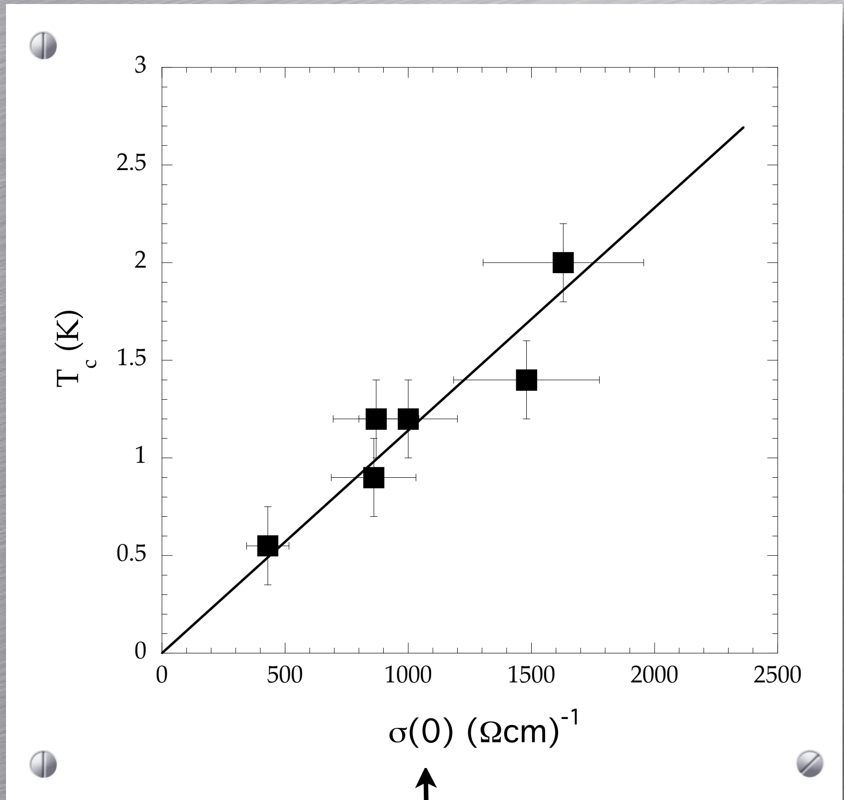
confirmed on homoepitaxial films

E.Bustarret 04





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



normal state conductivity extrapolated to zero

$T_c \sim \sigma(0)$???

enhanced superconductivity due to reduced screening close to the MIT ???

Soulen - Osofsky et al.

Hole doping of the σ bands leads to very efficient electron-phonon interaction potentiel

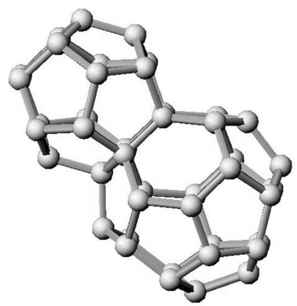
+ large DOS due to 2D character (sp2) in MgB_2 => $T_c \sim 40K$

superconducting is also "induced" in the π band -> two gap superconductivity

anomalous field and temperature dependence of the superconducting properties

can explain the onset of superconductivity in B-dopecd diamond in, which "reduced" DOS => $T_c \sim$ a few K

superconductivity appears in the vicinity of a MIT



large T_c values predicted in C clathrates ($X_8@C_{46}$)

$\lambda \sim 1.4$ & $\omega \sim 1500K$

=> T_c between 50

and ...150K !!!

(depending on screening coefficient)

Connetable et al. 2003