Ordered Supercell & Virtual Crystal approximation : On Heavy Carbon Doping of MgB₂

Deepa Kasinathan, Kwan-Woo Lee, Warren E. Pickett Dept. of Physics. University of California - Davis

Experimental Facts :

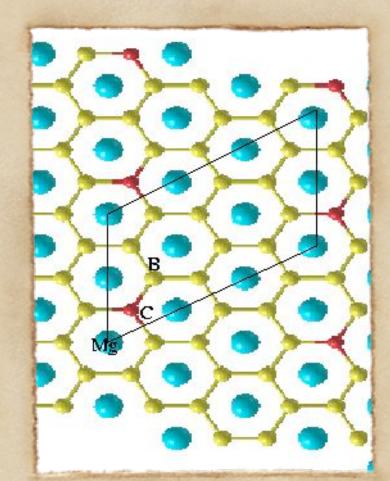
- MgB₂ a real possibility for a high field conductor, due to high parallel and perpendicular critical fields
- Mg_{1-y}Al_yB₂ ---> upto y = 0.10 T_c decreases
 smoothly ; 0.10 < y < 0.25 two phase behavior;
 y = 0.25 back to single phase with vanishing T
- Carbon doped MgB₂ highly mixed phase;
 miscibility of C really small; dT_c /dx = 1 K/%C
- Substituional C doping upto 10% still retains the two-band superconductivity

Calculational Method :

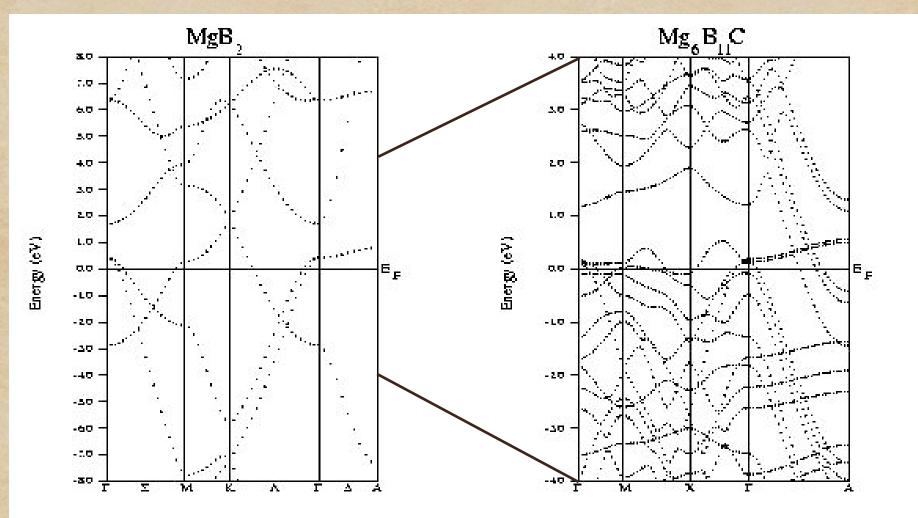
- Full-potential LAPW code WIEN2K
 P.Blaha, K.Schwarz, G.K.H.Madsen, D.Kvasnicka,
 J.Luitz, J.Phys. Chem. Sol. 63, 2201 (2002)
- Exchange-correlation potential approximated using GGA
- RK_{max} = 7.00 (good for s-p electron systems)
- k-mesh : 432 irreducible k points
- Lattice parameters Avdeev et al. (both supercell and virtual crystal)

Ordered $Mg(B_{1-x}C_x)_2$, x = 0.0833

- Maximum separation of C atoms – supercell Mg₆B₁₁C
- B₁₁C layer is 2 ×3
 times that of MgB₂
- a = 9.16 A^o, b = 6.11A^o
 c = 3.525 A^o
- Carbon has 3 first, 5 second & 3 third N.N B atoms

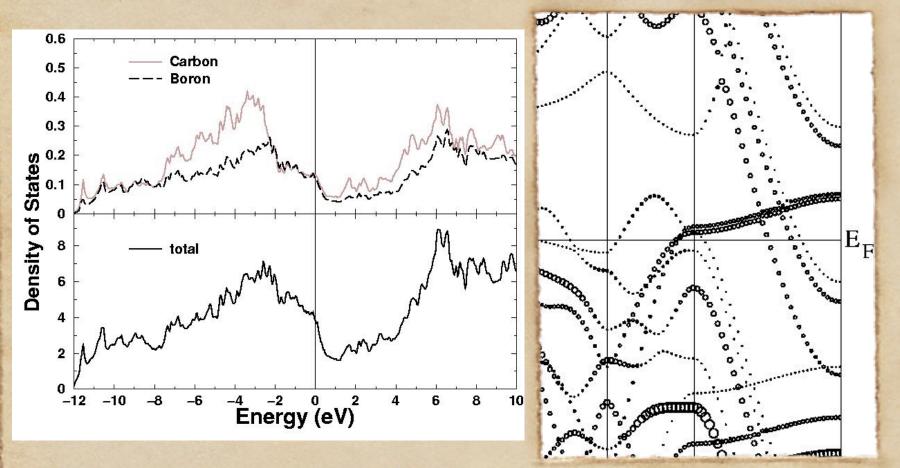


Bandstructure

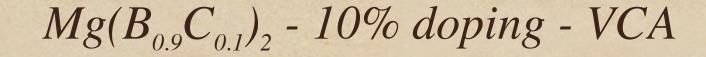


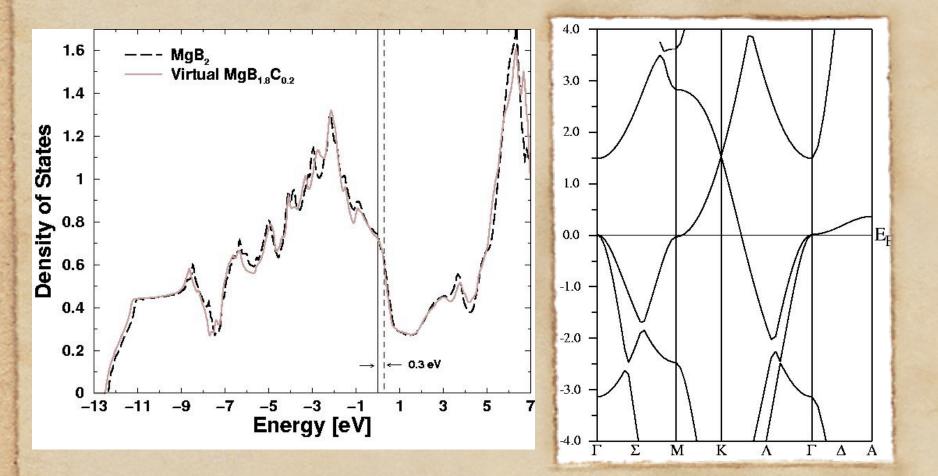
C doping - Degenerate σ bands split by 60 meV along Γ - A

Projected DOS & Bandstructure



C potential – pulls down the lower split band Energy scale for σ -band broadening $\Upsilon_{o} \approx 7$ meV /% C Charge transfer for 0.095e⁻ to C from the 3 first N.N B's





1% increase in occupied bandwidth; Fermi level raised by 0.3eV. Both cylindrical Fermi surfaces have shrunk to a point at Γ.

σ Hole Concentration

	No. of holes (holes/cell)
MgB ₂	0.11
8.33% doping Mg ₆ B ₁₁ C supercell	0.070
10% doping MgB _{1.8} C _{0.2} Virtual crystal	0.0463
8.33% doping MgB _{1.833} C _{0.167} extrapolation	0.057

Fermi surfaces are still intact – consistent with two-band superconductivity and substantial T_c observed in expts.

Virtual Crystal : Carbon = Boron + e ! Not very reliable.