Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Anisotropy breaking and superconductivity in MgB_2 SABINA RUIZ, PABLO DE LA MORA, Facultad de Ciencias, UNAM, Mexico, D.F. — When magnesium is replaced by aluminium an extra 3p electron is added to the system, this 3p-electron perturbs the σ-band structure slightly, while the replacement of magnesium by scandium a 3d electron is added, this 3d electron has a large effect on the electronic structure. With aluminium replacement T_c diminishes almost linearly and disappears at $\sim$0.53Al this corresponds to the point where the Fermi level fills up the σ-bands. The electrical conductivity in the direction of the plane due to the σ-bands (σ_a^σ) diminishes with a very similar trend. In this case these bands electrical anisotropy (a-direction vs. c-direction, $\sigma_a^\sigma/\sigma_c^\sigma$) also diminishes. On the other hand, in ScB_2 the σ-bands lose their electrical anisotropy ($\sigma_a^\sigma/\sigma_c^\sigma \approx$3.9), but the addition of an extra 3d electron does not raise the Fermi level above the σ-bands. Our results show that at first the anisotropy diminishes with scandium addition until $\sim$0.3Sc and then it remains almost constant, this shows a interesting parallelism with the T_c-experimental results of Agrestini et al. (2004 J. Phys. and Chem. Sol. 64, 1479), in which T_c diminishes with scandium and disappears at 0.3Sc.

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Date submitted: 30 Nov 2004 Electronic form version 1.4