Anisotropy breaking and superconductivity in MgB₂

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 $\sigma$-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 $\sim 0.53\text{Al}$ this corresponds to the point where the Fermi level fills up the $\sigma$-bands. The electrical conductivity in the direction of the plane due to the $\sigma$-bands ($\sigma^\sigma_a$) diminishes with a very similar trend. In this case these bands electrical anisotropy (a-direction vs. c-direction, $\sigma^\sigma_a/\sigma^\sigma_c$) also diminishes. On the other hand, in ScB₂ the $\sigma$-bands lose their electrical anisotropy ($\sigma^\sigma_a/\sigma^\sigma_c \approx 3.9$), but the addition of an extra 3d electron does not raise the Fermi level above the $\sigma$-bands. Our results show that at first the anisotropy diminishes with scandium addition until $\sim 0.3\text{Sc}$ and then it remains almost constant, this shows an 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 $0.3\text{Sc}$.