Observation of Non-Rigid-Band Alloying of Al- and C-doped MgB$_2$ by Electron Energy-Loss Spectroscopy

ROBERT Klie, LANCE COOLEY, QIANG LI, ARNOLD MOODENBAUGH, ROBERT SABATINI, ANTONIO ZAMBANO, YIMEI ZHU, Brookhaven National Laboratory — Angular-resolved electron energy loss spectroscopy in a scanning transmission electron microscope was used to study the B K-edge in pure and doped MgB$_2$. We have shown that the p$_{xy}$ states have a high density up to 0.8 eV above the Fermi level before dropping to near zero and then starts to rise again 5 eV above the Fermi level; the density of p$_z$-states changes only very little over the first 10 eV. The incompletely filled p$_{xy}$ states at the Fermi level are believed to play an important role in the superconductivity of MgB$_2$. Samples with carbon substituted for boron display a shift of the B K-edge towards lower energy but leave the pre-peak structure undisturbed, thus suggesting that carbon’s extra electron enters mainly the $\sigma$ band and has little effect on the $\pi$-band states. Samples with aluminum substituted for magnesium display dramatic changes in the B K-edge pre-peak, which implies that the Mg site dopant contribute strongly to $\pi$-band states and only weakly to the $\sigma$-band states. These site-specific changes in local density of states are discussed in terms of intra- and interband scattering scenarios.

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