Abstract Submitted for the MAR06 Meeting of The American Physical Society

Studying the electronic structure in pure and electron doped  $MgB_2^1$  Y. ZHU, R.F. KLIE, L. WU, J.C. ZHENG, Center for Functional Nanomaterials, L.D. COOLEY, Dept. Cond. Matt. Phys. & Mat.Sci., Brookhaven National Lab — We use high-energy electrons to reveal electronic structure information to understand the effects of electron doping in MgB<sub>2</sub> superconductors. Angle-resolved electron energy-loss spectroscopy was used to investigate the difference in the excited states, while image-coupled quantitative electron diffraction was used to map the valence electron distribution, in pure and Al-doped  $MgB_2$ . The results were compared with density functional theory calculations. We found significant changes in the B K-edge fine structure as a function of electron doping concentration, suggesting the corresponding  $\sigma$  and  $\pi$  bands are being filled simultaneously. The filling of the  $\sigma$ -band states near the Fermi level reduces the critical temperature T<sub>c</sub> of highly doped MgB<sub>2</sub> to a level comparable to that of other  $\pi$ -band superconductors such as intercalated graphite. Valence electron maps reveal that electron doping causes considerable charge transfer and accumulation in charge density between both Al-B and B-B bonds. This results in a shortened c-axis of the unit cell and higher phonon frequency, which eventually quenches superconductivity altogether. The relationship between charge transfer and inter-band scattering are also examined.

<sup>1</sup>Work supported by the U.S. Department of Energy under contract DE-AC02-98CH10886

Y. Zhu

Date submitted: 03 Dec 2005

Electronic form version 1.4