Bonding changes in compressed superhard graphite

MAO W. L., MAO H. K.^{*}, ENG P.¹, KAO C. C.², SHU J. F.^{*}, HEMLEY R. J.^{*}

Los Alamos National Lab ^{*}Geophysical Lab ¹University of Chicago ²Brookhaven National Lab

Inelastic x-ray scattering spectroscopy (IXSS) or x-ray Raman was used to study the near K-edge structure of carbon at high pressure. IXSS reveals that at approximately 17 GPa, half of the π -bonds between graphite layers convert to σ -bonds while the other half remain as π -bonds in the high-pressure form. The x-ray diffraction pattern of the high-pressure form is consistent with a distorted graphite structure in which bridging carbon atoms between graphite layers pair and form σ -bonds, while the non-bridging carbon atoms remain unpaired with π -bonds. The high-pressure form is superhard, capable of indenting cubic diamond single crystals with potential materials science application. The resulting work finally solved the mystery of what happens to cold-compressed graphite, a problem that had puzzled scientists for nearly four decades, and demonstrates the potential for studying the near K-edge structure of low-Z materials at extreme conditions.