Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Pressure-Constrained Deformation and Superior Strength: Compressed Graphite versus Diamond[1] YI ZHANG, CHANGFENG CHEN, Department of Physics and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, WEI ZHOU, HONG SUN, Department of Physics, Shanghai Jiao Tong University, China — The discoveries of compressed carbon phases and their ability to crack diamond anvil have generated great interest in the mechanical properties of carbon allotropes under high pressure. Significant progress has been made recently in structural identification of compressed graphite; however, its surprisingly high strength approaching or exceeding that of diamond remains unexplained. Here we explore this novel phenomenon and show by first-principles calculations that high-pressure confinement suppresses usual ambient or low-pressure deformation modes toward low-density carbon allotropes, and promotes alternative mechanisms for structural evolution leading to high-density compressed graphite phases that exhibit superior strength surpassing that of diamond. This finding explains the puzzling experimental observation and suggests new principles for structural deformation under high-pressure confinement. It also imposes stringent tests on widely used empirical hardness formulas that are unable to account for changes in pressure-constrained structural evolution and their influence on material strength.

[1]This work was supported by DOE Grant No. DE-FC52-06NA26274 at UNLV and NNSF of China Grant No.11174200 at SJTU.

Yi Zhang
Department of Physics and High Pressure Science and
Engineering Center, University of Nevada, Las Vegas

Date submitted: 05 Nov 2012 Electronic form version 1.4