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First-Principles Theoretical Analysis of Carbon Allotropes and Nanostructures TEJINDER SINGH, University of Massachusetts, Amherst, MICHAEL J. BEHR, ERAY S. AYDIL, University of Minnesota, Minneapolis, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We analyze the various crystalline phases of C observed upon exposing carbon nanotubes to H2 plasmas, which produces an amorphous carbon matrix with carbon nanocrystalls embedded in it. Structural characterization with electron diffraction and high-resolution TEM yields three distinct crystalline phases of C consistent with a fcc lattice with lattice parameter a = 4.25 Å, a bcc lattice with a = 3.0 Å, and a diamond lattice with a = 3.57 Å. Using first-principles density functional theory (DFT) calculations, we have analyzed the structure of several allotropes of pure carbon and we discuss our results in the context of the experimental findings. In addition, we consider the possibility of H incorporation in these C phases. According to our DFT calculations, incorporation at proper concentrations of H in interstitial sites of cubic phases of C provides interpretations for the experimentally observed crystalline C phases.

Tejinder Singh
University of Massachusetts, Amherst

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