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Atomic-scale Analysis of the Interactions Between Atomic Hydrogen and Multi-walled Carbon Nanotubes ANDRE R. MUNIZ, TEJINDER SINGH, DIMITRIOS MAROUDAS, University of Massachusetts at Amherst — We present a detailed atomic-scale analysis of the interactions of atomic hydrogen with the internal layers of multi-walled carbon nanotubes (MWCNTs). The analysis is based on a synergistic combination of classical molecular dynamics (MD) with first-principles density functional theory (DFT). The Adaptive Interatomic Reactive Empirical Bond Order (AIREBO) potential is employed in the MD simulations of H-MWCNT interactions and the resulting structural relaxations. Parameters that have been varied in our analysis include nanotube diameters, number of nanotube walls, inter-wall spacing, and temperature. The MD simulations reveal that, under certain conditions, H chemisorption onto internal MWCNT walls and H diffusion in the space between walls can induce the formation of inter-shell sp^3 C-C bonds. The MD mechanisms are in good agreement with our DFT calculations of optimal pathways of C-C bond formation and provide interpretations for the formation of nanocrystalline carbon, which has been observed experimentally upon H_2 plasma exposure of MWCNTs.

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