MAR05-2004-000439

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Optimization of the Properties of Carbon Nanotube-Based Structures by Electron and Ion Beam Irradiation[1]

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There is considerable interest in building new nanostructures for electronic devices and incorporating nanostructured fibers and particles into composites. Here, classical molecular dynamics simulations are used to study the production of new carbon nanotube junctions or cross-links through electron irradiation, in addition to the chemical modification of carbon nanotube-based structures and composites through ion and polyatomic ion beam deposition. In particular, electron irradiation is used to produce junctions between carbon nanotubes. The specific reactions that lead to junction-formation and the mechanical and electronic properties of the resulting junctions will be discussed. Additionally, the chemical modification of multi-walled nanotubes, single-walled and multi-walled nanotube bundles, nanopeapods, and nanotube-polymer composites from polyatomic fluorocarbon ions, which are commonly present in low-energy fluorocarbon plasmas, and Ar will be presented. Multi-walled carbon nanotubes usually fail through the so-called "sword-and-sheath" mechanism and nanotube-polymer composites often fail through nanotube pullout. In both cases the failure mechanism is due to the weak van der Waals bonds between either the nanotube shells in the multi-walled tube or between the nanotubes and polymer matrix in the composite. The simulation results show that ion beam deposition produces cross-links between shells in multi-walled nanotubes and between otherwise unfunctionalized nanotubes and polymer backbone chains, which ultimately toughens the composites. The conditions that are predicted to be optimum for effective chemical modification of the system will be discussed.

[1]This work was supported by the National Science Foundation through grant CHE-0200838