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Molecular Dynamics Simulations of Carbon Nanotubes Cross-Bonding by Proton Irradiation

N. J. Lee, C.R. Welch[1]

Summary

Carbon nanotubes have significant potential as the basis for super infrastructure material. The shear modulus of carbon nanotube ensembles is relatively low, comparable to graphite, as the carbon nanotubes interact via weak van der Waals forces. Unmodified, their intermolecular interactions are insufficient to take full advantage of the extraordinarily high strengths predicted for carbon nanotube-based fibers. Thus, a key to their use in high-strength materials is developing strong bonds between these molecules. In this study, we examine the potential development of covalent bonds between carbon nanotube pairs cross-bonded by proton bombardment using molecular dynamics simulation. Covalent bond formation between aligned pairs of carbon nanotubes of the same diameter and helicity is studied as a function of beam intensity, ambient temperature, and exposure time. Calculations are performed using the Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential. We present the simulation results and compare these to recent experimental data.

keywords: Single-walled carbon nanotubes, molecular mechanics, proton bombardment, cross-linking, nanofibers.

[1]U.S. Army Engineer Research and Development Center, Vicksburg, MS, U.S.A