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Simulation of Hydrogenated Boron Nitride Nanotube's Mechanical Properties for Radiation Shielding Applications

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Abstract : Radiation shielding is an obstacle in long duration space exploration. Boron Nitride Nanotubes (BNNTs) have attracted attention as an additive to radiation shielding material due to B10's large neutron capture cross section. The B10 has an effective neutron capture cross section suitable for low energy neutrons ranging from 10-5 to 104 eV and hydrogen is effective at slowing down high energy neutrons. Hydrogenated BNNTs are potentially an ideal nanofiller for radiation shielding composites. We use Molecular Dynamics (MD) Simulation via Material Studios Accelrys 6.0 to model the Young's Modulus of Hydrogenated BNNTs. An extrapolation technique was employed to determine the Young's Modulus due to the deformation of the nanostructure at its theoretical density. A linear regression was used to extrapolate the data to the theoretical density of 2.62g/cm3. Simulation data shows that the hydrogenated BNNTs will experience a 11% decrease in the Young's Modulus for (6,6) BNNTs and 8.5% decrease for (8,8) BNNTs compared to non-hydrogenated BNNT's. Hydrogenated BNNTs are a viable option as a nanofiller for radiation shielding nanocomposite materials for long range and long duration space exploration.

Keywords : boron nitride nanotube, radiation shielding, young modulus, atomistic modeling
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