MECHANICAL PROPERTIES OF NANOTUBES AND CNT/EPOXY COMPOSITES USING MOLECULAR DYNAMICS

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by

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Abstract

This work is divided into two broad sections. In the first section the mechanical properties of Nanotubes(Boron Nitride Nanotubes) are analysed. These BNNTs/CNTs will then be incorporated in a polymer matrix which will be the second part of the thesis.

Firstly, the thermal buckling behavior of pre-compressed Boron-Nitride nanotubes (BNNTs) using molecular dynamics simulations with Tersoff interatomic potential is studied. Critical buckling strains at near zero temperature is evaluated, and subsequently the nanotubes precompressed at a certain fraction of this value followed by temperature ramping. The critical buckling temperature, T_{cr}, is marked by a sudden decrease of the internal force.

In the second study, the length and the temperature dependent sensitivity of pre-compressed armchair Boron-Nitride nanotubes towards their use as sensors is studied. A nanomechanical resonator based sensor works by detecting small changes in the natural frequency of the device in presence of external agents. The vibrational data obtained using molecular dynamics simulations, is analysed for its frequency content through the Fast Fourier transformation. As the temperature of the system rises, the vibrational spectrum becomes noisy, and the modal frequencies show a red-shift irrespective of the length of the nanotube, suggesting that the nanotube based sensors calibrated at a particular temperature may not function desirably at other temperatures. Temperature induced noise become increasingly pronounced with decrease in the length of the nanotube. For the shorter nanotube at higher temperatures, we observe multiple closely spaced peaks near the natural frequency, creating a masking effect and reducing the sensitivity of detection. However, longer nanotubes do not show these spurious frequencies, and are considerably more sensitive than the shorter ones. The effect of precompression is also analyzed.

In the second part of the thesis, the mechanical porperties (elastic constants, fracture properties, thermal conductivities and viscoelastic properties) will be evaluated using molecular dynamics and ab-initio simulations.