TUNING THE PROPERTIES OF CARBON NANOTUBES BY FILLING, ELECTRON IRRADIATION, AND CHEMICAL FUNCTIONALIZATION

Susan B. Sinnott
University of Florida

Classical molecular dynamics simulations with many-body empirical potentials [1] have been used to study the tuning of the properties of carbon nanotubes through chemical functionalization of the sidewalls, electron irradiation, and through filling. First the effect of filling nanotubes with C_{60}, CH_4 or Ne is considered. The simulations predict that the buckling force of filled nanotubes can be larger than that of empty nanotubes, as shown in Fig. 1, and the magnitude of the increase depends on the density of the filling material [2]. An additional important finding is that the buckling force of empty nanotubes depends on temperature. Filling the nanotube disrupts this temperature effect so that it is no longer present in some cases. However, filling the nanotube is not predicted to influence the electronic properties of the nanotube. Important changes to the properties of crossed and aligned nanotubes are predicted from electron irradiation and chemical functionalization through ion beam deposition (see Fig. 2). Both the electron and the ion irradiation is done at relatively low energies of 5 eV for the electrons and 3-80 eV for the ions. Fusing of the nanotubes is predicted in the case of electron irradiation and this process is found to depend on the chirality of the nanotubes [3]. Polyatomic ion beam deposition is predicted to lead to efficient functionalization and cross-linking of crossed nanotubes, as shown in Fig. 3, and nanotubes aligned in a bundle [3-5]. This work illustrates the manner in which the properties of carbon nanotubes can be tuned to meet the requirements of a particular application. The support of the National Science Foundation through grant CHE-0200838 is gratefully acknowledged.

References

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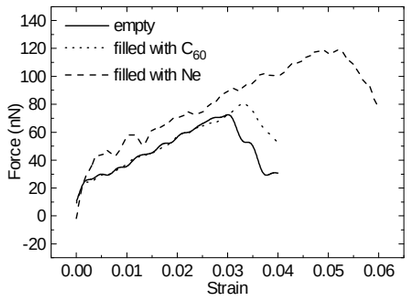

Fig 1: Force curves for compression of empty and filled 20 nm (10,10) nanotubes at 300 K. The data plotted is the average force from five trajectories that has been smoothed for clarity.

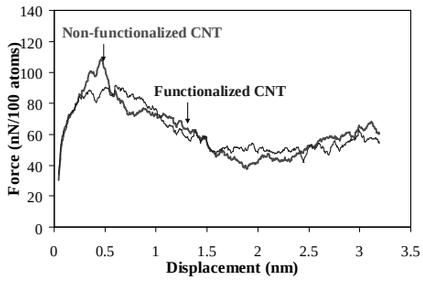

Fig. 2: Comparison of buckling force of functionalized and unfunctionalized (10,10) nanotubes.

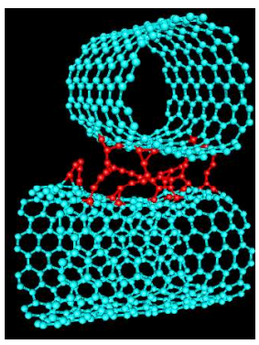

Fig 3: Cross-links formed between two crossed (10,10) nanotubes as the result of ion beam deposition at 3 eV/ion at 300 K.