INFLUENCE OF RANDOM DEFECTS ON THE MECHANICAL BEHAVIOR OF CARBON NANOTUBES THROUGH ATOMISTIC SIMULATION

by

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ABSTRACT

Carbon nanotubes (CNTs) have drawn great interest and shown great promise in recent years in the areas of composite materials, sensors, and small electronic devices owing in a large part to their extraordinary mechanical properties. Yet an enormous scatter is observed in available laboratory results on the stiffness and strength of CNTs. Surface defects including vacancies, pentagon and heptagons have been commonly observed in CNT samples, and are found to have significant influence on the mechanics of CNTs. However, any link between the randomness in CNTs mechanical properties and CNT defects has not been investigated systematically before. Moreover, the fracture of CNTs due to mechanical loading is an important issue likely to affect the durability and reliability of CNT-based materials and devices; yet, based on the author's knowledge, the fracture resistance of CNTs has not been quantified before.

This dissertation, trying to build up these missing links, studies the effects of randomly distributed vacancies and Stone-Wales (SW or 5-7-7-5) defects on the mechanical properties of single-walled nanotubes (SWNTs) using the technique of atomistic simulation (AS), and quantifies the fracture resistance of zigzag SWNTs with fracture mechanics concepts.

Basic principles and key issues of atomistic simulation and multiscale modeling are reviewed. A series of displacement controlled tensile tests of CNTs are modeled with atomistic simulation. Armchair and zigzag SWNTs, with and without defects are studied. A modified Morse potential is adopted to model the interatomic

forces. Time histories of energies, displacements and forces are generated from the simulations, and three mechanical properties – stiffness, ultimate strength and ultimate strain - are further calculated. Effects of loading speed and geometry are discussed. Further details of CNT structure changes, especially the evolution of defects during the loading process are monitored.

In studying the fracture resistance of CNTs, the strain energy release rate, G, is computed through a series of simulated mechanical loading of zigzag SWNTs with preexisting cracks of various lengths. A significant dependence of the critical strain energy release rate, G_c, on crack length, a, is observed: G_c increases with a initially, and tends to reach a constant value as a becomes large. The temperature dependence of G_c is also investigated up to 500K: G_c drops substantially as temperature increases for all tube diameters.

In studying the effects of random defects, proper random field description (homogeneous Poisson field for vacancies, Matern hard-core field for SW defects) are used to model the defects distribution on the finite, cylindrical tube wall. Groups of CNT samples with various mean values of defects are loaded to failure. The statistics of CNT mechanical properties, namely stiffness, ultimate strength and ultimate strain are analyzed for each group. The randomness resulting solely from the initial velocity distribution was rather insignificant at room temperature. The mean values of stiffness, strength and ductility of the tube decreased as the average number of defects increased. The influence of SW defects seems to be more significant than that of vacancies. The zigzag tube was found to be more brittle and show larger c.o.v. (coefficient of variation) in its stiffness and ductility compared with the armchair tube although the strength has roughly the same c.o.v. in either configuration.