ATOMISTIC SIMULATIONS OF SINGLE WALLED CARBON NANOTUBE OSCILLATORS

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Carbon nanotubes (CNT) are thin long tubes made from rolled up single sheets of graphite. They are truly nanometer size in diameter and can be grown in lengths ranging from a few nanometers to hundreds of microns. With respect to conventional NEMS (NanoElectroMechanical Systems), CNTs are extremely light, and have a high Young's Modulus (~1TPa).

Carbon nanotubes have enormous potential for a variety of applications, many still to be explored. Experiments have been conducted in several areas, such as the electrical actuation and detection of the guitar-string-like oscillation modes of doubly clamped nanotube oscillators.

For a typical CNT of 100nm length and 1nm in diameter the total mass is four orders of magnitude smaller than conventional NEMS, hence, assuming all other properties being equal, CNT resonators are expected to reach the ultimate mass sensitivity required for detecting small molecules.

While the wonderful world of the nanoscale can be probed in experiment, it can be observed completely in simulation. Experiments at the nanoscale and especially at an atomistic scale are much harder to carry out than experiments at longer length scales. Simulations at the atomistic or nanoscale are much easier to do than simulations at larger length scales. We present the first, preliminary results of a vibration analysis of the single walled carbon nanotube. We have carried out these Atomistic Simulations using the Brenner-Tersoff potential in order to help in understanding and obtaining insight into the experimental results.

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