Atomistic simulations of single-walled carbon nanotube oscillators

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NEMS

Various Nano-Electro-Mechanical Systems (NEMS) are under study currently in order to realize ultra-sensitive mass resonators, and to achieve the ultimate single molecule detection limit . The detection scheme for mass sensing with a mechanical resonator is achieved by monitoring the resonance frequency of one of the modes. The dependence of the normal mode frequency on the effective mass M allows for sensitive detection of additional mass being adsorbed on the surfaces of the resonator. Ekinci et al [1] recently showed that the sensitivity of such mass sensors depends on the effective mass, quality factor, resonance frequency and measurement averaging time. Typical NEMS are usualy nanomechanical bridges or cantilevers made out of silicon, silicon nitride etc. The change in mass is detected by monitoring the frequency shift as molecules are adsorbed onto the resonators.

TYPICAL NANORESONATOR

The highest measurable mass sensitivity ~ $0.4 \cdot 10^{-21}$ kg is achieved by 10MHz silicon beam (of lengh 4 micrometers) with a qulaity factor of ~ 2,500, M ~ $5 \cdot 10^{-16}$ kg.Recently, the mass of a single DNA molecule ~1600 base pairs ($1.6 \cdot 10^{-21}$ kg) was measured, by a silicon nitride cantilever [2]. The sensitivity required for detecting a single small molecule (~10 atoms) is about 10^{-25} kg, 4 orders of magnitude smaller than the world record. There are technical limitations to manufacturing lighter nanomechanical beams with conventional photo or e-beam lithography techniques, and degradation is expected in the quality factor as the surface-to-volume ratio increases.

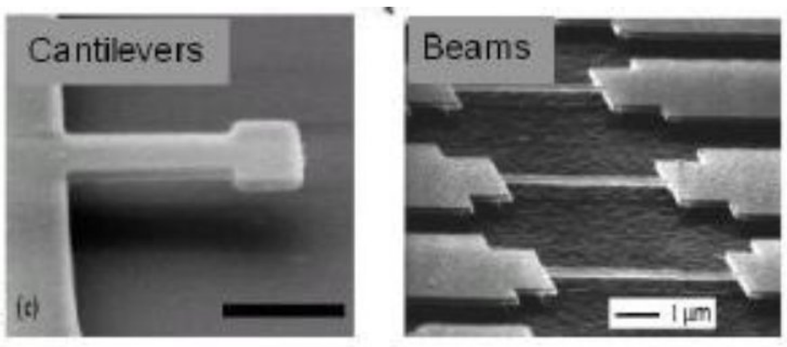


Figure 1: NEMS: Cantilevers of Aluminium Nitride [2] and Beams of Silicon Nitride [3].

CARBON NANOTUBES AS NEMS

With respect to conventional NEMS, NTs are extremely light, have a high Young's Modulus (~1TPa), and since there are no dangling bonds (all the carbon atoms are connected to each other) their anticipated quality factors are expected to be high (recent measurements indicate that the quality factor of the radial breathing mode of a NT is as high as 10^5). For a typical NT 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, NT resonators are expected to reach the ultimate mass sensitivity required for detecting small molecules.

APPLICATIONS

NEMS based on NTs promise a broad range of applications, from ultra-sensitive mass spectrometers that can be used to detect hazardous molecules, through biological applications at the level of a single DNA base-pair, to the study of fundamental questions such as the interaction of a single pair of molecules. NEMS based on Single Walled Carbon nanotubes (SWCNTs) have a potential to develop ultra sensitive mass and force sensors. Atomistic Simulations will be helpful to understand the underlying physics of such NEMS.

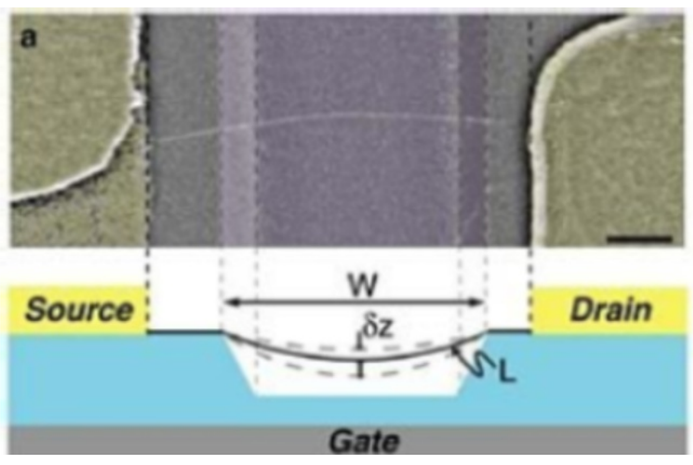


Figure 2: A doubly clamped Carbon Nanotube oscillator, device and geometry.[4]

THIS PROJECT

The starting point of this research was the work of Vera Sazonovva, Yuval Yaish et al. [4] who studied a suspended NT, clamped at both ends (Fig. 2). In this method a high frequency signal applied to a gate electrode electrostatically excites the mechanical vibration of a suspended NT. It was observed that the suspended SWCNT behaved as a tunable electromechanical oscillator, with resonance frequencies ranging between a few to 200 MHz, quality factors ranging between 50 to 200.

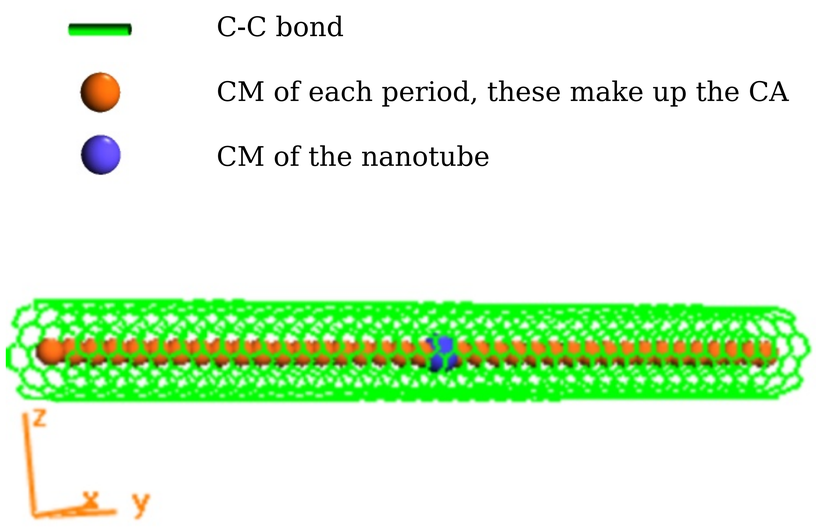


Figure 3: Single Walled Carbon Nanotube (green), center of mass (CM) for each period of nanotube (red), blue atom indicates CM of the nanotube. The image generated with AViz.

ATOMISTIC SIMULATIONS

We have begun atomistic simulations to prepare data for the SWCNTs in order to find and tune the frequencies to obtain improved sensitivity of NT devices. We started with a small model of a 98.38Å armchair nanotube with a diameter of 9.4A and a chiral vector of (7,7) clamped at both ends. We use the Brenner interatomic potential [5] and solve Newton's equations of motion using the Verlet algorithm.

The Brenner interatomic potential is an analytic potential energy function for solid carbon and hydrocarbon molecules based on a reactive empirical bond order (REBO) formalism. This formalism allows for covalent bond breaking and creation with associated changes in atomic hybridization within a classical potential, producing a powerful method for modeling complex chemistry in large many-body system.

VISUALIZATION

The AViz package was created by Geri Wagner and Adham Hashibon, based on earlier OpenGL routines written by David Segev (Saada) and implemented by Irina Rosenblum amongst others [7]. AViz requires an .xyz file of atomic coordinates, and draws balls at the atomic sites and then adds bonds of specific lengths between specific atoms, thus enabling us to directly observe bond lengths and angles.

PRELIMINARY RESULTS

Our first numerical experiments are monitoring thermal vibrations of such a NT at 300K. We let the nanotube vibrate during 626 psec with a time step of 0.5 fsec. The center of mass for each period of the nanotube (28 atoms in each period) was calculated (red dots in Figure 3), we call this line of points the Centered Axis (CA). We analysed the vibrations of CA and near center of mass of the nanotube with clamped ends (3 periods in each end do not move). The moving part of the nanotube has lenght of 83.62A. The tube axis is in the Y direction, X and Z are perpendicular.

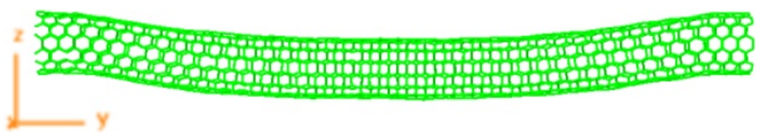
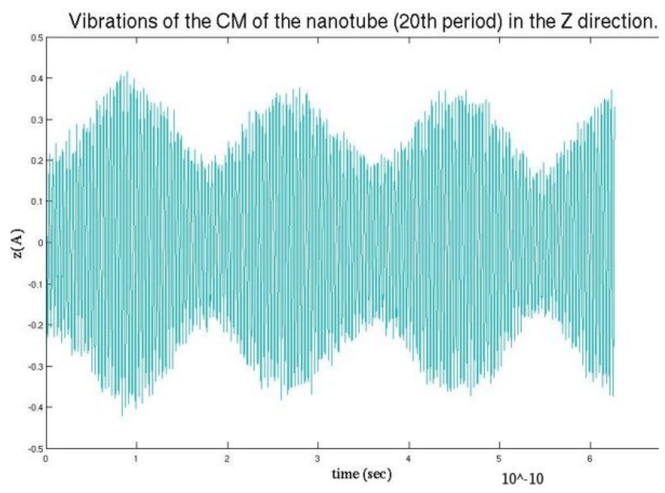


Figure 4: Nanotube vibrating in the Z direction. Three periods at each end are clamped in position.



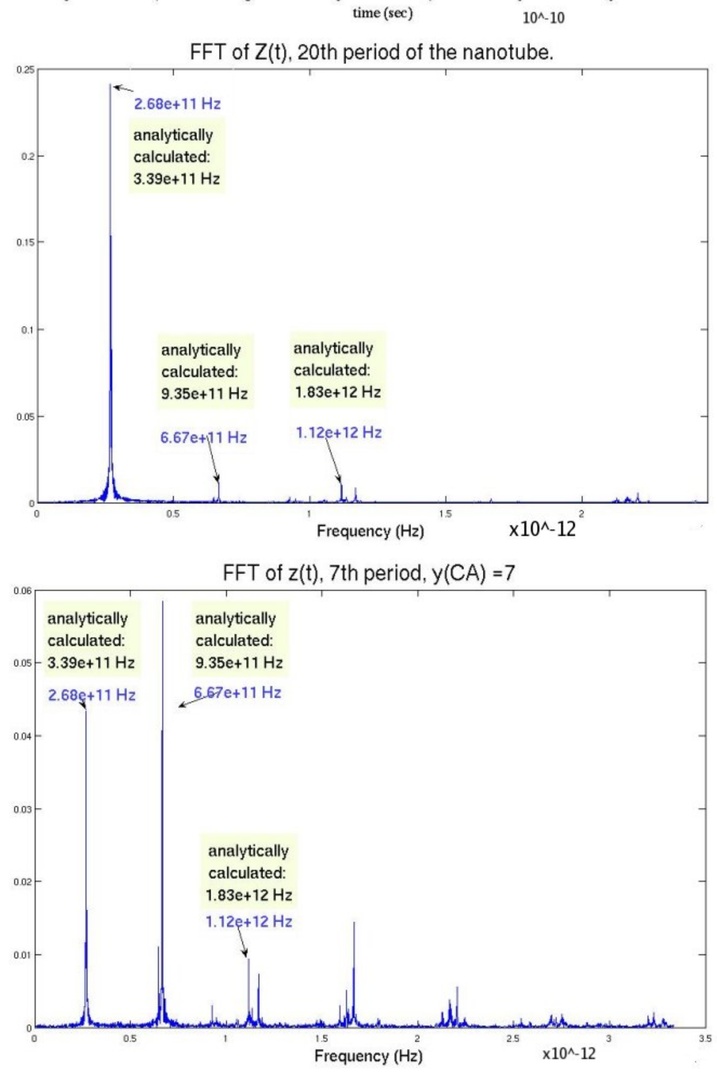


Figure 5: Analysis of the thermal vibrations in the Z direction of the nanotube shown in Figure 4. Upper image - vibrations of the CM at L/2, middle image - FFT of the upper image, lowest image - FFT of the vibrations at the 7th period of the nanotube. Results from an analytic model with L equal to the moving atoms are shown for comparison.

We have calculated analytic frequencies [6] from a nanotube model that takes into account the average density of a nanotube (1TPa) connected to walls at its sides at a single point of infinitesimal length. These are slightly higher than the simulated ones if the model nanotube has a length equal to the unclamped atoms of the simulation system. The 3 clamped periods (28 atoms in each period) that do not move do exert forces on the moving atoms and thus the connection has a finite length. If we calculate the analytic values for a nanotube equal to the unclamped length plus two extra periods at each end the values agree to two significant figures.

CONCLUSIONS

This results indicate that our first steps are in the right direction. We will now improve our FFT resolution and undersanding and monitor the vibration of tensioned SWCNTs before switching to larger systems.

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