

Atomistic simulations of single-walled carbon nanotube oscillators

Polina Pine^a, Yuval Yaish^b and Joan Adler^c

^a Russell Berrie Nanotechnology Institute, Technion, Haifa 32000 Israel

^b Electrical Engineering Department, Technion, Haifa 32000 Israel

^c Physics Department, Technion, Haifa 32000 Israel



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. Ekinici 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 usually 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 $\sim 0.4 \cdot 10^{-21}$ kg by 10MHz silicon beam (of length 4 micrometers) with a quality factor of $\sim 2,500$, $M \sim 5 \cdot 10^{-16}$ 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.

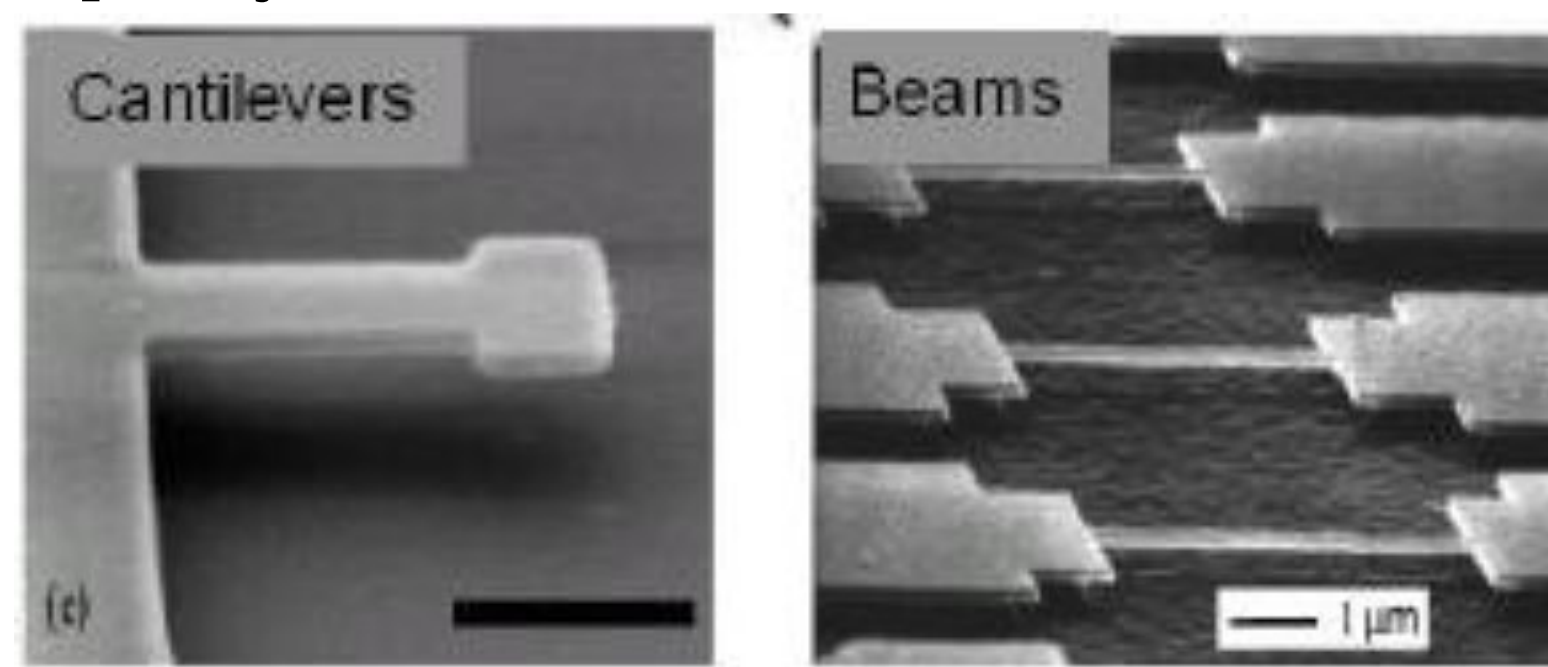


Figure 1: NEMS: Cantilevers of Aluminium Nitride [2] and Beams of Silicon Nitride [3].

CARBON NANOTUBES AS NEMS

As in [2] authors used NTs that were clamped at one end and free to move at the other. The detection was performed using TEM or SEM, and the reported mass sensitivity was in the attogram (10^{-21} kg) range. Carbon nanotubes 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, NTs are extremely light, have a high Young's Modulus (~ 1 TPa), 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.

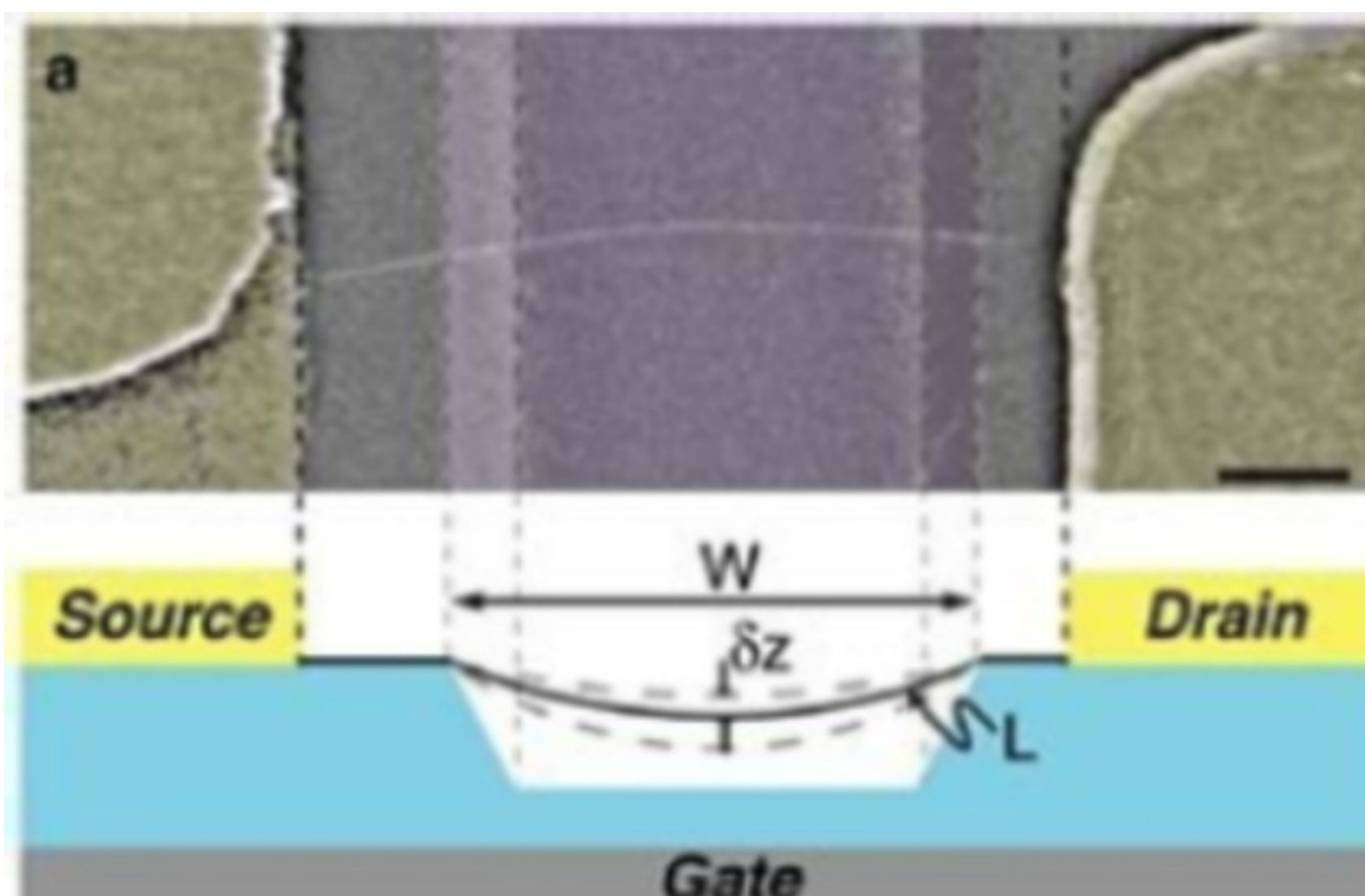


Figure 2: A doubly clamped Carbon Nanotube oscillator, device and geometry.

REFERENCES

1. K.L. Ekici, Y.T. Yang, M.L. Roukes, J. Appl. Phys., 95, 5, 2682 (2004).
2. B. Ilic, Y. Yang, K. Aubin, R. Reichenbach, S. Krylov and H.G. Craighead, Nano Lett., 5, 925 (2005).
3. A.N. Cleand, M. Pophristic, I. Ferguson, Appl. Phys. Lett, 79(13), 2070 (2001).
4. V. Sazonova, Y. Yaish, H. Ustunel, D. Roundy, T. A. Arias, and P. L. McEuen, Nature 431, 284 (2004)
5. D.W. Brenner, Phys. Rev. B 42, 9458 (1990)
6. L.D. Landau, E.M. Lifshitz, Theory of Elasticity; Pergamon Press: New York (1970)
7. AViz homepage: <http://phycomp.technion.ac.il/~aviz/>

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.

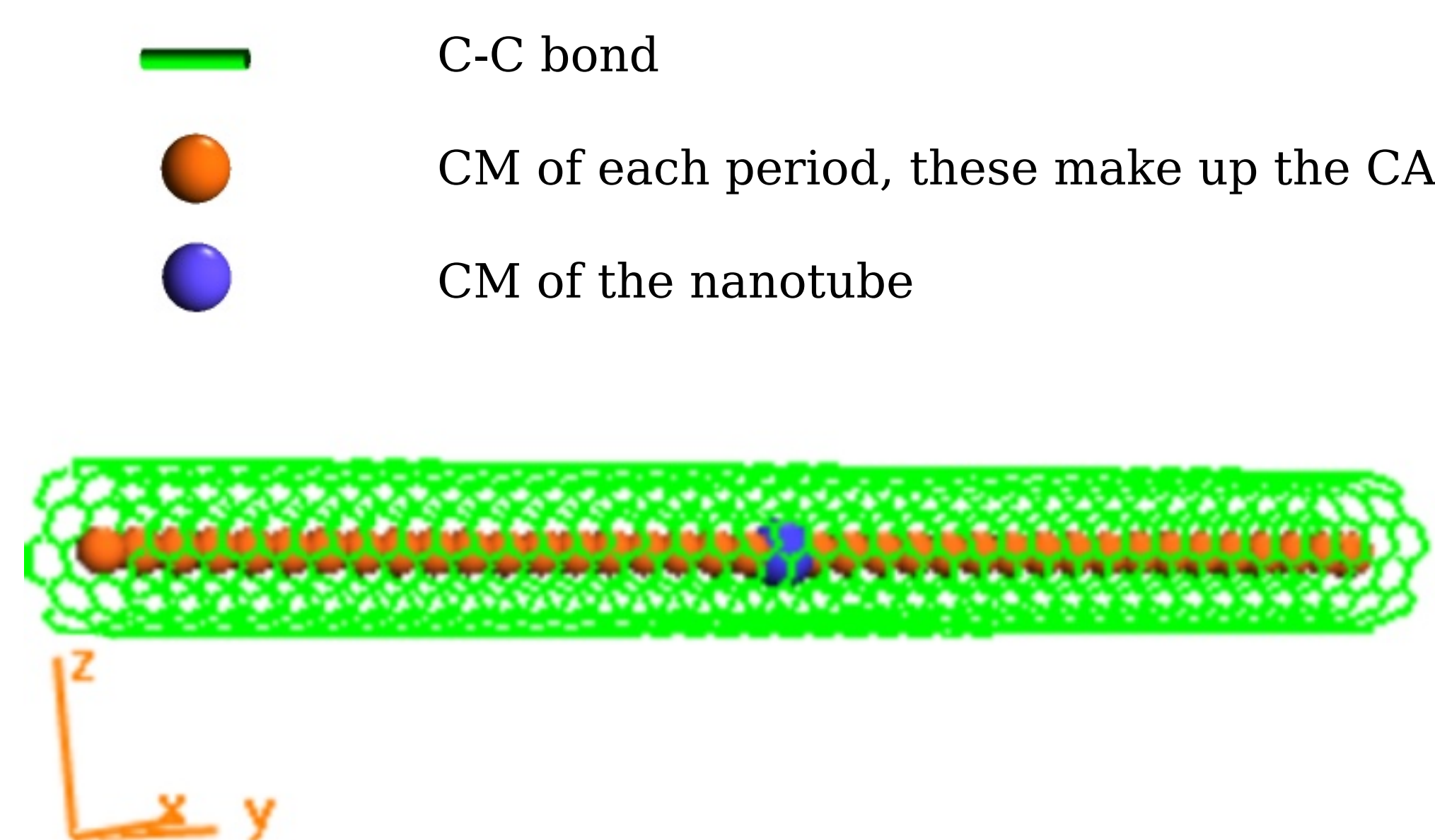


Figure 3: Single Walled Carbon Nanotube (green), center of mass (CM) for each period of nanotube (red), blue atom indicates CM of the nanotube. The image generated with AViz.

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 9.4Å and a chiral vector of (7,7) clamped at both ends. We used the Brenner interatomic potential [5] between the atoms and solve Newton's equations of motion using the Predictor-Corrector 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.

VISUALISATION

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 were monitoring thermal vibrations of such a NT at 10K. We let the nanotube vibrate during 187.5 psec with a time step of 0.5 fsec. The center of mass for each period of the nanotube was calculated (red dots in Figure 3), we call this line of points the Centered Axis (CA). We analysed the vibrations of CA and center of mass of the nanotube. The tube axis is in the Y direction, X and Z are perpendicular.

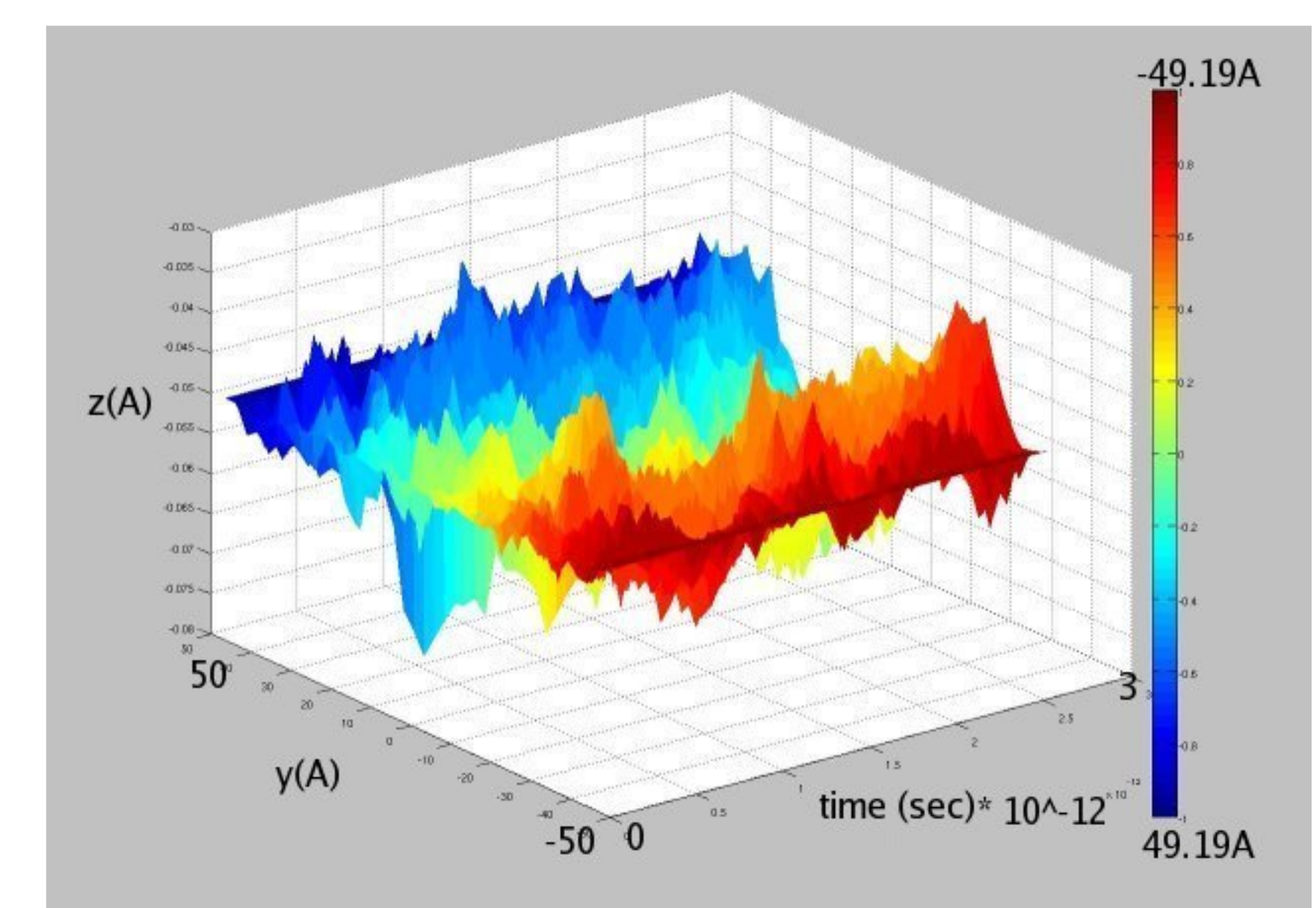


Figure 4: Thermal Vibration of the Centered Axis (CA) of the nanotube in the Z direction. The Z axis is the amplitude in z-direction, the colored axis (Y) is the axis of the nanotube (in our case it is the axis of CA) and the X axis is the time axis.

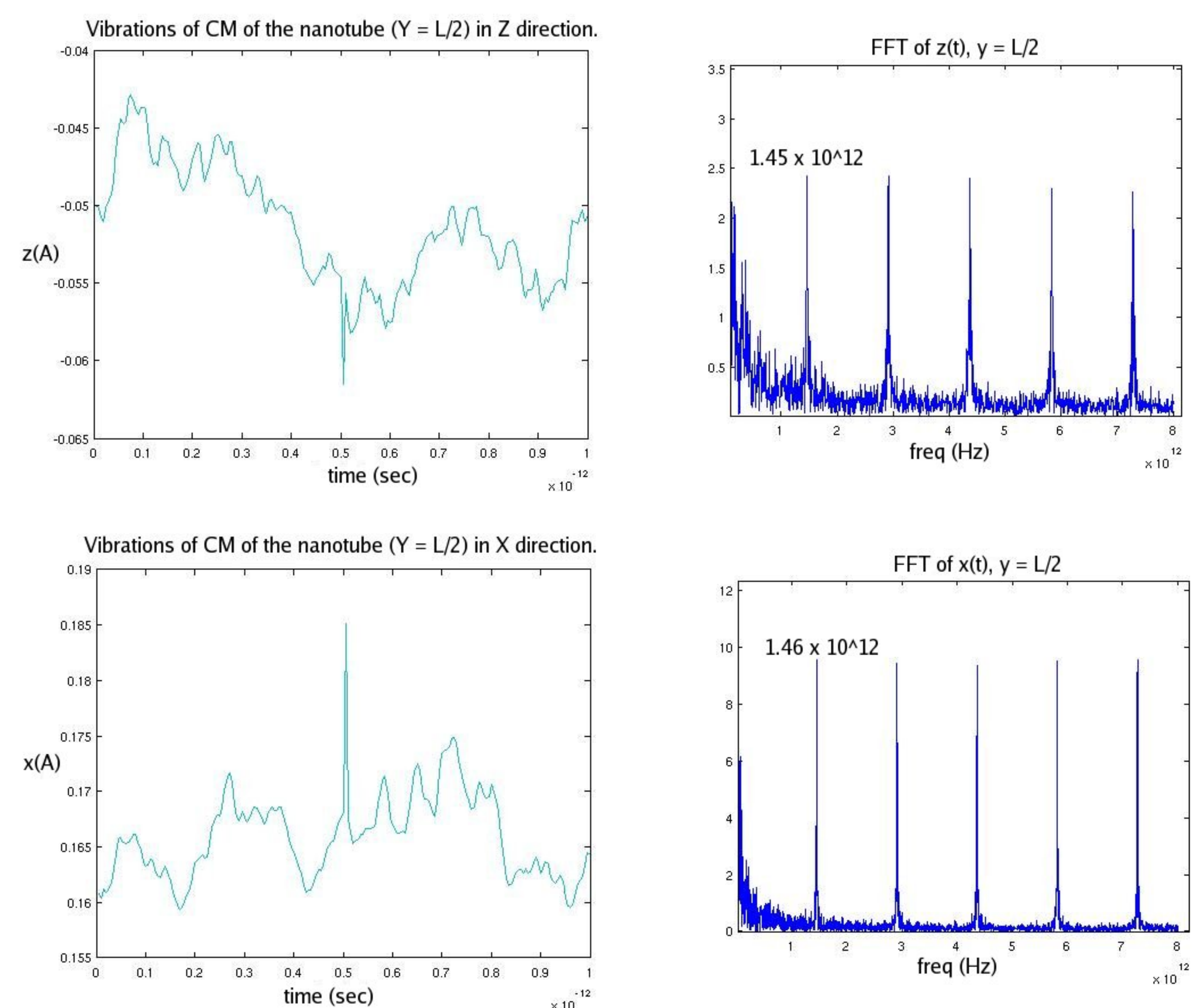


Figure 5: Thermal vibrations of the CM at $Y = L/2$ in the Z (X) directions upper (lower) left and their FFTs upper (lower) right. The upper left curve is the same as the one at the center of the Figure 4.

IT IS KNOWN THAT

The natural frequency of vibration of such a system is $\text{freq} \sim 25 \cdot 10^6 \cdot (D/L^2)$, where D is the diameter in nm and L is the length of the tube in micrometers [6]. Hence, the analytically calculated frequency of the first normal mode is about $2.5 \cdot 10^{12}$ Hz.

CONCLUSIONS

Our preliminary results for the frequency of the first mode in the X(Z) directions are $1.45 \cdot 10^{12}$ Hz ($1.46 \cdot 10^{12}$ Hz) and it is in good agreement with the analytically calculated value. This indicates that our first steps are in the right direction. We will now improve our FFT resolution and understanding and monitor the vibration of tensioned SWCNTs before switching to larger systems.

ACKNOWLEDGMENTS:

P.P. wants to thank Tali Mutat and Eduardo Warszawski for a helpful introduction to scientific computing and Pavel Bavli for a helpful introduction to Matlab.