Vibrational Analysis of Thermal Oscillations of SWCNT.

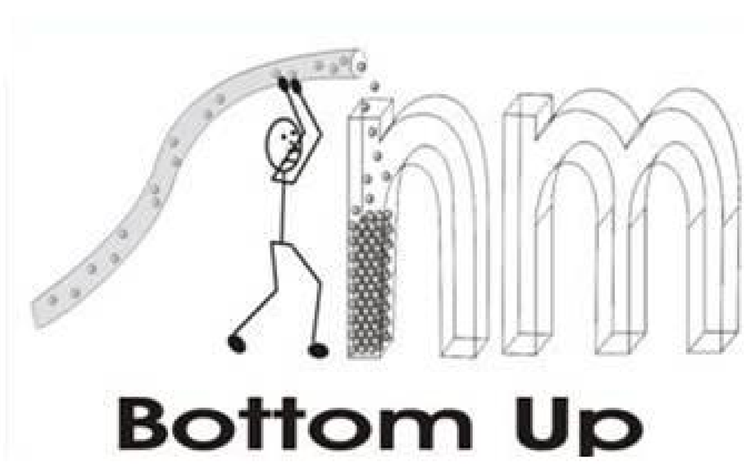
Polina Pine[a], Yuval Yaish[b] and Joan Adler[c]

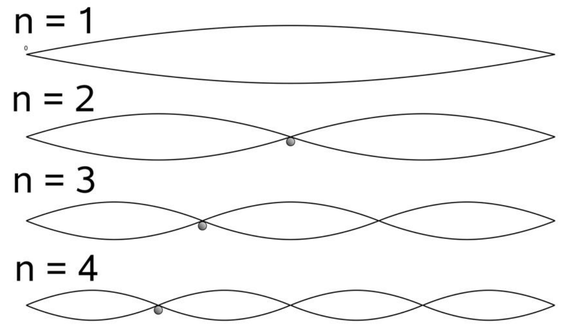
[a] Russell Berrie Nanotechnology Institute, Technion, Haifa 32000 Israel

[b] Electrical Engineering Department, Technion, Haifa 32000 Israel

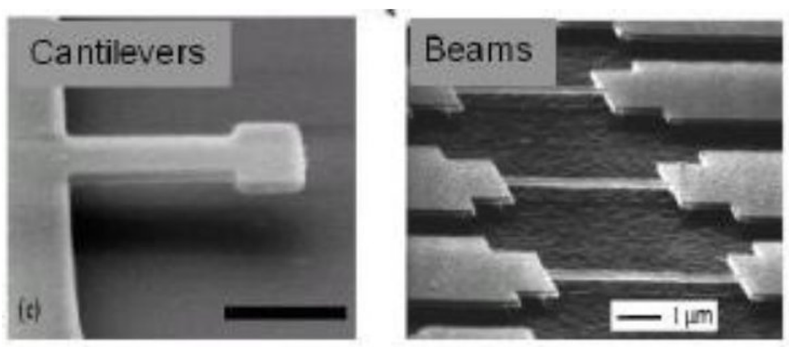
[c] Physics Department, Technion, Haifa 32000 Israel

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 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.

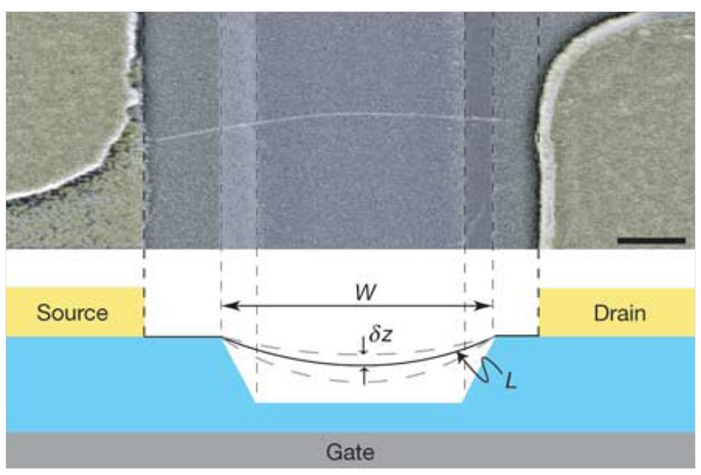




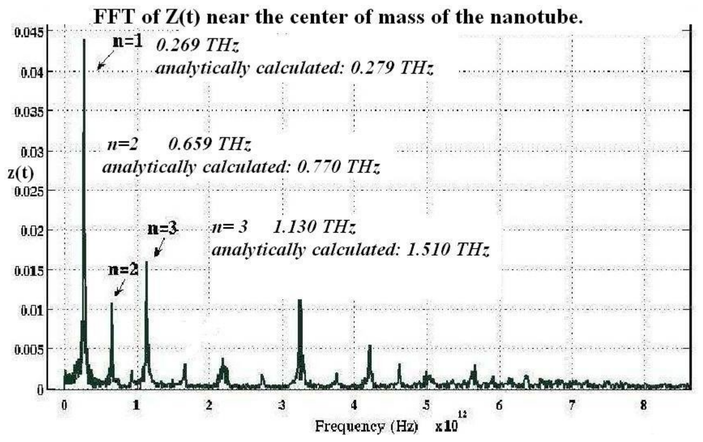
Vibration and standing waves: the fundamental and the first modes (n = 1,...,4)



NEMS: Cantilevers of Aluminium Nitride (above left) [2] and Beams of Silicon Nitride (above right) [3].



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



ANALYTICAL MODEL:

$$EI\frac{\partial^4 z(y,t)}{\partial z^4} + \rho A\frac{\partial^2 z(y,t)}{\partial t^2} - T\frac{\partial^2 z(y,t)}{\partial z^2} = 0$$

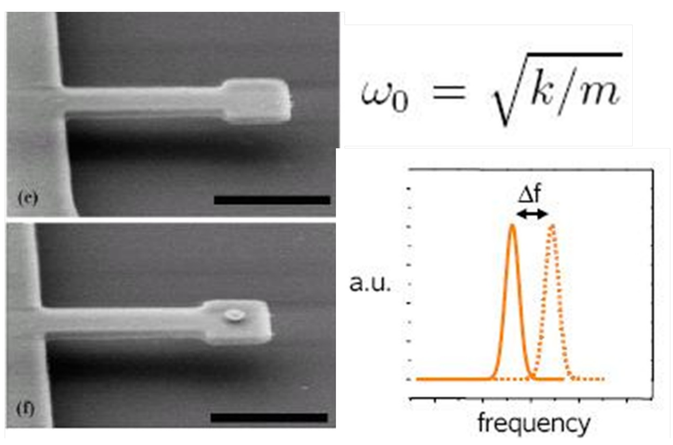
Bending Term Tension Term

For low deformations the tension term is neglected (T = 0)

APPLICATIONS:

Mass, Force and Presure Sensors

EFFECT OF ADDITIONAL MASS:



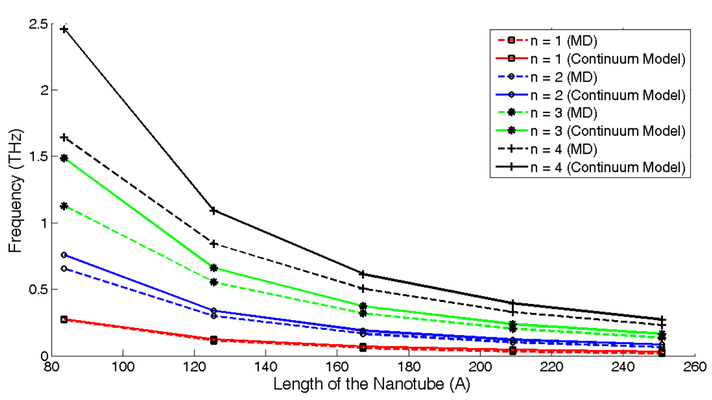
AIMS:

* Simulate nanotube vibrations to deduce optimal parameters for NEMS based on carbon nanotubes.

* Study qualitatively and quantitatively the modes of vibration in order to tune such a NEMS.

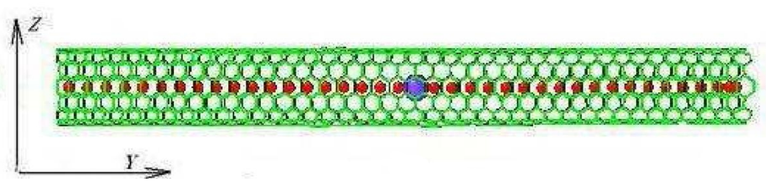
For this purpose we need to separate vibrations of the nanotube into different modes and study the effect of varying nanotube length and radius.

An analytical model from the solution of the equation above using standard parameters . Graphs of the frequencies of the first 4 modes as functions of nanotube length and radius from both the simulations and the model are shown below.



NEMS BEST RESULTS:

Mass of the NEMS ~ 10^{-13} g	Cantilivered[2]	Doubly Clamped[3]
Highest mass Sensitivity (g)	$0.23 \cdot 10^{-18}$	$0.39 \cdot 10^{-18}$
Q (quality factor)	3000 - 5000	2500 - 4500
Length of the NEMS (μm)	3.5	4.0

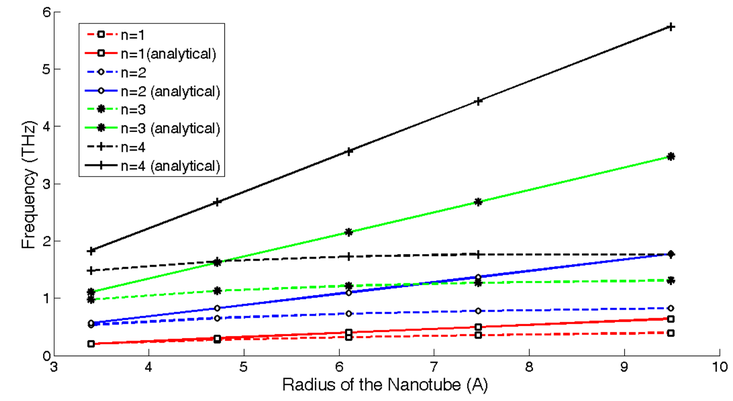


C-C bond

CM of each period, these make up the

CM of the nanotube

(7,7) Single Walled Carbon Nanotube, center of mass (CM)for each period of nanotube (red), blue atom indicates CM of the nanotube. Image generated with AViz.



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COMPUTATIONAL DETAILS:

Molecular Dynamics with REBO potential [5], using Velocity Verlet algorithm of integration. T = 300K, Ends of the nanotube are clamped in their positions. The simulations were made on NANCO and other computers for times of up to 10000 psec for nanotubes of lengths of 83.62, 147.57, 196.76, 245.95, 295.14 A and radius 4.75A and for the length of 83.62 A and radii 3.39, 4.75, 6.10, 7.46 and 9.49 A. The vibrations of the CM were recorded and Fourier transformed to seperate them into modes.

CONCLUSIONS:

* As the nanotube length increases the difference between MD and analytic values becomes smaller for all modes of vibration. For the shorter nanotubes, the disagreement between the two methods is very small for the first mode (n = 1) but increases as n increases

* The most surprising observation is that the widely used elastic continuum model which does not take into account the tension term, fails to completely describe the vibrational and elastic behavior of short nanotubes, or of those whose length/radius ratio is small.

ACKNOWLEDGMENTS:

P.P. wants to thank Tali Mutat and Eduardo Warszawski for a helpful introduction to scientific computing, Pavel Bavli for a helpful introduction to Matlab, Avi Abramov for help in the result analysis and acknowledges support from RBNI.