Atomistic simulations of vibration of carbon nanotubes:

is it possible to measure the mass of a single atom?

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Carbon nanotubes are long thin tubes made from rolled up single sheets of graphene. Nanotube resonators have already reached the mass sensitivity required to measure the mass of single molecules, but in order to detect smaller (atomic) masses these devices must be further optimized. For this, a deep understanding of their operational mechanism is required, but simple analytic models and previous simulations have internal contradictions leading to questions such as whether the Young's modulus of nanotubes is a well defined concept.

We have made careful, extensive, atomistic Molecular Dynamics simulations [1] of nanotubes using the Brenner potential. The nanotube vibrations were recorded at selected points and decomposed into vibrational modes using a Fourier Transform technique. The nanotubes were first slowly thermalized to 300 degrees K with periodic boundary conditions then clamped to retain its at the mean length. Different lengths and radii were studied and we developed protocols for dealing with the large quantity of data generated. (Each nanotube is allowed to vibrate 1000 times more than the period of its lowest frequency and we use a timestep of 0.5fm).

The simulations provide clear evidence for the failure of simplistic analytic models to accurately extract resonance frequencies as a function of the ratio between the tube's radius and length as the latter increases. Our results agree with the Timoshenko beam model (which includes the effect of both rotary inertia and of shearing deformation) and partially resolve Yakobson's paradox concerning the Young's modulus, and provide an upper cutoff estimate for the effective wall thickness. We have further [2] made a comparison of the vibrational behavior of different types of nanotubes: zigzag, armchair and two chiral types. This gives the surprising result that nanotube structure/chirality does not affect the vibrational frequencies under double clamping conditions. In the laboratory, nanotubes are not fully clamped as in models and some simulations. Only atomistic simulations can truly model partial clamping. Our latest simulations with partial clamping [3] show that under such conditions the degeneracy lifts and we can propose which type of nanotube would be the best candidate to progress towards weighing single atoms.

[1] P. Pine, Y. Yaish and J. Adler, ``Simulational and vibrational analysis of thermal oscillations of single-walled carbon nanotubes", Phys. Rev. B (2011)83 155410.
[2] P. Pine, Y. Yaish and J. Adler, ``Thermal oscillations of structurally distinct nanotubes", submitted.
[3] P. Pine, Y. Yaish and J. Adler, "The affect of boundary conditions on the vibrations of armchair, zigzag and chiral single walled carbon nanotubes", in preparation.