Molecular Dynamics Simulation of Carbon Nanotubes as Gigahertz Oscillators

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From the discovery of carbon nanotubes by Iijima [1] as a by-product of fullerene synthesis, the carbon science has experienced an intense growth. These discoveries revealed that carbon solid is capable of forming novel nanosize structures [2]. Similarly to graphite, the intershell interaction in multiwall carbon nanotubes (MWNT) is predominantly van der Waals [1], and since the interlayer corrugation is small [3,4], it is expected that individual cylinders of MWNTs might easily slide or rotate one with respect to the other. In the area of technological applications, carbon nanotubes are playing a special role. In particular, the fabrication of nanomechanical systems operating in gigahertz order frequencies is now a possible achievement.

Recently, Cumings and Zettl [5] demonstrated the controlled and reversible telescopic extension of MWNT, thus reaching ultralow-friction nanoscale linear bearing. This exploit was possible due to the discovery of a method [6] whereby the ends of a MWNT can be carefully opened in a way that the core nanotubes are left fully intact and protruding.

Using static models on a slightly modified Cumings and Zettl set up, Zheng et al. [7,8] have showed that multishelled nanotubes could lead to gigahertz nanooscillators. Once the reliability of such nanodevices depends on the consideration of effects as temperature and time fluctuations, we have carried out the first molecular dynamics studies for these systems on the framework of classical mechanics with standard molecular force fields [9,10]. The calculations were performed considering structures containing up to 6,000 carbon atoms. Our results show that telescopic extension and retraction movements are possible for a large combination of tube diameters and types. However, sustained oscillation are only possible when the radii differences between inner and outer are of ~3.4Å, independently of tube type.

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