

MECHANICAL PROPERTIES OF NANOTUBES AND FULLERENES

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Introduction

One of the most attractive properties of carbon nanostructures is their high mechanical stability. This is of particular interest as these structures have a low mass density and high temperature resistance. Many applications are possible in this context. A number of experimental and theoretical studies were performed on the strain, torsion and buckling of carbon nanotubes (Yakobson et al. 2001, Ruoff et al. 2003, Srivastava et al. 2003). First applications of carbon nanotubes are as filler materials for composite reinforcement [Coleman]. As some carbon nanotubes are metallic they can be used as tips for scanning probe microscopes and as elements of nanoelectromechanical systems (Bhushan 2004).

A further interesting mechanical property of nanotubes, C_{60} and C_{70} fullerenes are their lubrication properties (Blau et al. 1992, Zhao et al. 1996). In spite of preceding speculations, which attribute the low friction in these nanostructures to their spheroidicity and high “molecular” moduli, the frictional properties are indeed similar to graphite or even a little bit higher due to the interfullerene interactions.

The effects of the mechanical response of nanotubes on a load orthogonal to the tube axis are not less important to understand the mechanical properties, e.g. in nanotube composites or in AFM studies of single nanotubes. Theoretical studies of mechanical properties of nanotubes include investigations of tube deformations within their bundles or isotropic radial compression of single tubes (Chesnokov et al. 1999, Xiao et al. 2006). Here we present the results of molecular dynamics investigations on the behaviour of carbon nanotubes and fullerenes under anisotropic (nonhydrostatic) pressure, using a combined quantum mechanical (QM) – classical (molecular mechanics – MM) treatment.

Methods

The molecular dynamics simulations were performed using a QM/MM scheme. The nanostructure was treated by the quantum mechanical density-functional based tight-binding method (DFTB) (Porezag et al. 1985, Seifert et al. 1986) with dispersion corrections (Zhechkov et al. 2005), applying periodic boundary conditions. The quantum-mechanical (QM) part included the nanoobject (a supercell of a nanotube or a fullerene with up to 300 atoms).

The grips are modelled as rigid metal plates (6 atomic (001) planes, 1296 atoms per unit cell) and the grip-nanostructure interaction has been treated by Lennard-Jones parameters as given by the Universal Force Field (UFF)(Rappe et al. 1992).

A detailed description of DC-DFTB method can be found in the original papers (Elstner et al. 2001, Zhechkov et al. 2005). Previous studies showed the reliability of this approach to estimate the interaction energies for numerous number of carbon systems (Frauenheim et al. 2000, Elstner et al. 2000).

Results

Nanotubes: phenomenology of the squeezing

Our calculations demonstrate that the behaviour of nanotubes under anisotropic pressure is very sensitively depending on the chirality of tubes. We have considered the single-walled nanotubes of *armchair* (5,5) and *zigzag* (9,0) chiralities.

The evolution of a (5,5) nanotube under compression (views from top and side, Fig. 1a) goes from the unperturbed spherical cross section to a flat structure of two graphene stripes, interconnected at the edges. In this phase, the deformation is reversible (elastic deformation). The irreversible destruction starts with a spontaneous defect in a tube wall, which initiates a „zipper“ mechanism. The break at the tube walls creates dangling bonds and zigzag-like graphene edges, and finally two parallel stripes, which glide on top of each other and form quite well-ordered graphene nanostripes with zigzag-like edges.

The (9,0) nanotube behaves under compression quite different (Fig. 1b). The elastic part of the compression is similar to that of the armchair tube. At a later stage, sp^3 -hybridized carbon atoms appear, connecting the opposite tube walls. The destruction of the tube in this state starts with decomposing of the walls from the edges. But, in contrast to the (5,5) nanotube, there is no separation of the tube into two slices because of the numerous chemical bonds between the opposite parts of the tube. Instead, the opposite walls form a nanostripe with a disordered haeckelite-like structure.

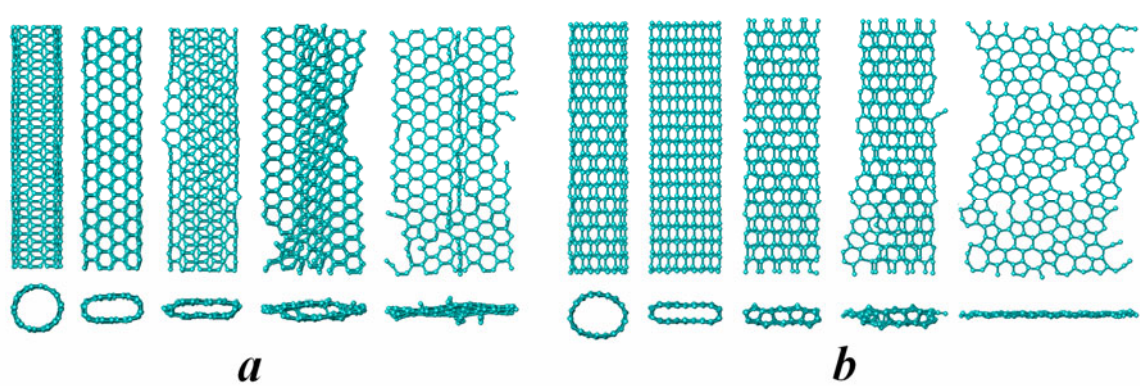


Figure 1. Evolution of *armchair* (5,5) (**a**) and *zigzag* (9,0) (**b**) carbon nanotubes with decreasing grip distance (left to right).

Fullerenes: phenomenology of the squeezing

The study of the response of fullerenes on load was performed for single-walled I_h fullerenes (C_{60} , C_{80} , C_{180} , C_{240}) and for double-walled $C_{60}@C_{240}$.

As typical example, the evolution of the structure of a C_{240} fullerene under compression are shown in Fig. 2a (views from top and side). The 5-fold axis of the fullerene cage between the gripes is oriented perpendicular to the surfaces of the gripes. With increasing pressure the fullerene wall bursts from one side under the formation of a „*packman*“ -like structure. Further, the fullerene wall bursts from the other side, sometimes under formation of carbene-like chains. Later, the carbon chains and wall fragments form an amorphous phase which ends up in a disordered carbon plane.

The behaviour of a $C_{60}@C_{240}$ onion under compression on the first steps does not differ so much from the case of the single walled fullerenes (Fig. 2b). The destruction of the whole fullerene starts with breaking the inner C_{60} . The dangling bonds of C_{60} connect to the wall of C_{240} and accelerate its fast breaking. It is intriguing, that in the next step, the fullerene wall of C_{60} incorporates into the hole of C_{240} („*mouth of a C_{240} packman*“) and the cracking process is continued as for single walled fullerenes. The observed destruction process might be very important for understanding the breaking process of multi-walled particles: inner fullerenes can fill the holes of outer fullerene walls (coalescence) and heal even large defects. This might be of interest for future studies and applications of these or similar particles as lubricants.

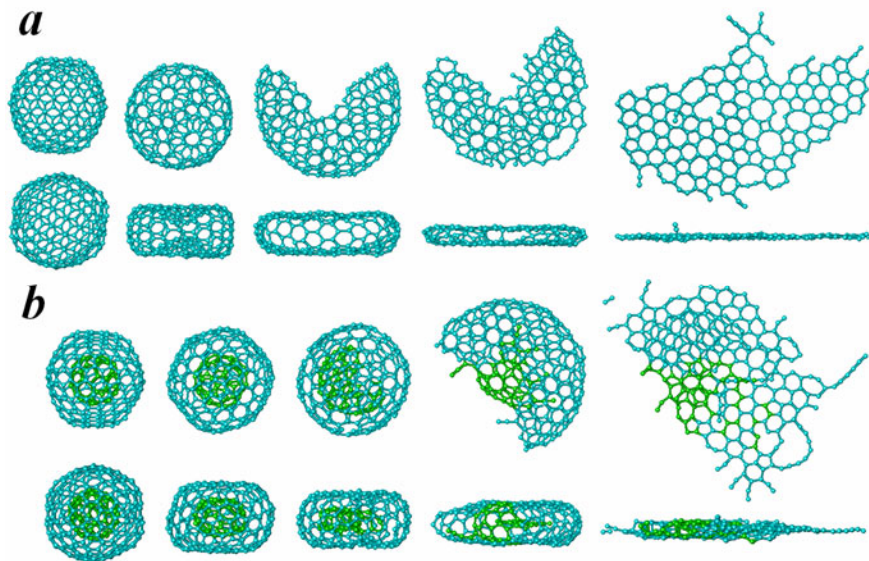


Figure 2. Evolution of a C_{240} (**a**) and $C_{60}@C_{240}$ (9,0) (**b**) carbon fullerenes with decreasing grip distance.

Conclusions

Our calculations indicate a rather different behaviour of carbon nanostructures against anisotropic compression. While a similar deformation process is observed in the elastic region, the destruction process is quite different for the different nanostructures studied in this work:

- 1) a “zipper” mechanism with the formation of zigzag-like edges for armchair nanotubes,
- 2) the formation of an interlinked double layer via sp^3 -hybridized atoms for zigzag nanotubes and
- 3) the formation of an amorphous phase for fullerenes.

After destruction, the armchair tubes form ordered graphene stripes, while fullerenes and zigzag tubes form disordered haeckelite-like stripes or platelets.

Calculations of the mechanical behaviour under compression for multiwalled nanotubes and fullerenes are in progress.

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