

MECHANICAL PROPERTIES OF ORDERED SINGLE WALLED CARBON NANOTUBE NETWORKS

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Many attempts have been made in order to develop procedures to controllably assemble large number of single walled carbon nanotubes (SWCNTs) in terms of position and orientation [1-4]. The achievement of such procedures would allow the fabrication of ordered SWCNT networks representing a breakthrough in the “bottom-up” manufacturing approach. These ordered networks would open possibilities to design new materials with desirable electronic and mechanical properties.

We present here results of classical molecular dynamics simulations of the mechanical response of carbon nanotube networks (CNNs) under different types of mechanical tests. The interactions between carbon atoms were described by the adaptive intermolecular reactive empirical bond-order potential [5]. The CNNs were constructed connecting SWCNTs through Y- or X-like junctions yielding to hexagonal and crossbar networks, respectively. Figure 1(a) shows an example of a crossbar CNN. Our results showed that CNNs exhibit very high flexibility dependent on the network architectures, showing elasticity modulus ~10-100 GPa and bulk modulus ~10 GPa. Due to the network topology involving SWCNTs and junctions, different response mechanisms under normal deformation for suspended networks are expected. They are associated with the carbon nanotube stretching and nanotube-junction-nanotube angle bending which differently contribute depending on the degree of deformation of the network. The symmetry presented by the junctions that constitute the network and the network disorder are important aspects on the resulting mechanical properties [6].

Using the same heuristic method for generating SWCNTs from a graphene layer, CNNs can be rolled up to form CNNs with a tubular geometry. The resulting structures, the so-called 'super' carbon nanotubes (STs) [7], which are carbon nanotubes made of SWCNTs. Similarly to a (n,m) SWCNT, $[N,M]$ ST with different chiralities can be constructed. The STs are represented as $[N,M]@(n,m)$ and characterized by: the (n,m) SWCNT used to form them; the necessary junctions to weld consecutive SWCNTs; and the distance between these junctions. Figure 1(b) shows an example of a ST.

From tensile tests of impact loads, we have found that STs are more flexible than the SWCNT used to form them but in some cases they show comparable tensile strengths (Figure 1(c)). The ST Young's modulus have been predicted to have an inverse dependence on the ST radius. During tensile deformations the shape and aperture of pores in ST sidewalls can be modified providing a way to vary the accessible channels to the inner parts of STs through the application of mechanical loads. The ST rupture occurs basically at regions near the SWCNT junctions and it is influenced by the ST chirality. Based on the predicted geometrical and mechanical properties, STs may represent hypothetical candidates for novel porous, flexible, and high-strength materials.

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Figures:

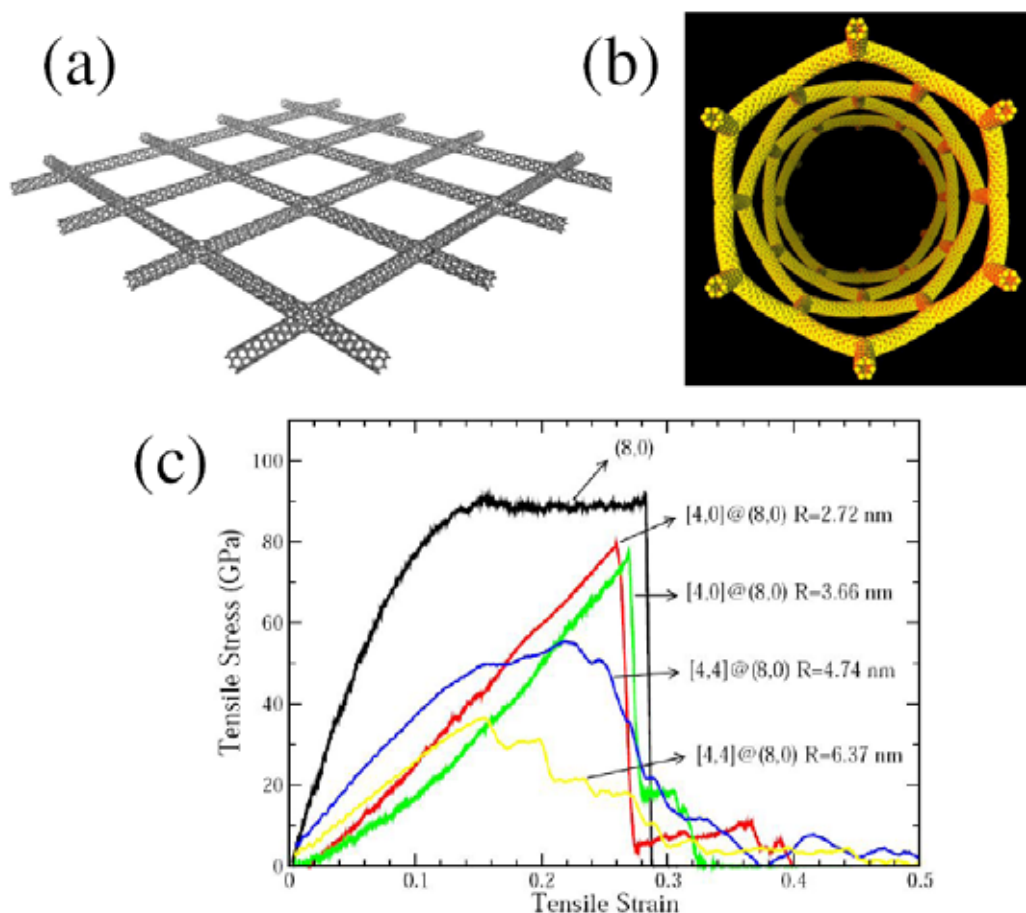


Figure 1: (a) Crossbar ordered single walled carbon nanotube network. (b) Configuration of a [6,0]@(6,0) super carbon nanotube. (c) Tensile failure behavior for super carbon nanotubes with different chiralities and radii (R) and for the (8,0) SWCNT at 300 K.