Fracture of Low-dimensional Nanomaterials

Wanlin Guo*, Yufeng Guo, Chun Tang and Liangzhi Kou

State Key Laboratory of Mechanics and Control of Mechanical Structures and Key Laboratory for Intelligent Nano Materials and Devices of MOE, Institute of Nanoscience, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, China

* Corresponding author: wlguo@nuaa.edu.cn

Abstract We found different failure mechanisms and mechanical properties for single-walled carbon nanotubes (SWCNTs) when subjected to electric fields and that subjected to tensile load by quantum mechanics calculations. The electric field induced breaking in SWCNT begins from the outmost carbon atomic layers while the tensile load breaks the nanotube near its middle. When a tube is tensioned in an electric field, the critical tensile strength of the tube decreases significantly with increasing intensity of the electric field. It is interesting to be shown that a piece of graphene sheet formed by unwrapping the SWCNT can also be stretched up to 2.5% by applied electric field and fractured at it edges. We also studied the mechanical response and structural evolution of graphene with topological line defect under tensile strain by using first-principles calculations. We studied the superelongation and fracture of carbon nanotubes at high temperatures by molecular dynamics simulations, and found that the nearly simultaneous activation and wide distribution of a large number of defects near the elastic limit play a key role in impeding the formation of localized predominant instability and facilitating large tensile elongation of carbon nanotubes at high temperature.

Keywords Carbon nanotubes, mechanical and electric coupling, failure, quantum mechanics

Carbon nanotubes (CNTs), a novel form of carbon materials, have been recognized as particularly important nanoscopic systems. The exceptional mechanical properties of carbon nanotubes have been the subject of numerical experimental and theoretical studies. Electric field will impose significant influence on the electronic and structural properties of carbon nanotubes. Electric field induced failure of carbon nanotubes as well as the corresponding mechanisms are key issues for nanotube applications in nanoelectromechanical devices. By using semi-empirical quantum mechanical calculations as well as quantum-molecular dynamics techniques based on the Roothaan–Hall equations and the Newton motion laws, we [1] found different failure mechanisms and mechanical properties for single-walled carbon nanotubes (SWCNTs) when subjected to electric fields and that subjected to tensile load. The electric field induced breaking in SWCNT begins from the outmost carbon atomic layers while the tensile load breaks the nanotube near its middle. Electronic polarization and mechanical deformation induced by an electric field can significantly change the electronic properties of a SWCNT. Under electric field, the SWCNT can be stretched but the toughness is much lower than that under mechanical loading. When a tube is tensioned in an electric field, the critical tensile strength of the tube decreases significantly with increasing intensity of the electric field, as shown in Fig. 1.

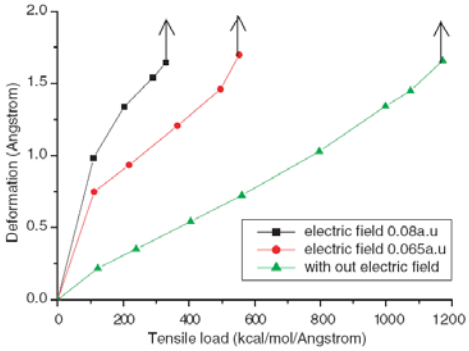

Figure 1. Deformation of SWCNTs versus the tensile load in the absence and presence of electric fields [1].

On the other hand, the mechanical behaviors and the electric and electronic properties of carbon nanotubes are always coupled with each other. By using Hartree-Fock and density functional quantum mechanics simulations, we [2] demonstrated a large axial electrostrictive deformation in short SWCNTs under electric field [Fig. 2 (a)]. The external field induced axial strains in armchair and zigzag tubes can be greater than 10% for a field strength within 1 V/Å. The corresponding volumetric and gravimetric work capacities of the SWCNTs are predicted to be three and six orders higher than those of the best known ferroelectric, electrostrictive, magnetostrictive materials and elastomers, respectively. Further study indicated the significant effect of axial electrostrictive deformation on the electronic properties of SWCNTs. It is also found that the band structures of SWCNTs change in electric fields and the change can be significantly enhanced by the electrostrictive deformation. The polarization of the orbital charge densities and the variation of the dipole moment are also enhanced by the electrostriction. The coupled mechanical and electrical behaviors of CNTs might lead to wider applications of nanotubes in nanoelectromechanical systems. It is interesting to be shown [2] that a piece of graphene sheet formed by unwrapping the single walled carbon nanotube can also be stretched up to 2.5% by applied electric field [Fig. 2 (b)].

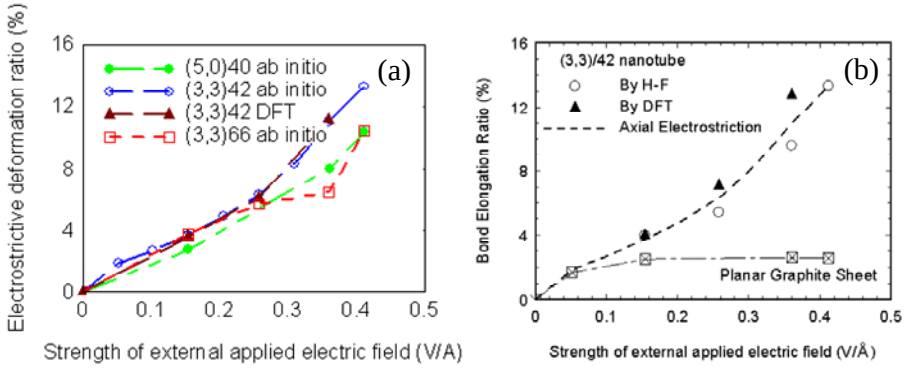

Figure 2. (a) Axial electrostrictive deformation ratio induced by external applied electric field in (3, 3) metallic single walled nanotubes of different lengths and a (5, 0) semi-metallic tube. (b) Average elongation ratios of the C-C bonds having a contribution to the deformation along the direction of the external electric field for the (3, 3)/42 tube and the corresponding single layer planar graphite sheet by unwrapping the nanotube. [2].

A recent experiment discovered that SWCNTs become superplastic and can accommodate extremely large plastic strains with a total elongation of 280% when being tensile loaded at high temperatures [3]. Similar ductile behaviors have been observed in individual double-walled and triple-walled carbon nanotubes at high temperatures above 2000 oC, with tensile elongation of 190% and diameter reduction of 90% [4]. However, several fundamental questions concerning the mechanism for superelongation of CNTs remain. By using molecular dynamics (MD) simulations, we [5] found that the nearly simultaneous activation and wide distribution of a large number of defects near the elastic limit play a key role in impeding the formation of localized predominant instability and facilitating large tensile elongation of carbon nanotubes at high temperature, as shown in Fig. 3. Intricate interplay between nanotube sizes and defect nucleation and motion determine the overall deformation pattern.

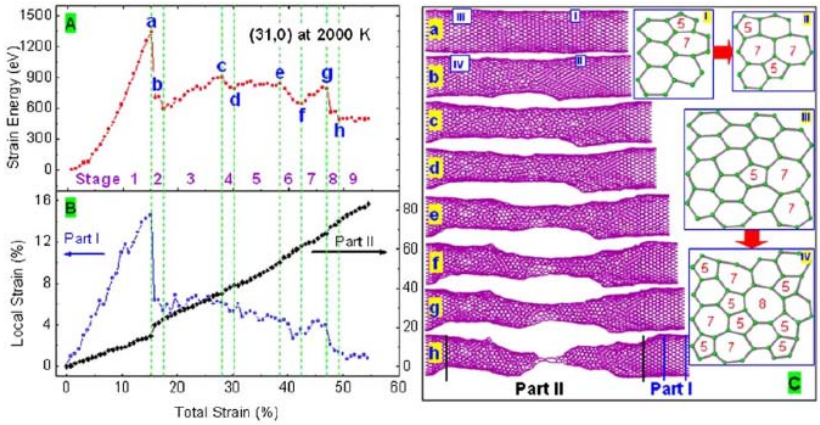

Figure 3. A (31,0) SWCNT subjected to tensile loading at 2000 K. The tube is 10.6 nm in length and 2.43 nm in diameter. (a) Strain energy. (b) Variation of local strain in two distinct parts of the tube: the elastic (part I) and plastic (part II) as shown in (c). (c) a–h: Selected snapshots of stretched SWCNT from the MD simulation; the insets show the 5-7-7-5 dipole and other defect formation and motion, and the rearrangement of local atomic structure during the deformation [5].

Graphene, a two-dimensional honeycomb carbon layer of sp2 hybridized carbon atoms, exhibits exceptional electronic, magnetic, optical and chemical properties. As the carbon-carbon bond is one of the strongest covalent bonds in the world, the mechanical behaviors of graphene have attracted enormous scientific interests from experimental and theoretical studies. We studied the mechanical response and structural evolution of graphene with topological line defect under tensile strain by using first-principles calculations, as shown in Fig. 4 [6]. It is seen that, before the strain reaches the critical value of about 12%, both bond lengths l1 and l2 increase monotonically with strain. It is interesting to note that when strain reaches about 4% the two bond lengths intersect. When the strain exceeds 12%, the two bond lengths experience an abrupt change: l1 suddenly increases while l2 sharply decreases. Such sudden variations of bond lengths induce significant redistribution of spin-polarized electrons at the defected part, which indicates that the magnetism of defected graphene can be tuned by strain.

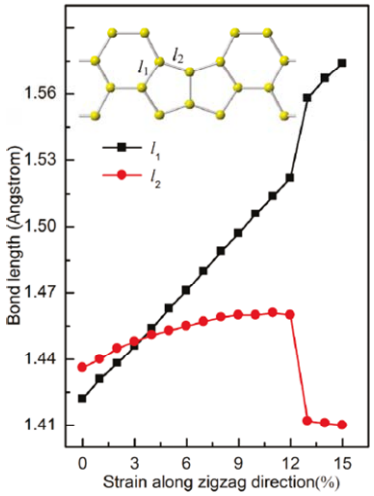

Fig. 4. Local bond length variation of defected graphene around the line defect region with strain [6].

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