ON THE STRUCTURAL AND DYNAMICAL FEATURES OF CARBON NANOSCROLLS

Vitor R. Coluci[1,2], Scheila F. Braga[1], Sergio B. Legoas[3], Ronaldo Giro[1], R. H. Baughman[2], and Douglas S. Galvão[1]
[1]Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas
CP 6165, 13083-970 Campinas, SP, Brazil
[2]NanoTech Institute and Department of Chemistry, University of Texas
Richardson, Texas 830688, U.S.A.
[3]Departamento de Física, Universidade Federal do Amazonas
69077-000, Manaus, AM, Brazil
E-mail: galvao@ifi.unicamp.br

Carbon-based materials present an enormous variety of forms and properties. Among these structures we can mention graphite, diamond, carbon fibers, fullerenes, carbon onions, and carbon nanotubes (CNTs) [1]. Recent developments in synthesis using graphite intercalation/exfoliation structures have provide a simple, low-temperature, and efficient chemical route to a new carbon-based structure. This structure, named carbon nanoscroll (CNS) [2], is formed by curling up an isolated exfoliated graphite sheet (grapheme). The route to obtain these structures consists on the graphite intercalation with potassium metal followed by exfoliation with ethanol forming a dispersion of carbon sheets which, after energy assisted process (sonication), leads to CNSs. As CNSs do not have end caps they present a larger accessible surface area in comparison to equivalent CNTs. Such aspect can be useful for technological applications such as hydrogen storage and energy harvesting in super-capacitors.

In this work we report atomistic molecular dynamics results of the structural and dynamical properties of different families of CNSs. We have used classical molecular dynamics methodologies with standard molecular force fields [3,4]. We have analyzed both neutral and charge CNSs in order to investigate the effects of charge injection on scroll conformations. Electroactuation has been observed for CNTs and CNSs can exhibit a new type of actuation (scroll unwinding).

Our results show that CNS formation is dominated by two major energetic contributions: the elastic energy increase caused by bending the graphite sheet (decreasing structural stability) versus the free energy decrease generated by the van der Waals interactions of overlapping regions. CNS structures can be more stable (in terms of energy per carbon atom) than its related graphite sheet. CNS formation is a self-sustained curling process after a critical overlap area is reached [5]. Consistent with experimental observations our results show that CNSs having inner diameters smaller than 20 Å are instable with respect to an increase in their diameters and conical scrolls can be trapped as meta-stable states. For larger structures both tubular and conical shape scrolls can be formed. Fig. 1 shows a simulated CNS obtained from a rectangular ghaphite sheet of 21.5 x 23.0 nm and containing about 20,000 carbon atoms. The obtained structural features are in very good agreement with the available experimental data [2]. We also observed that charge injection causes unwinding of the CNSs (Fig. 2), which might be an important feature to use CNSs as nano-mechanical actuators.

References:

[1] M. S. Dresselhaus, G. Dresselhaus, and P. C. Ecklund, *Science of Fullerenes & Carbon Nanotubes*, Academic Press, New York (1996).

[2] L. M. Viculis, J. J. Mack, R. B. Kaner, Science **299** (2003) 1361.
[3] R. H. Baughman and D. S. Galvão, Nature (London) **365** (1993) 735.
[4] Universal 1.02 Molecular Force Field, available from Accelrys, Inc. as part of the Cerius suite programs. http://www.accelrys.com.
[5] S. F. Braga, V. R. Coluci, S. B. Legoas, R. Giro, D. S. Galvão, and R. H. Baughman, Nano Lett. – *in press*.

Figure 1. Three dimensional view of a Carbon Nanoscroll obtained from molecular dynamics simulations.

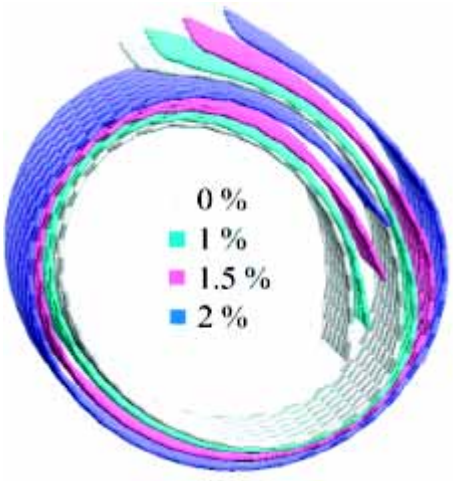

Figure 2. Nano scroll structure as a function of charge-per-carbon injection (expressed as percentages). The scroll unwinding as a function of increasing charge injection is clearly seen.

Work supported in part by the Brazilian Agencies FAPESP, CNPq, IMMP/MCT, CAPES, and the Robert A. Welch Foundation.