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Structure and Dynamics of Boron Nitride Nanoscrolls

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Abstract

Carbon nanoscrolls (CNSs) are structures formed by rolling up graphene layers into papyruslike shape. CNNs have been experimentally produced by different groups. Boron nitride nanoscrolls (BNNSs) are similar structures formed from rolling up boron nitride layers. In this work we report molecular mechanics and molecular dynamics results for the structural and dynamical aspects of BNNS formation. Similar to CNS, BNNS formation is dominated by two major energy contributions, the increase in the elastic energy and the energetic gain due to the van der Waals interactions of the overlapping surface of the rolled layers. The armchair scrolls are the most stable configurations, zigzag ones are metastable structures that can be thermally converted to armchair ones. Chiral scrolls are unstable and tend to evolve to zigzag or armchair scrolls depending on their initial geometries. The possible experimental routes to produce BNNSs are also addressed.

In order to address the structural and dynamical aspects of BNSs we have carried out molecular and molecular dynamics simulations using the well-known molecular universal force field (UFF)[1,2] as implemented in Cerius and Materials Studio[3] software. Boron and nitrogen atoms were assumed as having partial double bonds and sp2 hybridization. We investigated structures containing up to ~ 20,000 atoms, which precludes the use of full quantum methods. The evolution of the scroll structure was simulated using molecular dynamics (MD) methods for different temperatures (up to 300 K) within the NVT ensemble making use of a Nosé thermostat. The nanoscroll structures were generated by rolling a graphene or BN layer into a truncated Archimedean-type spiral, by rotation around the y1 axis defined by the angle θ shown in Fig. 1.

We have investigated the energetics and dynamical aspects of Boron Nitride Nanoscrolls (BNNSs) using molecular mechanics and molecular dynamics methods. Our results show that the BNNS formation mechanisms are quite similar to the Carbon Nanoscrolls (CNSs) ones[4]. Similar to CNS, BNNS formation is dominated by two major energy contributions, the increase in the elastic energy due to the bending of the initial planar structure (decreasing structural stability) and the energetic gain due to the van der Waals interactions of the overlapping surface of the rolled layers (increasing structural stability). There is a critical diameter value for scroll stability and reaching this limit the scrolled structure can be even more stable than its parent planar structures. The armchair scrolls are the most stable configurations (Fig. 2), zigzag ones are metastable structures that can be thermally converted to armchair ones. Chiral scrolls are unstable and tend to evolve to zigzag or armchair scrolls depending on their initial geometries.

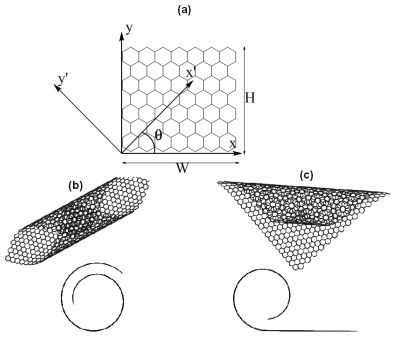

Figure 1 - (a) The unwrapped honeycomb lattice of a single layer (width *W* and height *H*). Here x_1 and y_1 are the scroll axes, which are rotated by an angle θ with respect to the reference coordinate system *xy*. The scroll is generated by wrapping the sheet around the axis y_1. Examples of (b) α and (c) β-type CNSs (with θ=45°) and their cross sections are shown.

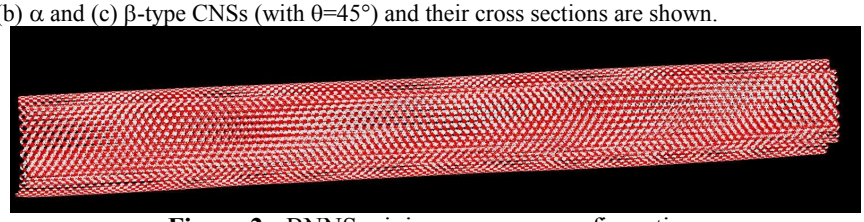

Figure 2 - BNNS minimum energy configuration.

[1] Goldberg D, Bando Y, Tang C, Zhi C 2007 *Adv. Mater.* **19** 2413
[2] Rappe A K, Casewit C J, Colwell K S, Goddard III W A and Skiff W M 1992 J. *Amer. Chem. Soc*. **114** 10024
[3] Root D, Landis C and Cleveland T 1993 *J. Amer. Chem. Soc.* **115** 4201
[4] Braga S F, Coluci V R, Legoas S B, Giro R, Galvao D S and Baughman R H 2004 *Nano Lett.* ***4*** 881