Boron Nitride Nanoscrolls

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Recently, based on computer simulations, it has been proposed that stable boron nitride nanoscrolls (BNNSs) can exist. In this work we show that the BNNSs stability mechanisms follow the same simple physical principles proposed for carbon nanoscrolls (CNSs). For both classes of scrolls, the mechanical stability arises as the result of the interplay between attractive van der Waals forces and the elastic (bending) deformations. The topology (chirality) of the scrolled single-layer membranes plays an important role defining BNNS stability. A controled way to produce BNNSs is also addressed.

I. INTRODUCTION

Carbon nanoscrolls (CNSs) are structures composed of only carbon atoms, such as, graphite, fullerenes[1], nanotubes[2] and graphene[3]. CNSs were first observed by Bacon[4] decades before the disovery of fullerenes and nanotubes, but did not attract much attention. Only recently advances were made on the low-themperature synthesis of these structures[5, 6] which sparked new interest on these nanostrucures [7–10]. CNS structures consist of rolled up graphene sheets with both ends opened, as in a papyrus scroll. Thus, they present great radial flexibility and a large accessible surface area, with many potential technological applications[8–10]. Considering that the boron nitride (BN) fullerenes-like [11], BN nanotubes [12, 13] and single BN monolayers [14, 15] have already been obtained, we can expect that BN nanoscrolls (BNNSs) should also exist. In fact, that stable BNNSs can exist have been proved based on computer simulations [16]. Here we briefly discuss the BNNSs stability mechanisms and possible fabrication approaches.

II. METHODOLOGY

We carried molecular mechanics (MM) and molecular dynamics (MD) simulations using the classical force field Universal Force Field (UFF)[17] as implemented on Accelrys Materials Studio[18]. UFF includes bond stretching, angle bending, torsion, inversion, and van der Waals terms. Both boron and nitrogen atoms were assumed as having sp^2 hybridization and no explicit charges. Dynamics were carried out using the NVT ensemble and a Nosé thermostat. The scrolls were generated by rolling a rectangular BN honeycomb sheet into a truncated Archimedean spiral-like structure, which is described by the parametric equation $r = a\phi + a_0$, where a and a_0 are non-zero constants and r and ϕ are the usual polar coordinates. The interlayer spacing d is related to a by $a = d/2\pi$ and we used d=3.4Å in accordance to the interlayer spacing of BN crystals. The chirality of the scroll is defined by the angle θ defined by the rolling axis y', as shown in figure 1, $\theta = 0$ being a zigzag scroll, $\theta = 90$ an armchair one and $0 < \theta < 90$ a chiral scroll. The values of W and H determine scroll dimensions.

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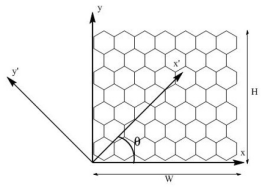

Figure 1: Scroll geometric parameters and the definition of the θ angle.

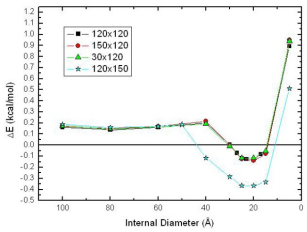

Figure 2: Energy profile of bent sheets with respect to its diameter. ΔE is the energy difference per atom between the bent and the planar sheet configurations. Sheet dimensions are given in the HxW form

III. RESULTS AND CONCLUSIONS

Similarly to CNSs[7], the stability of BNNSs is due to the interplay between van der Waals and elastic forces. When a planar sheet is bent, there is an increase in energy due to the elastic forces, which tend to unbend the sheet, but when the curvature is high enough as for the sheet ends to overlap each other, there is a decrease of the energy due the van der Waals attraction between overlapping layers. Under certain configurations the balance between these opposing forces can produce a stable structure, even more stable than the planar sheet, as shown in figure 2. We can also see that scroll stability depends on its dimensions, in the case of zigzag (armchair) scrolls the important dimension being W (H) which is the dimension responsible for the number of overlapping layers, while the other one only controls scroll length. This balance between both forces becomes more evident when we look at the van der Waals and the bending energy contributions separately, as shown in figure 3 (for a 120 Åx120 Åsheet). As the sheet is being bent its bending energy continuously increase, but as soon as opposing sheet ends begin overlapping the van der Waals contribution rapidly decreases and thus a stability valley is formed.

The stability dependence on the chirality becomes evident

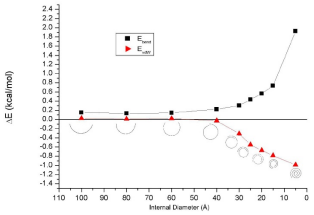

Figure 3: van der Waals and bending energy evolution during the process of scrolling a planar sheet.

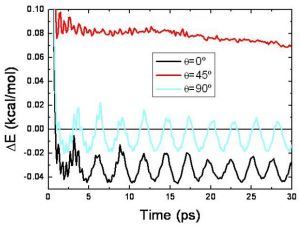

Figure 4: ΔE time evolution for scrolls of different chirality. See text for discussions.

when we analyze the time evolution of scrolling sheets with different θ values. As scrolled sheets with inner diameter values close to those of stability evolve freely in time we compute the energy difference ΔE and plot them in figure 4. It becomes evident that zigzag ($\theta = 0$) scrolls are the most stable ones, while armchair ($\theta = 90$) are metastable states and chiral ($0 < \theta < 90$) are unstable, evolving to zigzag scrolls after some time.

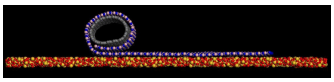

Figure 5: Snapshot of BNNSs formation initiated by a CNT.

Recently, an all-dry route to fabricating CNSs has been proposed based on results from molecular dynamics simulations[19]. They showed that the scrolling of a graphene sheet deposited over SiO_2 substrates can be initiated by a CNT. Since recently BN monolayers have been obtained [14, 15] we investigated the possibility of using the same approach to synthesize BNNSs in laboratory. As our simulations show[20], the method is quite promissing for the synthesis of both CNSs and BNNSs under special conditions in which the CNT presence alter the energy balance and favors the scrolling of the deposited sheet. A snapshot of on of these simulations is shown in figure 5.

IV. ACKNOWLEDGMENTS

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