Boron nitride nanotube peapods at ultrasonic velocity impacts: a fully atomistic molecular dynamics investigation

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Abstract
Boron nitride nanotube peapods (BNNT-peapod) are composed of linear chains of $C_{60}$ molecules encapsulated inside BNNTs, they were first synthesized in 2003. In this work, we investigated the mechanical response and fracture dynamics of BNNT-peapods under ultrasonic velocity impacts (from 1 km s$^{-1}$ up to 6 km s$^{-1}$) against a solid target. We carried out fully atomistic reactive molecular dynamics simulations using a reactive force field. We have considered the case of horizontal and vertical shootings. Depending on the velocity values, we observed tube bending, tube fracture, and $C_{60}$ ejection. Furthermore, the nanotube unzips for horizontal impacts at certain speeds, forming bi-layer nanoribbons ‘incrusted’ with $C_{60}$ molecules. The methodology used here is applicable to other nanostructures. We hope it motivates other theoretical investigations on the behavior of nanostructures at ultrasonic velocity impacts and aid in interpreting future experimental results. It should be stressed that similar experiments and simulations were carried out on carbon nanotubes trying to obtain nanodiamonds. The present study expands these investigations to include BNNT.
1. Introduction

The hypervelocity impact (HVI) of single- and double-walled carbon and boron nitride nanotubes (BNNTs) have been extensively investigated, theoretically and experimentally. In these experiments, nanotubes collide with solid substrates at ultrasonic velocities (usually between 2 and 8 km s\(^{-1}\)). The resulting impact forces induce significant structural deformations that can result in new structures, depending on parameters such as impact angle and speed, number of layers, and material composition, among other factors [1–6]. These initial investigations also compared the results of molecular dynamics (MD) simulations with experiments. This comparison revealed that both methodologies produced similar structures after the impact of nanotubes with a substrate [4–6].

For single-walled carbon nanotubes (SWCNTs), the high-velocity impacts generate (due to structural deformations) localized stress at the edges of the tubes, breaking C–C bonds in almost perfect lines, unzipping the tubes and producing carbon nanoribbons [4]. Similarly, double-walled carbon nanotubes become completely unzipped (two walls at the same time) through stress accumulation at the edges of the structure, as structural deformations are now constrained by the second wall [7]. On the other hand, double-walled boron nitride nanotubes exhibit a different pattern, unzipping one wall at a time due to the higher hardness of the inner core and the brittle character of boron nitride (BN) materials [8].

The above-cited works were carried out for nanotubes of the same composition (carbon or boron nitride). Theoretically, \textit{ab-initio} investigations can elucidate the stability [9], mechanical properties [10], and even reaction pathways [11] for structures of varied composition. Experimentally, hybrid tubes with different wall compositions (external and internal) have already been synthesized. One example is the hybrid BN-C nanotube (composed of concentric carbon and boron-nitride walls), experimentally realized by Nakanishi’s group [12]. A study of the high-velocity impacts of these new hybrid nanotubes has already been reported, in which the authors predicted the elastic response of the individual walls [13]. The authors showed that they have remarkably different elastic properties in relation to carbon nanotubes (CNTs) and BNNTs. For example, the tubes can decouple, and the carbon nanotube can unzip. These results opened up a new perspective for synthesizing nanostructures with different topologies and compositions.

Carbon nanotube peapods are an interesting example of hybrid carbon-based nanostructures, and they are composed of fullerenes encapsulated in carbon nanotubes. They have been synthesized through different experimental techniques [14–17], and exhibit interesting chemical and physical properties [18–20]. They can even present higher thermal conductivity than SWCNT [21]. These remarkable properties have been exploited in many applications in nanotechnology, which include transistors [22], solar cells [23], nano-memory devices [24], and supercapacitors [25]. A previous HVI study [26] showed that peapods exhibit remarkable resilience under high strain rate conditions. The simulations showed large structural deformations and multiple fracture pathways, depending on the impact velocity and relative nanotube-substrate orientation during the impacts.

Another hybrid nanostructure already synthesized is the BNNT peapod [27]. These structures are composed of C\(_{60}\) fullerenes encapsulated in BNNTs [28] (figures 1(a)–(c)). These structures have received less attention in the literature than their carbon nanotube counterparts. In particular, a comprehensive study on their structural deformation behavior at HVI impacts is still missing. One of the objectives of the present work is to carry out this study.
2. Computational methodology

In this work, we carried out fully atomistic reactive MD simulations to analyze the structural deformations and fracture patterns of BNNT-peapods at HVI against a rigid target. The target used in the simulations is a rigid van der Waals (vdW) wall, a mathematical construct, not a real wall composed of atoms. As a BNNT-peapod approaches the rigid wall, its atoms interact with the target according to the 12-6 Lennard–Jones potential:

\[ E = 4 \epsilon \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \]  

where \( r \) is the distance between an atom and the vdw wall, \( \epsilon = 0.07 \) kcal mol\(^{-1}\), and \( \sigma = 5.0 \) Å. We have considered two impact orientations (see figures 2(a) and (b)): (a) vertical shooting, where the angle between the main axis of BNNT and the plane of the target is 90°; (b) lateral shooting, where this angle is 0°. For both cases, we considered impact velocities ranging from 1 km s\(^{-1}\) (low speed) up to 6 km s\(^{-1}\) (ultrasonic speed), with a step velocity increase of 1 km s\(^{-1}\).

The simulations were carried out using the set of parameters for C/B/N atoms defined for the reactive force field (ReaxFF), as implemented in the LAMMPS code [39]. The reactive force field allows the breaking and formation of chemical bonds and was previously used to study the mechanical behavior of nanostuctures at ultrasonic impacts [30–32]. ReaxFF produces results in good agreement with quantum simulation methods in describing carbon-based nanostructures [33, 34].

For all simulations, we considered a 14.9 nm long (12,12) BNNT, containing an encapsulated linear arrangement of 10 C\(_{60}\) molecules. Without considering the vdw radius, the diameter of the (12,12) BNNT is 1.66 nm, and the diameter of the C\(_{60}\) molecule is 0.70 nm. For reference, the vdw radii of C, B, and N is 0.170, 0.192, and 0.155 nm, respectively. To create the BNNT-peapod, we added a fullerene at one end of the BNNT, and added more fullerenes separated by a constant distance of 0.837 nm (see figures 2(a) and (b)). We stopped adding fullerenes when the next one would be outside of the BNNT. An asymmetric configuration can occur as there is incommensurability between the fullerene distances and tube length (fullerenes closer to the tube end experience a different force from the ones at the tube center). In total, the hybrid system contains 3480 atoms.

A time step of 0.025 fs was used to integrate the equations of motion. This small step was used because the atom positions evolve quickly during the impacts. The BNNT-peapods were first equilibrated with an NVT ensemble (constant number of particles, volume, and temperature) at 300 K for 1.0 \( \times \) 10\(^3\) time-steps, using a chain of three Nosé–Hoover thermostats [35]. Then, we turned off the thermostat and added a vertical component to the velocity of each atom in the structure. The system is then free to evolve for \( 5 \times 10^{5} \) time steps using an NVE ensemble (constant number of particles, volume, and energy). This approach has been successfully applied to many theoretical investigations of nanostructures at HVI [4, 13, 31, 32].

We analyzed in detail the BNNT-peapods during and after the impacts. During the impacts, the BNNT-peapods experience pressure-induced deformations. The pressure values can be evaluated, as a function of time, using the following expression: [36, 37]:

\[ P_{\text{atoms}} = Nk_{\text{B}}T - \left( \frac{1}{V} \right) \frac{1}{3} \sum_{l=1}^{N} \sum_{m=1}^{N} \sum_{m'=1}^{N} r_{lm} \frac{d\phi}{dr_{lm}} \]  

where in the first term, \( N \) is the number of atoms, \( k_{\text{B}} \) is the Boltzmann constant, and \( T \) is the temperature. The second term is related to the interatomic forces among the atoms, whose elements are the contribution of the force and the position vector components between the \( l \) and \( m \) atoms in the BNNT peapods. In this term, \( V \) is the volume and \( \phi \) is the potential energy. We also calculated the time evolution of the hydrostatic stress, which is equal to one-third of the trace of the stress tensor [38]:

\[ \sigma_{hh} = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3} \]  

the hydrostatic stress can be negative (for compressive stress) or positive (for tensile stress). A similar methodology was successfully used in other studies [4–6, 13, 26, 31, 39].

3. Results and discussions

Representative MD snapshots of the temporal evolution for vertical shooting (90° with the target) at three different speeds...
Figure 3. Representative MD snapshots for vertical shooting (90° with the target) at three different impact velocities values. The numbers presented along each snapshot correspond to the time elapsed since the shooting.

(1, 2, and 3 km s\(^{-1}\)) are presented in figure 3. The results show that structural deformations and fractures occur mainly on the nanotubes. Moreover, they reveal that, as expected, the degree of deformation/fracture depends on the impact velocities. For low values (1 km s\(^{-1}\)), the conversion of kinetic energy into elastic energy causes mainly nanotube bending (figure 3(a)). As the velocity increases, the tube is fractured, with an increasing number of broken bonds (figure 3(b)), resulting in a fast release of kinetic energy. For \(v = 2\) km s\(^{-1}\), the impact causes both BNNT bending and bond breaking, while...
Figure 4. Representative MD snapshots for horizontal shooting (0° with target) at three different impact velocity values. The numbers presented along each snapshot correspond to the time elapsed since the shooting.

for \( v = 3 \text{ km s}^{-1} \), the impact essentially leads to extensive bond breaking and C\(_{60}\) ejection (figure 3(c)). These results are similar to those reported in the literature for nanotubes, which show that vertical impact can induce extensive fractures due to a high accumulation of energy in a small number of atoms and bonds \([4–6, 13, 26, 31, 39]\).

We also considered the results for horizontal shooting. In figure 4 are presented some representative MD snapshots. It is possible to see that there is a better distribution of the kinetic energy during the impact, reducing the number of atoms ejected from the structure. The C\(_{60}\) remain intact for impact velocities of up to 3 km s\(^{-1}\). For the BNNTs, the level of structural fragmentation again depends on the impact velocity value. For \( v = 1 \text{ km s}^{-1} \), the nanotube is deformed without fracture, and for \( v = 2 \text{ km s}^{-1} \), some bonds break, forming defects on the BNNT wall. On the other hand, for \( v = 3 \text{ km s}^{-1} \), the BNNT fractures are extensive. Careful inspection of the results reveals that the bonds break mainly near the C\(_{60}\) within the nanotubes. We further discuss this result in more detail below.

From 4 km s\(^{-1}\) (figure 5), the number of broken bonds in the BNNT wall increases, and the impact also start fracturing
the C$_{60}$. The dynamics of this process can be visualized with the aid of supplementary movie S1 (MD trajectory displaying the lateral impact of a BNNT-peapod with a rigid substrate at $v = 4.0$ km s$^{-1}$. The color indicates the local stress value). In figure 6, we present the percentage of broken bonds as a function of the simulation time, corroborating this assertion. For better analyses, the system is divided into four regions: (i) the bottom and (ii) the top of the BNNT; (iii) the bottom and (iv) the top of the C$_{60}$. These results reveal a clear relationship between impact velocity and fracture patterns. From figure 6(a), we can see that for velocity values equal to or below 3 km s$^{-1}$, there is no particular region for the nanotube fracture. For both the bottom and the top areas, the percentage of broken bonds graph presents a plateau of around 7%. However, as the impact velocity increases, an asymmetry emerges in the bond break between the upper and lower regions. For instance, for $v = 5$ km s$^{-1}$, the difference is around 11% points. Thus, for higher impact velocities, the presence of C$_{60}$ induces an increase in broken bonds at the bottom of the nanotubes, preserving the top area. This effect enables the possibility of obtaining nanoribbons from unzipped nanotubes. For C$_{60}$, a similar asymmetry emerges between the top and bottom regions (figure 6(b)). As mentioned above, for the most part, fullerenes remain intact after impact for velocity values below 4 km s$^{-1}$. At $v = 4$ km s$^{-1}$, around 15% of the bonds in the bottom part of the C$_{60}$ break, compared to 32% for the bottom of the BNNT. On the other hand, for an impact velocity of 6 km s$^{-1}$, C$_{60}$ fractures are more extensive than those of the nanotubes. The C$_{60}$ are almost completely fragmented at this critical velocity value.

Similar to CNTs, BNNT-peapods at high-velocity impacts could, in principle, also result in unzipped nanotubes. To investigate this possibility, we selected velocity values between 3 km s$^{-1}$ (where the asymmetry in bond breakage is small) and 4 km s$^{-1}$ (where the fracture is already extensive). The results below are for a shooting velocity of 3.3 km s$^{-1}$, and the corresponding MD trajectory is presented in supplementary movie S2 (MD trajectory displaying the lateral impact of a BNNT-peapod with a rigid substrate at $v = 3.3$ km s$^{-1}$). In figure 7, we present the hydrostatic stress values as a function of the simulation time. We selected an example in which the tube unzipping occurred. To investigate the propagation of stress in detail, we divided the system into four regions and calculated the average stress in each part at each instant. In part (a) of figure 7, the orange/red curves correspond to the average stress in the lower/upper part of the BNNT, while the gray/black curves correspond to the average stress at the lower/upper part of the C$_{60}$. One advantage of using hydrostatic stress is that its sign differentiates compressive (negative) and tensile (positive) stresses. We also analyzed local stress patterns, and in figures 7(b)–(e), we used a color scale ranging from red to blue to indicate the local values of the hydrostatic stress.

Before the collision with the substrate (indicated with the blue dotted line in figure 7(a)), we find that, as expected, the stress values are low throughout the system (figure 7(b)). Since the lower part of the BNNT collides first with the substrate, the stress increases in this region immediately after impact, leading to the first compressive peak in orange in figure 7(a). Figure 7(c) presents the corresponding stress distribution in this region, and we find that the entire lower part of the BNNT is under compression at this time. The stress then propagates upward, towards the lower part of the C$_{60}$ (gray peak in figure 7(a)), and then towards their upper parts (black peak in figure 7(a)). Directly after this compressive spike, we noticed a sharp tensile stress peak in the upper part of the BNNT, reaching 74.6 GPa, as the C$_{60}$ push this region up (see figure 7(d)). Consequently, a partial fracture occurs through this BNNT region, as shown in figure 7(e). Figure 7(f) provides further insights into the partial unzipping process. In this figure, we made part of the nanotube transparent to highlight the C$_{60}$ configuration inside the BNNT during the collision. Notice in the frame obtained at $t = 0.72$ ps that the C$_{60}$ presses against the upper part of the BNNT, leading to fractures of the nanotubes in the areas where the fullerenes are present ($t = 1.10$ ps).
In all cases, we only observed partial unzipping as a result of the presence of distance gaps between the fullerenes. Finally, note that the stress values at the BNNT-C_{60} points of contact are certainly higher than the numbers presented in figure 7(a), which provides values averaged over regions of the system.

To understand the role of the fullerenes at impact, comparing HVI results for BNNTs with and without fullerenes is instructive. For this comparison, we use BNNT results from the literature [6]. Comparing results for single-walled BNNTs with (without) C_{60}, for a lateral impact at $v = 4.0 \text{ km s}^{-1}$, we find the percentage of broken bonds is 28.7% (29.6%). Hence, the presence of fullerenes slightly reduces fracture, although adding an inner BNNT to the outer nanotube has a more pronounced effect, reducing the percentage to 24.3%. Regarding the propagation of stress and the morphology after impact, the BNNT-peapods have an outcome closer to double- and multi-walled BNNTs. In both instances, the impact stress propagates through the inner layers toward the top of the external nanotube, where tension causes unzipping. However, in the
4. Conclusions and remarks

Fully atomistic reactive MD simulations were carried out to investigate the dynamics of high-velocity ballistic impacts of BNNT-peapods against a solid target for the cases of vertical and horizontal collisions. For low velocity vertical (1 km s$^{-1}$) shootings, the major structural deformations are in the BNNTs (mainly tube bending). With increasing velocity, the tube is fractured with $C_{60}$ ejections. The stress is better distributed for horizontal shootings, and BNNTs retain their structural integrity for small velocity values. Increasing the velocity values, the tube fracture became extensive, and bonds broke mainly near the encapsulated fullerenes. An interesting result is the formation of nanoribbon structures from unzipped tubes. For example, for a velocity impact of 3.3 km s$^{-1}$, the BNNT is unzipped with the formation of a bilayer nanoribbon “incrusted” with $C_{60}$. The nanostructures investigated here have already been synthesized, and we hope our results motivate further research on the response of BNNT-peapods to high-strain rate deformations. We also hope that the results obtained in this research article by the reactive classical MD method (ReaxFF) will motivate further research on the response of other complex nanostructures to high strain rate mechanical deformations.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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