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# A theoretical scenario for the mechanical failure of boron carbide nanotubes

Azam Salmankhani <sup>1</sup>, Zohre Karami <sup>2</sup>, Amin Hamed Mashhadzadeh <sup>2\*</sup>,  
Maryam Zarghami Dehaghani <sup>2</sup>, Mohammad Reza Saeb <sup>2</sup>,  
Vanessa Fierro <sup>3</sup>, Alain Celzard <sup>3,†</sup>

<sup>1</sup> Faculty of Mechanical Engineering, K. N. Toosi University of Technology, Tehran, Iran; [azamsalmankhani@gmail.com](mailto:azamsalmankhani@gmail.com); P.O.Code: 1969764499

<sup>2</sup> Center of Excellence in Electrochemistry, School of Chemistry, College of Science, University of Tehran, P.O. Box: 14155-6455, Tehran, Iran; [zohrekarami.2013@yahoo.com](mailto:zohrekarami.2013@yahoo.com) & [amin.hamed.m@gmail.com](mailto:amin.hamed.m@gmail.com) & [maryam\\_zz67@yahoo.com](mailto:maryam_zz67@yahoo.com) & [mrsaeb2008@gmail.com](mailto:mrsaeb2008@gmail.com)

<sup>3</sup> Université de Lorraine, CNRS, IJL, F-88000 Epinal, France; [vanessa.fierro@univ-lorraine.fr](mailto:vanessa.fierro@univ-lorraine.fr) & [alain.celzard@univ-lorraine.fr](mailto:alain.celzard@univ-lorraine.fr)

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\* Correspondence: [amin.hamed.m@gmail.com](mailto:amin.hamed.m@gmail.com) ,  
[amin.hamedmashhadzadeh@yahoo.com](mailto:amin.hamedmashhadzadeh@yahoo.com); Tel.: (+98-9113765114)

† Correspondence: [alain.celzard@univ-lorraine.fr](mailto:alain.celzard@univ-lorraine.fr); Tel.: (+33-372-74-9614)

## 23 **Abstract**

24 Although the volume of research on carbon nanotubes (CNTs) has increased over a short  
25 period, less attention has been paid to other types of carbon-based nano-objects such as boron  
26 carbide ( $\text{BC}_3$ ) nanotubes ( $\text{BC}_3\text{NTs}$ ). In the present article, we modeled  $\text{BC}_3\text{NTs}$  using  
27 molecular dynamics (MD) simulation to investigate the effects of chirality, wall number,  
28 diameter and temperature on the mechanical failure of  $\text{BC}_3\text{NTs}$ ,  $\text{BC}_3$  nanobuds and  $\text{BC}_3\text{NTs}$   
29 with different kinds of defects. In addition, we modeled the corresponding CNTs to validate  
30 the results and understand how the replacement of a quarter of the carbon atoms in the CNT  
31 by boron atoms affects the properties of the newly formed nanotube. The results showed that  
32 the variation of mechanical properties as a function of diameter and temperature was rather  
33 limited, regardless of chirality. The Young's modulus, failure stress and failure strain of the  
34 zigzag single-walled  $\text{BC}_3\text{NTs}$  ( $\text{SWBC}_3\text{NTs}$ ) were lower than the armchair ones, and were  
35 lower than those of the corresponding CNTs too. Furthermore, adding a second and third  
36 wall to the  $\text{SWBC}_3\text{NTs}$  significantly improved their mechanical properties. Finally, we  
37 modeled  $\text{BC}_3$  nanobuds with 1 to 4  $\text{C}_{60}$  attached to the surface of  $\text{SWBC}_3\text{NTs}$  and observed  
38 that the properties decreased as the number of fullerenes increased. Moreover, considering  
39 defective  $\text{SWBC}_3\text{NTs}$  revealed that two-atom vacancies and Stone-Wales defects resulted in  
40 the highest and lowest reduction of mechanical properties, respectively.

41 **Keywords:**  $\text{BC}_3$  nanotubes; Molecular Dynamics; Mechanical Properties; Nanobud; Defect

42

## 43 1. Introduction

44 Carbon nanotubes (CNTs) are best known for their excellent mechanical strength, high  
45 thermal and electrical conductivity and good sensing capability, making them excellent  
46 candidates for the development of technical materials and systems (see Figure 1S in the  
47 Supplementary Information, SI) [1, 2]. Chemical doping with heteroelements is a promising  
48 technique for improving their mechanical, electronic, optical and chemical properties [3-8].  
49 A particular type of boron-doped CNTs can be obtained when a quarter of the carbon in the  
50 graphene is replaced by boron atoms, resulting in a new structure called  $BC_3$  graphene. Like  
51 CNTs,  $BC_3$  nanotubes ( $BC_3$ NTs) are formed when a  $BC_3$  sheet is wound along its chiral  
52 vector [9-11]. For  $BC_3$  compounds, only the B-C and C-C bonds are considered stable, while  
53 the B-B bonds are neglected because they are less stable.  $BC_3$  nanosheets have good  
54 temperature resistance and are of high crystalline quality [12].

55 The mechanical properties and failure mechanism of the nanostructures are of great  
56 importance, particularly at high temperatures [13, 14]. Although  $BC_3$ NTs have been  
57 extensively studied from an electronic or chemical perspective, less attention has been paid to  
58 understanding the mechanical failure of  $BC_3$ NTs. In a recent work, we have modeled and  
59 simulated the mechanical properties of either defect-free or defective  $C_3N$  nanotubes  
60 ( $C_3$ NNTs) and their nanobuds, and analyzed and compared the results with the corresponding  
61 modeled CNTs as a reference/control geometry for validation [15].

62 In this framework, we have developed  $BC_3$  nanotubes by replacing a quarter of the CNTs  
63 atoms with boron atoms in order to explore the effect of chirality, tube diameter, number of  
64 walls and temperature on the elastic modulus, failure stress and failure strain of flawless and  
65 defective  $BC_3$ NTs, as well as  $BC_3$  nanobuds. Since no research has reported on the  
66 mechanical properties of  $BC_3$ NTs, the results of our previous work on corresponding CNTs  
67 with the same chirality and under the same loading conditions have been considered as a

68 reference to theoretically validate our new results obtained by Molecular Dynamics (MD)  
69 simulation [15].

70

## 71 **2. Computational design**

72 The molecular dynamics modeling in the present study was performed using the  
73 large-scale atomic/molecular massively parallel simulator (LAMMPS) package to predict the  
74 mechanical properties of BC<sub>3</sub>NTs in either armchair or zigzag chirality. To model C-C  
75 bonds, we selected the modified Tersoff potential presented by Lindsay and Broido [16].  
76 Moreover, to define the interaction of carbon and boron atoms, we used the Tersoff potential  
77 parameters developed by Kinaci et al. [17]. Armchair and zigzag BC<sub>3</sub>NTs with an  
78 approximate length of 5 nm were modeled and the results obtained were compared with those  
79 of the corresponding carbon nanotubes (CNTs) as reference materials from our previous  
80 article [15]. To calculate the mechanical properties, the stress-free structures at the simulated  
81 temperature were first performed with the isothermal-isobaric (NPT) ensemble at 300 K  
82 (pressure of 1 bar) with the time span of 100 ps. Next, the simulation box was stretched along  
83 the loading axial direction (z-direction) with the strain rate of 10<sup>9</sup> s<sup>-1</sup>. To measure the effects  
84 of temperature, single-walled nanotubes in either zigzag or armchair chirality were modeled  
85 and tested at temperatures varying from 300K to 900K. Besides, the effects of wall addition,  
86 fullerene attachment, and different types of defects on the elastic modulus, failure stress and  
87 failure strain of BC<sub>3</sub> nanotubes were determined under the same loading conditions. We have  
88 provided a brief flowchart of the total modeling process used in the present study in Figure 1.  
89 This flowchart follows the same procedure as that used in our previous article [15].

90

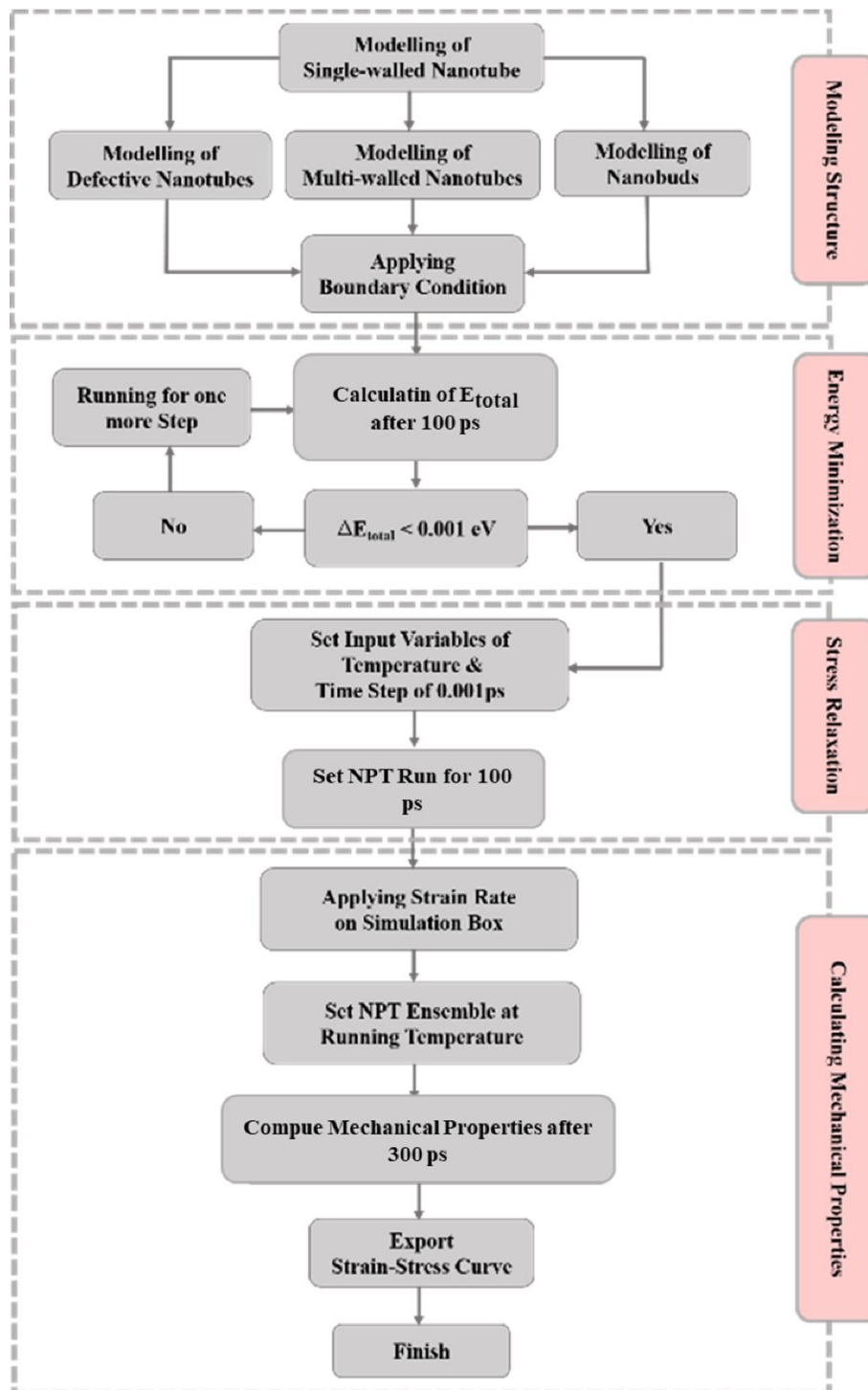
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## 92 **3. Results and discussion**

### 93 *3.1. Mechanical properties of single-walled BC<sub>3</sub>NTs*

94 To study the mechanical properties, we first modeled zigzag and armchair single-walled  
95 BC<sub>3</sub> nanotubes (SWBC<sub>3</sub>NTs) and their corresponding CNTs using molecular dynamics  
96 (MD) simulation. A schematic of the modeled SWBC<sub>3</sub>NTs and their stoichiometry are  
97 shown in Figure S2 and Table 1, both derived from the reference materials [15]. The values  
98 of radius corresponding to each chirality are tabulated in Table S1. In Figure S2 and Table 1,  
99 DWBC<sub>3</sub>NTs and TWBC<sub>3</sub>NTs refer to double-walled and triple-walled nanotubes,  
100 respectively. Next, all samples were subjected to uniaxial tensile loading with a strain rate of  
101 0.001 ps<sup>-1</sup> when the temperature was set at 300K, and the stress-strain ( $\sigma - \epsilon$ ) curves were  
102 extracted to calculate Young's modulus, failure stress, and failure strain. A schematic view of  
103 a (8,0) zigzag BC<sub>3</sub>NT under uniaxial tensile loading is shown in Figure S3.

104



**Figure 1.** Flowchart of the overall simulation steps including modeling, energy minimization and calculation of properties.

**Table 1.** Stoichiometry and chirality of SWBC<sub>3</sub>NTs, DWBC<sub>3</sub>NTs, TWBC<sub>3</sub>NTs.

Chirality	Number of Atoms	Chirality	Number of atoms
(4,4)	328	(4,4),(7,7)	902
(6,6)	492	(4,4),(8,8)	984
(8,8)	656	(4,4),(9,9)	1066
(10,10)	820	(4,4),(10,10)	1148
(12,12)	984	(4,4),(11,11)	1230
(8,0)	384	(4,4),(12,12)	1312
(10,0)	480	(8,0),(14,0)	1056
(12,0)	576	(8,0),(16,0)	1152
(14,0)	672	(8,0),(18,0)	1248
(16,0)	768	(8,0),(20,0)	1344
(18,0)	864	(4,4),(8,8),(12,12)	1968
(20,0)	960	(8,0),(14,0),(20,0)	2016

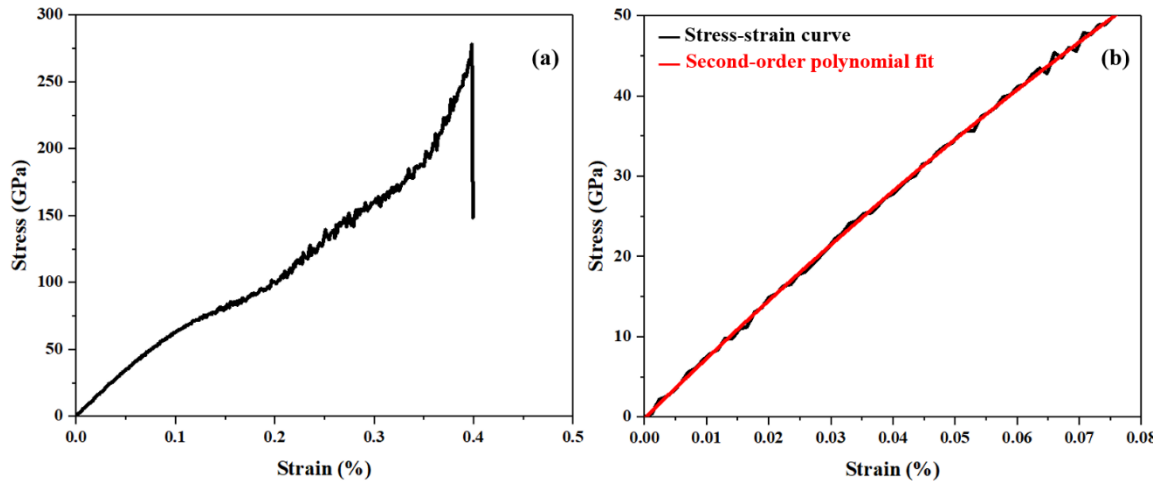
106

107 To obtain the Young's modulus, a second-order polynomial was fitted to the linear part  
108 of the stress-strain curves using the following equation [18].

$$\sigma = \frac{\partial U}{\partial \varepsilon} = D\varepsilon^2 + E\varepsilon + C \quad (1)$$

109 where  $E$ ,  $D$ , and  $C$  are the Young's modulus, third-order elastic modulus and residual stress  
110 of the nanotubes, respectively. A stress-strain curve plotted for a (6,6) armchair BC<sub>3</sub>NT is  
111 presented in Figure 2a, and Figure 2b shows a zoom of the linear part of the plot used for the  
112 second-order polynomial fit. As seen in Figure 2a, the highest stress obtained is observed at a  
113 strain rate of about 40%. Then, the stress drops to a considerably lower amplitude. Therefore,  
114 the coordinates of this point correspond to the values of failure stress and failure strain.





115

116 **Figure 2.** (a) Stress-strain curve for a (6,6) armchair BC<sub>3</sub>NT, and (b) zoom on the  
 117 second-order polynomial fit.

118

119 The same steps were repeated for all SWBC<sub>3</sub>NTs and the plots of the mechanical

120 properties are shown in Figure 3. According to Figure 3a, the Young's modulus of

121 SWBC<sub>3</sub>NTs is significantly lower than those of the reference SWCNTs [15], either in zigzag

122 or armchair structure. This could be associated with the stronger C-C bonds of CNTs

123 compared to B-C bonds of BC<sub>3</sub>NTs due to the shorter C-C bond (144.1 pm) compared to B-C

124 bond (153.5 pm). Furthermore, the Young's modulus of armchair SWBC<sub>3</sub>NTs was slightly

125 higher than zigzag structures of close radius. By increasing the size of the nanotubes, the

126 elastic modulus of armchair SWBC<sub>3</sub>NTs increased slightly from 724.8 GPa in structure (4,4)

127 to the maximum value of 780.5 GPa in structure (10,10) and then decreased to 776.7 GPa in

128 structure (12,12). Similarly, an upward behavior was observed in zigzag SWBC<sub>3</sub>NTs, i.e.,

129 the Young's modulus increased from the lowest value of 718.4 GPa in structure (8,0) to the

130 highest value of 751.7GPa in structure (16,0), and then decreased slightly to 741.5 GPa in

131 structure (20,0). By increasing the radius, the elastic modulus of the armchair and zigzag

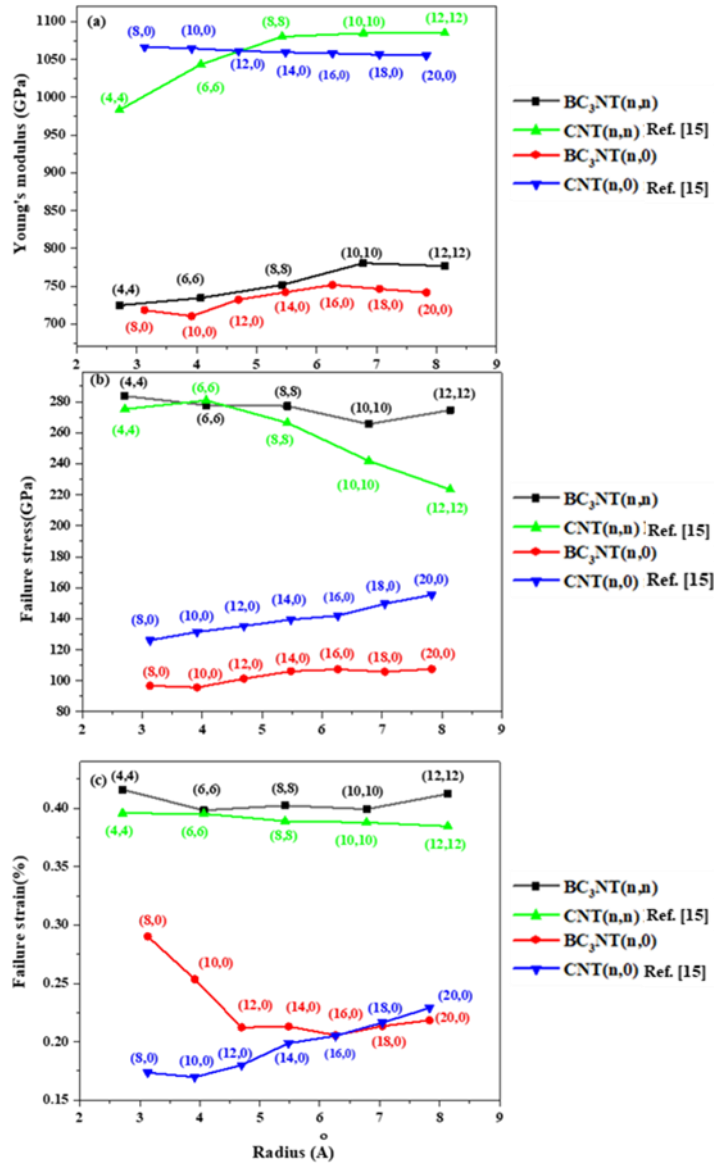
132 SWBC<sub>3</sub>NTs increased by approximately 7% and 4%, respectively. The same behavior was

133 observed for the Young's modulus of armchair SWCNTs while zigzag SWCNTs remained

134 almost unchanged by increasing the radius of nanotubes [15]. The results previously obtained

135 [15] with armchair and zigzag SWCNTs as reference materials were in the range of 1 TPa,

136 which is close to other data [19-21], thereby demonstrating the accuracy of the used model  
137 and the obtained results for SWBC<sub>3</sub>NTs. In their experimental study, Yu et al. reported the  
138 average modulus obtained for 8 SWCNT ropes using atomic force microscopy, equal to 1002  
139 GPa [22]. Furthermore, Treacy et al. calculated an elastic modulus in the range of 2TPa for  
140 individual SWCNTs of different lengths and radii [23]. Moreover, the failure stress plots in  
141 Figure 3b reveal that armchair SWBC<sub>3</sub>NTs have higher stress at break than zigzag  
142 SWBC<sub>3</sub>NTs (almost three times as high), and the same behavior was observed in armchair  
143 SWCNTs compared to zigzag ones as derived from reference samples [15]. The results  
144 obtained for armchair and zigzag SWBC<sub>3</sub>NTs and their corresponding SWCNTs are  
145 gathered in Tables S2 and S3, respectively.



**Figure 3.** (a) Young's modulus, (b) failure stress and (c) failure strain of armchair and zigzag structures of SWBC<sub>3</sub>NTs under uniaxial tensile tests at 300K and their corresponding reference SWCNTs materials (from [15]).

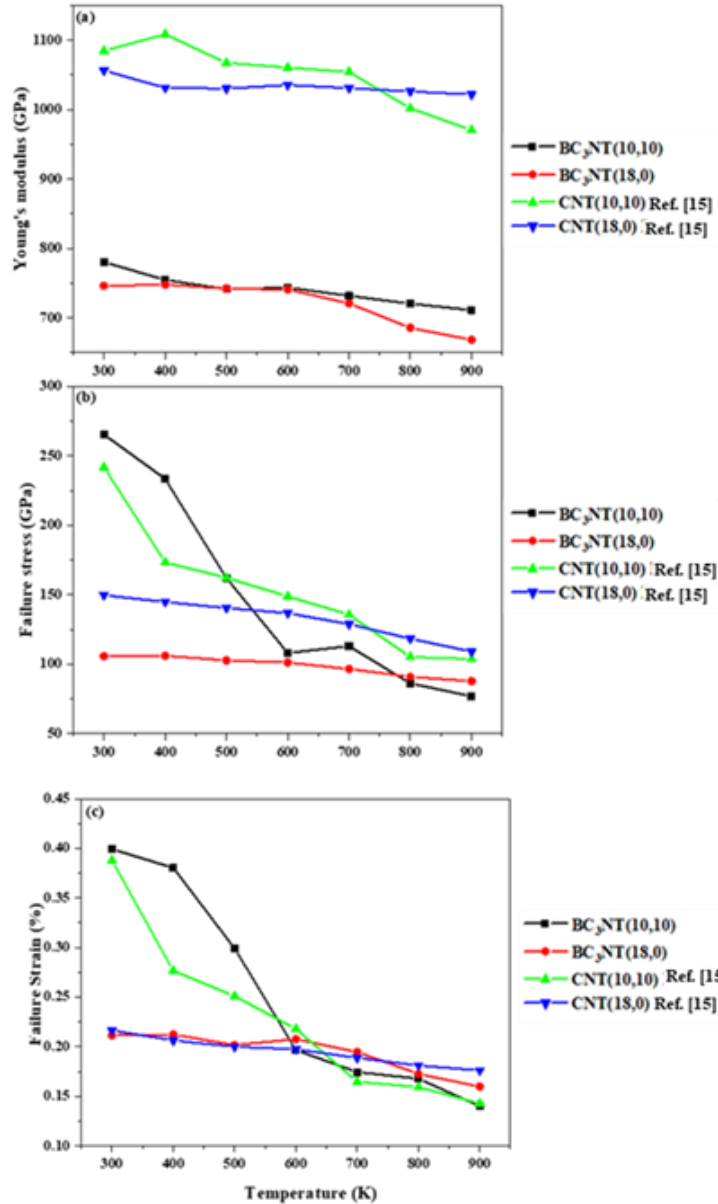
146

147 In addition, by increasing the radius of the nanotubes, the failure stress of the armchair  
 148 SWBC<sub>3</sub>NTs slowly decreased, while on the other hand, the failure stress of zigzag  
 149 SWBC<sub>3</sub>NTs increased (in the limits of certain fluctuations). The highest failure stress of the  
 150 armchair and zigzag SWBC<sub>3</sub>NTs obtained was observed in structures (4,4) and (20,0) with  
 151 values of 283.71 GPa and 107.6 GPa, respectively. Figure 3c shows the failure strain of the  
 152 SWBC<sub>3</sub>NTs and their corresponding reference SWCNTs (from [15]). According To this

153 figure, and as already noted for elastic modulus and failure stress, the failure strain of zigzag  
154 and armchair SWBC<sub>3</sub>NTs was higher than or very close to that of SWCNTs with close  
155 radius, and the failure strain of the armchair SWBC<sub>3</sub>NTs was higher than that of the zigzags.  
156 While the failure strain of the armchair SWBC<sub>3</sub>NTs and SWCNTs was almost unchanged,  
157 this property decreased significantly from the highest value of 0.295% in zigzag structure  
158 (8,0) to the lowest value of 0.205% in structure (16,0), followed by a small increase to 0.218%  
159 in structure (20,0). Overall, armchair SWBC<sub>3</sub>NTs exhibited higher mechanical properties than  
160 zigzag SWBC<sub>3</sub>NTs.

161 To understand the effects of temperature on the mentioned properties, we selected a  
162 zigzag and an armchair SWBC<sub>3</sub>NT with the closest radius, of structures (18,0) and (10,10),  
163 respectively, and examined their properties while the temperature was varied from 300K to  
164 900K as shown in Figure 4. We also used the results of our previous article for comparison  
165 with reference CNTs subjected to the same range of temperature [15]. This figure shows that  
166 temperature had a negative effect on the mechanical properties of both SWBC<sub>3</sub>NTs and  
167 SWCNTs. The Young's modulus of the armchair SWBC<sub>3</sub>NTs indeed constantly decreased  
168 from 780.5 GPa at 300K to 711.2 GPa at 900K (i.e., by 8%) while the modulus of zigzag  
169 SWBC<sub>3</sub>NTs was reduced from 746.4 GPa at 300K to 668.4 GPa at 900K (i.e., by 10%).  
170 Besides, Figures 4b and 4c reveal that, although the failure stress and failure strain of the  
171 armchair SWBC<sub>3</sub>NTs and SWCNTs were higher than for the corresponding zigzag structures  
172 at lower temperatures, these properties decreased sharply in armchair structures, reaching a  
173 lower value at higher temperatures compared to zigzag SWBC<sub>3</sub>NTs or SWCNTs. The  
174 minimum failure stress and failure strain were found in armchair SWBC<sub>3</sub>NTs at 900K with  
175 values of 76.85 GPa and 0.14%, respectively. The same kind of results were observed by  
176 Zahedi et al. for BC<sub>3</sub> single-layers [24]. They found that the Young's modulus of BC<sub>3</sub>

177 single-layers decreased by about 10% and 3% in armchair and zigzag directions at 900K  
 178 compared to 200K, respectively.



179 **Figure 4.** (a) Young's modulus, (b) failure stress and (c) failure strain of (10,10) and (18,0)  
 180 SWBC<sub>3</sub>NTs and SWCNTs reference materials (from [15]) under uniaxial tensile tests as a  
 181 function of temperature.  
 182  
 183

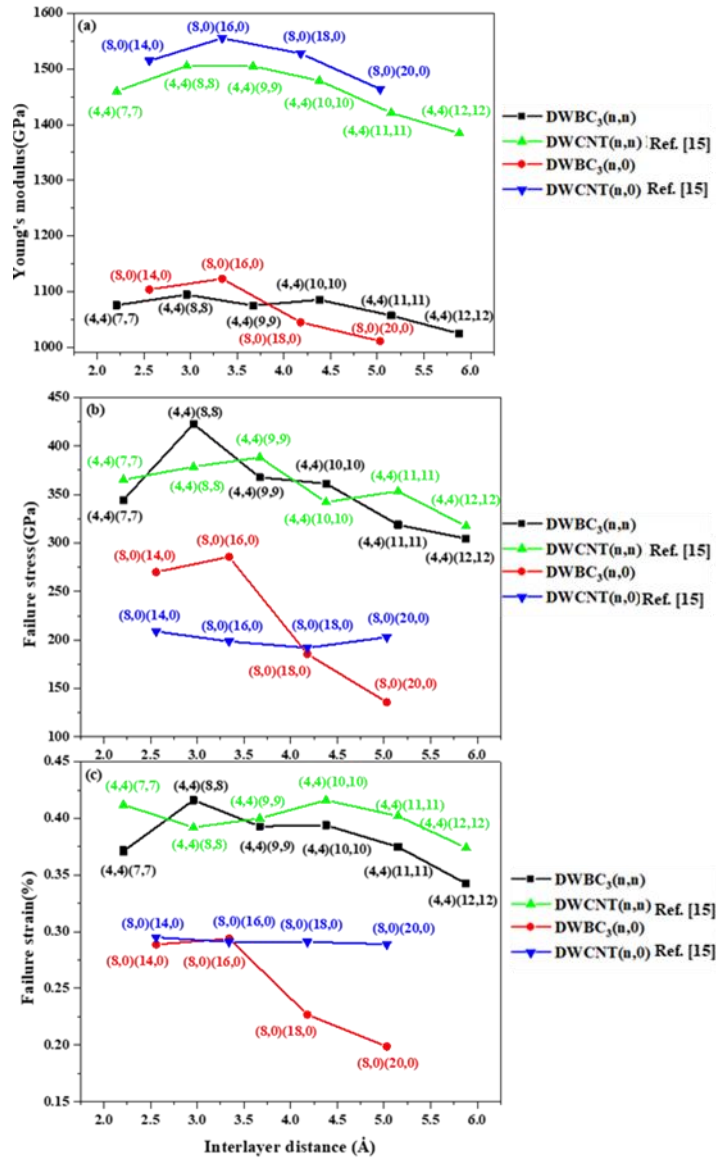
184 *3.2. Mechanical properties of double-walled BC<sub>3</sub>NTs*

185 In order to determine the effects of wall addition on the mechanical properties of  
 186 SWBC<sub>3</sub>NTs, six armchair and four zigzag double-walled (DWBC<sub>3</sub>NTs) were modeled and  
 187 tested, and the results were compared with those of the corresponding reference CNTs from

188 [15]. A schematic view of the designed DWBC<sub>3</sub>NTs is displayed in Figure S4, and the results  
189 of Young's modulus, failure stress and failure strain are presented in Figure 5. All tests were  
190 implemented at a constant temperature of 300K while the samples were subjected to uniaxial  
191 tensile loading. It should be mentioned that there are some limitations for modeling  
192 multi-walled nanotubes regarding interlayer distance. If the distance between layers exceeds  
193 a critical value, see Figure S5 for upper and lower limits of interlayer distance, no van der  
194 Waals interaction can take place between the layers and therefore no stable structure is  
195 formed. Otherwise, when the interlayer distance is below a certain value, the structure is  
196 unstable and collapses. Consequently, the distances shown in Figure S4 were selected to  
197 model stable armchair and zigzag structures with similar dimensions.

198 Figure 5a shows that by increasing the radius of the nanotubes, which is the consequence  
199 of the increase of the interlayer distance, the Young's modulus progressively decreased in  
200 both DWBC<sub>3</sub>NTs and reference DWCNTs samples from [15]. The elastic modulus of two of  
201 the zigzag DWBC<sub>3</sub>NTs including structures (8,0),(14,0) and (8,0),(16,0) was higher than  
202 those for armchair DWBC<sub>3</sub>NTs of a similar radius, including structures (4,4),(7,7) and  
203 (4,4),(8,8), and two others had a lower modulus than the corresponding armchairs  
204 DWBC<sub>3</sub>NTs. The maximum Young's modulus of the armchair and zigzag DWBC<sub>3</sub>NTs were  
205 1122.9 GPa and 1094.4 GPa, obtained for structures (8,0),(16,0) and (4,4),(8,8), respectively,  
206 and this property was about 8% and 5% lower in the thicker zigzag and armchair  
207 DWBC<sub>3</sub>NTs compared to the thinner ones. Comparison of the Young's modulus of  
208 DWBC<sub>3</sub>NTs and DWCNTs reveals the higher modulus of DWCNTs. The highest Young's  
209 modulus of DWCNTs was 1553.3 GPa, calculated for the structure (8,0),(16,0). This value is  
210 within the range of previous reports for DWCNTs, thus supporting the accuracy of the results  
211 of this study [25, 26].

212 Unlike Young's modulus, the failure stress of armchair DWBC<sub>3</sub>NT and DWCNT did not  
213 change significantly, as seen in Figure 5b. This property generally decreased in both  
214 structures by increasing the radius of double-walled nanotube despite some ups and downs.  
215 For the zigzag structures, it can be observed that as the radius increased, the failure stress of  
216 the zigzag DWCNTs remained virtually unchanged, while the failure stress of DWBC<sub>3</sub>NT  
217 with the same chirality dropped sharply to the lowest value obtained among all the  
218 double-walled nanotubes studied (135.81GPa). The highest failure stress of DWBC<sub>3</sub>NT was  
219 obtained 422.77 GPa and 285.74 GPa, obtained for structures (4,4),(8,8) and (8,0),(16,0),  
220 respectively, and this property decreased by about 50% and 11% in zigzag and armchair  
221 DWBC<sub>3</sub>NT, respectively.



**Figure 5.** (a) Young's modulus, (b) failure stress and (c) failure strain of armchair and zigzag DWBC<sub>3</sub>NTs 300K and their corresponding reference DWCNT from [15].

222

223

Besides, the examination of Figure 5c reveals that the failure strain of the armchair

224

DWCNTs and DWBC<sub>3</sub>NTs did not change significantly with the increase in the radius of the

225

nanotubes. However, like the failure stress, the failure strain of zigzag DWBC<sub>3</sub>NTs

226

decreased significantly (10%) as the radius of the nanotubes increases. The failure strain of

227

the armchair DWBC<sub>3</sub>NT was nearly twice as high as that obtained for the corresponding

228

zigzag DWBC<sub>3</sub>NT, and the highest failure strain of DWBC<sub>3</sub>NT was 0.416% and 0.293%,



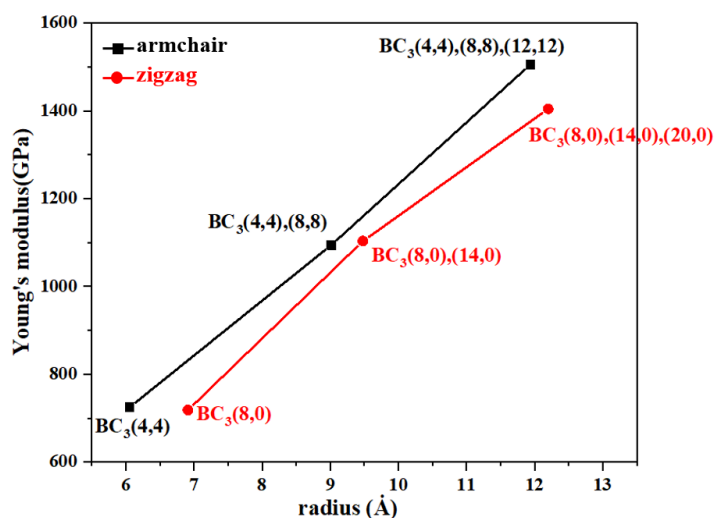
229 calculated for structures (4,4),(8,8) and (8,0),(16,0), respectively, similar to the failure stress.  
230 The results obtained for the armchair and zigzag DWBC<sub>3</sub>NT and DWCNT are summarized  
231 in Tables S4 and S5.

### 232 3.3. Effect of adding walls on the Young's modulus of BC<sub>3</sub>NTs

233 In order to measure the mechanical properties of BC<sub>3</sub>NTs with respect to the number of  
234 walls, a third wall was added to the DWBC<sub>3</sub>NT and a zigzag and an armchair TWBC<sub>3</sub>NT  
235 were modeled, while the results of the corresponding reference TWCNT of similar radius  
236 were used (from [15]). In other words, the main objective of this section is to examine how  
237 the addition of the second and third walls to a selected zigzag and armchair single-walled  
238 BC<sub>3</sub>NT could affect its Young's modulus. To this end, (4,4)(8,8)(12,12) armchair and  
239 (8,0)(14,0)(20,0) zigzag TWBC<sub>3</sub>NTs were modeled and tested under the same loading  
240 conditions at a constant temperature of 300K. A schematic view of the designed structures is  
241 shown in Figure S5, and the corresponding results are given in Table S6.

242 According to Figure 6, comparisons were made between the Young's modulus of  
243 BC<sub>3</sub>NTs having one, two, and three walls. In this figure, the Young's modulus of both zigzag  
244 and armchair SWBC<sub>3</sub>NT increased significantly as the number of walls increased from one  
245 to two and then to three. The addition of one wall to a (4,4) SWBC<sub>3</sub>NT improved its Young's  
246 modulus by about 33% (from 724.8 GPa to 1094.4 GPa), and the addition of another wall  
247 further increased the Young's modulus of the (4,4),(8,8) armchair structure by about 27%,  
248 reaching 1505.9 GPa in the structure (4,4),(8,8),(12,12), so that its total increase was about  
249 60%. Similarly, the modulus of the zigzag (8,0) SWBC<sub>3</sub>NT first increased by 34% to reach  
250 1103.5 GPa in the (8,0),(14,0) structure, followed by a further improvement of 21% to  
251 1404.4 GPa in the (8,0),(14,0),(20,0) structure. The same behavior was observed for  
252 TWCNTs confirms the reasonableness of the results presented. The results obtained  
253 demonstrate that increasing the number of walls has a synergistic effect on the Young's

254 modulus of the considered BC<sub>3</sub>NT, so that it could have the same effect on other BC<sub>3</sub>NTs of  
 255 different dimensions by adding more walls.

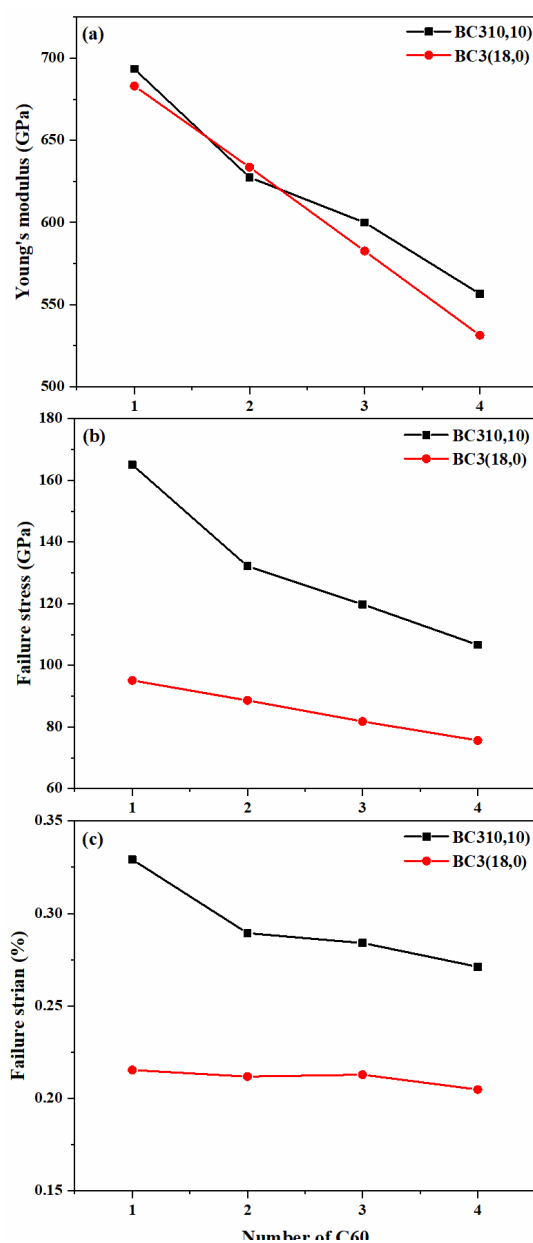


256  
 257 **Figure 6.** Young's modulus as a function of dimensions for different chiral single-, double- and  
 258 triple-walled BC<sub>3</sub>NT.  
 259

#### 260 3.4. Mechanical properties of BC<sub>3</sub> nanobuds

261 Recently, 3D nanostructures have received more attention. Nanobuds are a class of 3D  
 262 nanostructures that form once a fullerene or nanocage is attached to the outer surface of a  
 263 nanotube or graphene sheet. Research shows remarkable properties and applications of  
 264 nanobuds due to their porous shells and nanometric thickness [27-29]. In the present study,  
 265 C<sub>60</sub> fullerene was selected to model BC<sub>3</sub> nanobuds by attaching one, two, three and four C<sub>60</sub>  
 266 to the outer surface of SWBC<sub>3</sub>NT. An armchair and a zigzag single-walled BC<sub>3</sub>NTs with the  
 267 closest dimension, having (10,10) and (18,0) structures, respectively, were selected to model  
 268 nanobuds. These structures were selected because they have the closest dimensions when  
 269 we compared the dimensions of all the armchair and zigzag single-walled structures. Thus,  
 270 we were able to provide results that could be better compared. All samples were tested  
 271 under the same loading condition at a constant temperature of 300K. The graphs of the  
 272 Young's modulus, failure stress, and failure strain obtained in Figure 7 show that all  
 273 properties consistently decreased as the number of the attached fullerenes increased, whether

274 in armchair or zigzag chirality. This could be associated with the concentration of stresses  
 275 that exist around the regions where bonds form between the fullerene and the surface of the  
 276 nanotube. The higher the number of fullerenes, the higher the stress concentration and the  
 277 more the mechanical properties are degraded.



**Figure 7.** (a) Young's modulus, (b) failure stress, and (c) failure strain of BC<sub>3</sub> nanobuds under uniaxial tensile tests at 300K.

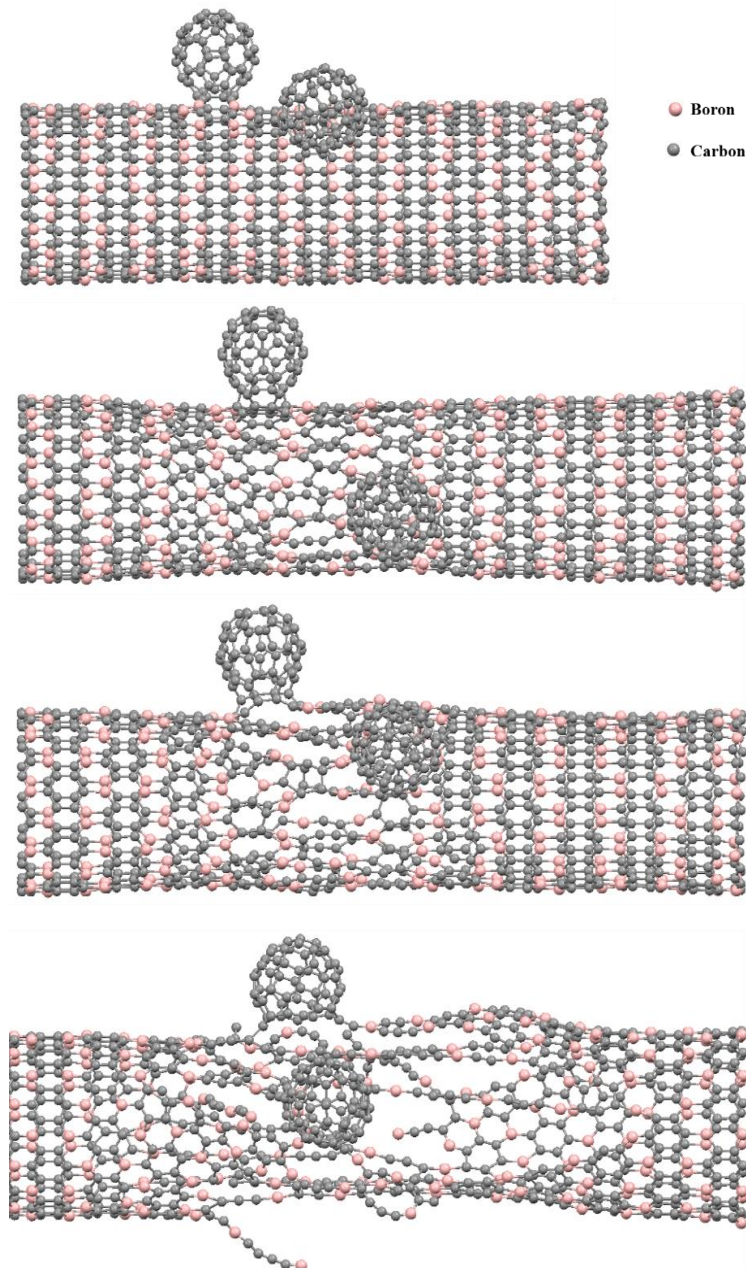
278

279 The Young's modulus, failure stress and failure strain of the armchair BC<sub>3</sub> nanobuds were  
 280 higher than for zigzag BC<sub>3</sub> nanobuds with the same number of fullerenes attached. In

281 addition, all mechanical properties of the armchair and zigzag nanobuds were less than or  
282 nearly identical to (except for the failure strain of zigzag-1C<sub>60</sub>) the corresponding  
283 SWBC<sub>3</sub>NT. The highest Young's modulus of the armchair and zigzag BC<sub>3</sub> nanobuds was  
284 693.4 GPa and 680 GPa, respectively, found in BC<sub>3</sub>-1C<sub>60</sub> structures, and the lowest modulus  
285 obtained was observed in BC<sub>3</sub>-4C<sub>60</sub> armchair and zigzag nanobuds with values of 556.6 GPa  
286 and 531.4 GPa. Both values were approximately 28% lower than the armchair and zigzag  
287 SWBC<sub>3</sub>NT. The same percentage reduction was found by comparing the failure stress of  
288 zigzag BC<sub>3</sub>-4C<sub>60</sub> nanobuds with that of the corresponding SWBC<sub>3</sub>NT (28%), while the  
289 failure stress of the armchair BC<sub>3</sub>-4C<sub>60</sub> was remarkably lower (nearly 60%) than that of the  
290 corresponding SWBC<sub>3</sub>NT (106.62 GPa against 265.52 GPa).

291 Similar results were reported in previous articles concerning other types of nanobuds.  
292 Thus, Ghorbanzadeh et al. [30] used DFT calculations to compare the mechanical properties  
293 of simple CNTs and CNT nanobuds. They found a tendency for the Young's modulus of  
294 zigzag and armchair CNTs to decrease after attaching one C<sub>60</sub> molecule. Mashhadzadeh et al.  
295 [31] reported in their DFT-based research that the Young's modulus of BeO nanobuds  
296 decreased considerably by increasing the number of attached nanocages. All values obtained  
297 for the mechanical properties of BC<sub>3</sub> nanobuds are shown in Table S7.

298 An overview of the failure process of a (18,0)-2C<sub>60</sub> nanobud under continuous tensile  
299 loading is provided in Figure 8. As can be seen, the failure started in the regions close to the  
300 attached fullerene molecules, due to higher concentration of stresses in these areas, which  
301 facilitates and accelerates crack formation and propagation.



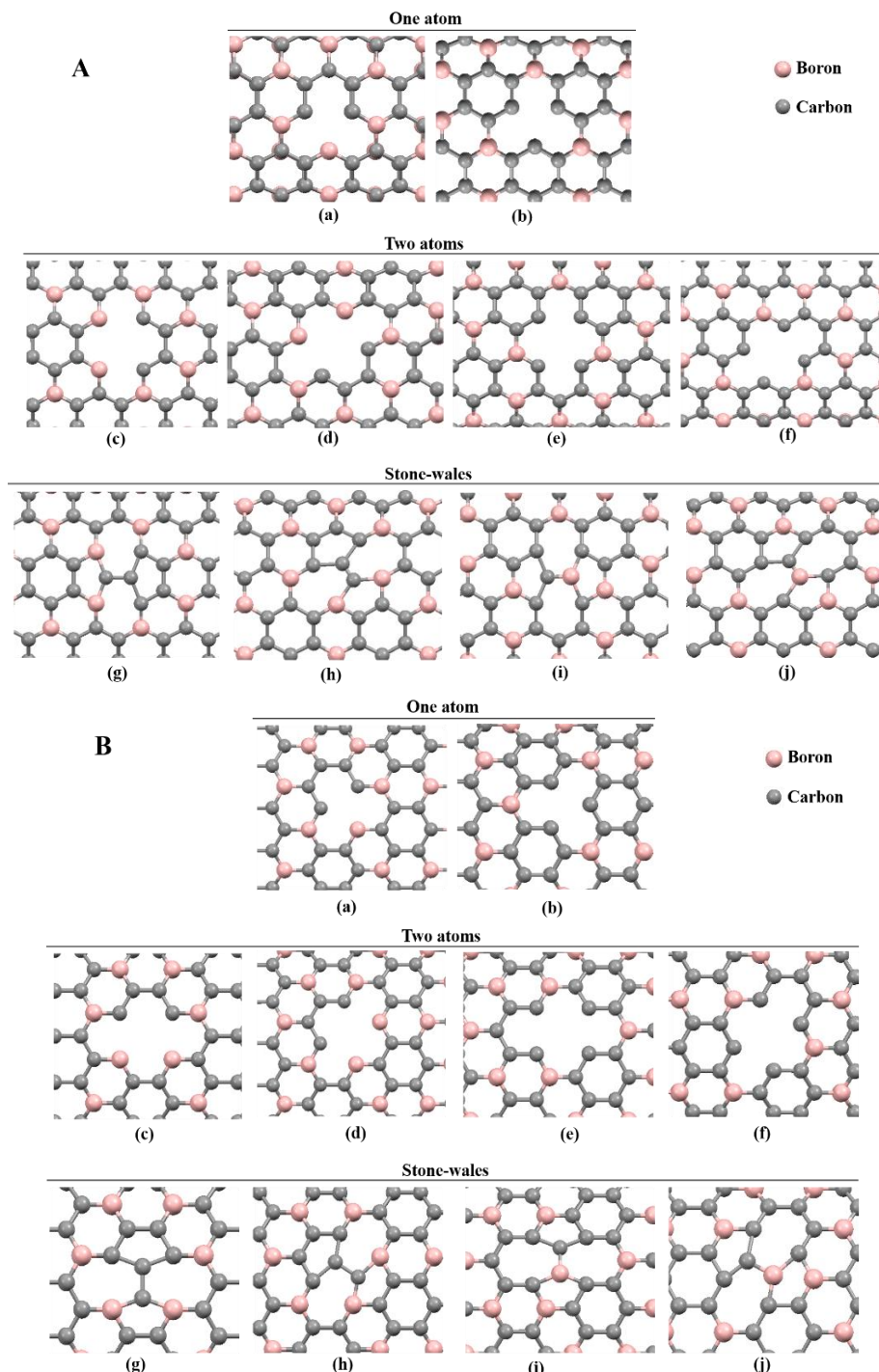
**Figure 8.** A snapshots of the failure process of a (18,0)-2C<sub>60</sub> BC<sub>3</sub> nanobud.

302

303 *3.5. Mechanical properties of defective BC<sub>3</sub>NT*

304 Finally, we investigated the mechanical properties of (10,10) armchair and (18,0) zigzag  
 305 SWBC<sub>3</sub>NT with point defects, including vacancies and Stone-Wales defects. Just as in the  
 306 previous subsection, these structures were selected because of their very close dimensions,  
 307 thus providing easy comparison. Schematic views of the modeled defective structures are  
 308 shown in Figure 9. This figure shows two types of Stone-Wales defects: type one (STW-1)

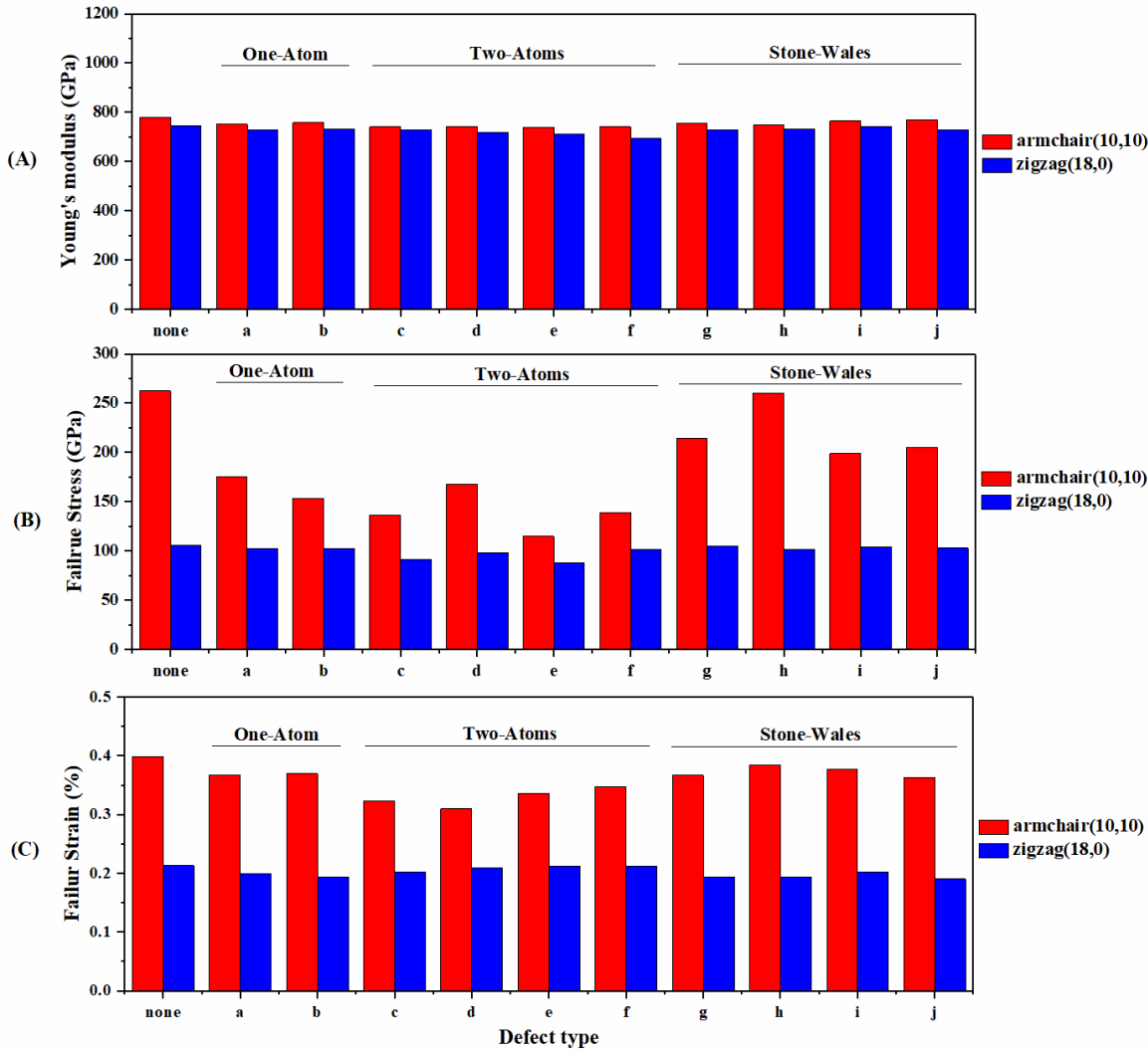
309 forms when a horizontal B-C (or C-C) bond rotates 90 degrees, and type 2 (STW-2) forms  
 310 when a skewed B-C (or C-C) bond rotates 90 degrees. The results calculated after testing all  
 311 samples at the constant temperature of 300K are presented in Figure 10 as bar graphs.



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**Figure 9.** (A) Embedded defects in armchair BC<sub>3</sub>NTs: (a) one carbon atom vacancy, (b) one boron atom vacancy, (c) and (d) two carbon atoms vacancy, (e) and (f) one-carbon, one-boron vacancy, (g) and (i) Stone-wales type 1, (h) and (j) Stone-wales type 2. (B) Same as (A) but for zigzag BC<sub>3</sub>NTs.



**Figure 10.** (a) Young's modulus, (b) failure stress, and (c) failure strain of defective (10,10) BC<sub>3</sub>NT and (18,0) BC<sub>3</sub>NT.

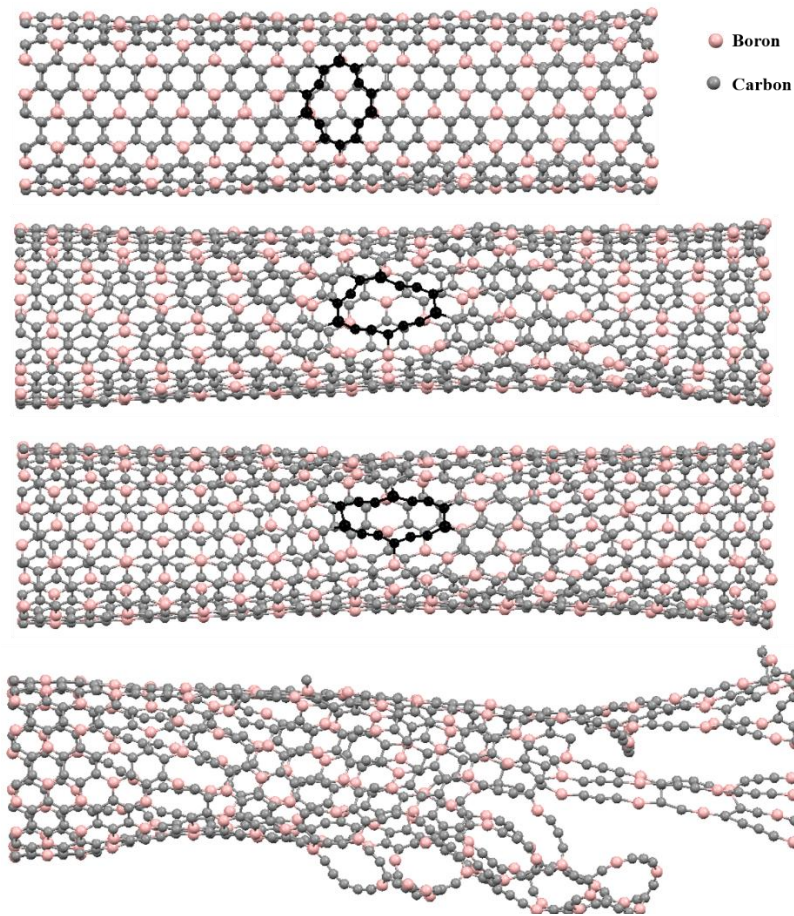
318

319 It can be seen that the mechanical properties of defective BC<sub>3</sub>NTs were lower than for  
 320 flawless SWBC<sub>3</sub>NTs, regardless of chirality. The variation in properties regarding the  
 321 number of missing atoms or the type of the Stone-Wales defect was rather limited and the  
 322 values obtained for each chirality were very close. BC<sub>3</sub>NTs with a Stone-Wales defect had  
 323 the smallest reduction in Young's modulus and failure stress, whatever the chirality, while  
 324 the two atom vacancies imposed the maximum reduction in these properties. In addition, the  
 325 failure strain of the defective armchair BC<sub>3</sub>NT with two missing atoms showed a greater  
 326 reduction than with only one missing atom or with Stone-Wales defects, while in zigzag

327 structures we found a greater reduction in the failure strain of BC<sub>3</sub>NT with Stone-Wales  
328 defects compared to those containing atom vacancies. The highest Young's modulus, failure  
329 stress, and failure strain calculated for defective BC<sub>3</sub>NTs of armchair structure with defect  
330 types j (STW-2) and h (STW-1) were 769.1 GPa, 260.32 GPa and 0.384%, respectively. In  
331 contrast, the lowest Young's modulus and failure stress of all studied defective BC<sub>3</sub>NT were  
332 found for zigzag structures with defect type e (one-carbon, one-boron): 711.2 GPa and 87.16  
333 GPa, respectively. Zigzag BC<sub>3</sub>NT with defect type j had the lowest failure strain of 0.19%.  
334 All the values obtained for the mechanical properties of defective BC<sub>3</sub>NT are shown in Table  
335 S8.

336 Previous research has also provided the same kind of results. Thus, Zahedi et al.  
337 investigated the effects of crack- and notch-type defects on the mechanical properties of BC<sub>3</sub>  
338 single layers and reported a greater reduction in tensile strength properties as crack or notch  
339 dimensions increased [24]. In their paper on molecular dynamics, Albooye et al. [18]  
340 demonstrated that the Young's modulus of defective BNNT was reduced by increasing the  
341 number of missing atoms, with the highest modulus being found in pristine structures while  
342 the lowest modulus was reported for structures with three-atom vacancies. In another  
343 MD-based research, Gupta et al. [32] studied the Young's modulus, failure stress, and failure  
344 strain of hybrid graphene single-layers and showed a downward trend in all the properties  
345 mentioned by creating Stone-Wales and nanopore defects compared to pristine single-layer  
346 graphene. Ghorbanzadeh et al. [33] investigated the effects of point defects on the properties  
347 of ZnO graphene-like surfaces in a DFT study, and also reported the negative effect of point  
348 defects on the mechanical properties of this material. Figure 11 presents a snapshot of the  
349 failure process of a (10,10) armchair BC<sub>3</sub>NT with two atom vacancies (defect type e). As  
350 expected, the failure occurred in the defective areas due to the higher stress concentration,  
351 and the process continued until the destruction of the nanostructure was complete.





**Figure 11.** Snapshot of the failure process of an armchair (10,10) BC<sub>3</sub>NT with two-atom defects (defect type e).

352

#### 353 **4. Conclusions**

354 In the present article, molecular dynamics (MD) simulation was used to study the  
 355 mechanical properties of BC<sub>3</sub> nanotubes. We examined the Young's modulus, failure stress  
 356 and failure strain of BC<sub>3</sub>NT, BC<sub>3</sub> nanobuds and BC<sub>3</sub>NT with different types of defects as a  
 357 function of factors such as chirality, size, number of walls and temperature. We also used the  
 358 results of CNTs of similar chirality and dimensions, obtained from a previous work, to  
 359 compare and validate the present results. Our results demonstrated that the addition of walls  
 360 to single-walled BC<sub>3</sub>NT increased the Young's modulus, failure stress, and failure strain  
 361 remarkably, regardless of chirality, so that triple-walled BC<sub>3</sub>NT had markedly better

362 properties than double-walled nanotubes, and double-walled nanotubes showed better  
363 properties compared to single-walled ones, again regardless of chirality. The highest  
364 Young's modulus obtained was observed for TWBC<sub>3</sub>NT and the lowest modulus was  
365 calculated for SWBC<sub>3</sub>NTs. In addition, armchair structures had higher mechanical properties  
366 than zigzag structures in most of the nanotubes studied, and BC<sub>3</sub>NT had lower properties  
367 compared to CNTs. The highest Young's modulus of the armchair and zigzag SWBC<sub>3</sub>NT  
368 was calculated to be 780.5 GPa and 751.7 GPa for (10,10) and (16,0) structures, respectively.  
369 The modeling of double and triple-walled BC<sub>3</sub>NTs based on structures (4,4) and (8,0), with  
370 the closest radius, revealed that the Young's modulus of the armchair (4,4),(8,8),(12,12)  
371 TWBC<sub>3</sub>NT and (4,4),(8,8) DWBC<sub>3</sub>NT was nearly 60% and 33% higher than (4,4)  
372 SWBC<sub>3</sub>NTs, respectively. Similarly, the Young's modulus of the zigzag (8,0),(14,0),(20,0)  
373 TWBC<sub>3</sub>NT and (8,0),(14,0) DWBC<sub>3</sub>NT was 55% and 34% higher than that of (8,0)  
374 SWBC<sub>3</sub>NT, respectively.

375 Furthermore, after modeling BC<sub>3</sub> nanobuds by attaching 1 to 4 C<sub>60</sub> molecules to the outer  
376 surface of SWBC<sub>3</sub>NT, we observed that all mechanical properties were slightly reduced by  
377 increasing the number of attached fullerenes. Thus, the lowest Young's modulus, failure  
378 stress and failure strain of each chirality were obtained in nanobuds with four attached  
379 fullerenes. The lowest Young's modulus of the armchair and zigzag BC<sub>3</sub> nanobuds was  
380 calculated at 556.6 GPa and 531.4 GPa for structures (10,10)-4C<sub>60</sub> and (18,0)-4C<sub>60</sub>,  
381 respectively, and were 28% and 30% lower than the corresponding pristine SWBC<sub>3</sub>NTs,  
382 respectively. In the end, we modeled and tested SWBC<sub>3</sub>NTs with embedded one-atom and  
383 two-atom vacancies as well as Stone-Wales defects and found that Stone-Wales defects  
384 imposed the smallest reduction in Young's modulus and failure stress, regardless of chirality,  
385 while two-atom vacancies resulted in the largest reduction in these properties. With respect to  
386 failure strain, the greatest reduction was observed for two-atom vacancies and Stone-Wales

387 defects in the case of armchair and zigzag structures, respectively. We calculated the highest  
388 Young's modulus, failure stress, and failure strain of the defective BC<sub>3</sub>NTs in armchair  
389 structures with defect types j (STW-2) and h (STW-1), and the corresponding values were  
390 769.1 GPa, 260.32 GPa, and 0.384%, respectively. Overall, the outstanding results of this  
391 study could provide a new prospect for the wider use of 1D carbon-based materials in a  
392 variety of applications.

### 393 **Data availability**

394 The raw/processed data required to reproduce these findings cannot be shared at this  
395 time as the data also forms part of an ongoing study.

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