Mechanical Properties of C\textsubscript{3}N Nanotubes from Molecular Dynamics Simulation Studies

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Received: 18 April 2020; Accepted: 3 May 2020; Published: 7 May 2020

Abstract: Although the properties of carbon nanotubes (CNTs) are very well-known and are still extensively studied, a thorough understanding of other carbon-based nanomaterials such as C\textsubscript{3}N nanotubes (C\textsubscript{3}NNTs) is still missing. In this article, we used molecular dynamics simulation to investigate the effects of parameters such as chirality, diameter, number of walls, and temperature on the mechanical properties of C\textsubscript{3}N nanotubes, C\textsubscript{3}N nanobuds, and C\textsubscript{3}NNTs with various kinds of defects. We also modeled and tested the corresponding CNTs to validate the results and understand how replacing one C atom of CNT by one N atom affects the properties. Our results demonstrate that the Young’s modulus of single-walled C\textsubscript{3}NNTs (SWC\textsubscript{3}NNTs) increased with diameter, irrespective of the chirality, and was higher in armchair SWC\textsubscript{3}NNTs than in zigzag ones, unlike double-walled C\textsubscript{3}NNTs. Besides, adding a second and then a third wall to SWC\textsubscript{3}NNTs significantly improved their properties. In contrast, the properties of C\textsubscript{3}N nanobuds produced by attaching an increasing number of C\textsubscript{60} fullerenes gradually decreased. Moreover, considering C\textsubscript{3}NNTs with different types of defects revealed that two-atom vacancies resulted in the greatest reduction of all the properties studied, while Stone–Wales defects had the lowest effect on them.

Keywords: C\textsubscript{3}N nanotubes; molecular dynamics; mechanical properties; nanobuds; defects

1. Introduction

In recent decades, rapid progress has been made in the development of new classes of 2D and 1D materials, and these materials have entered almost all fields of science and technology. Graphene and CNTs as the most famous 2D and 1D nanostructures have been extensively used in a wide range of mechanical, electronic, optoelectronic, and medical applications [1–8]. The success of these materials relies on their extraordinary properties such as good electrical conductivity, excellent electron mobility, and high mechanical strength arising from their ultra-thin sp\textsuperscript{2} network along with high specific surface area [9–11].

The outstanding properties of carbon-based nanostructures have prompted researchers to focus on other types of carbon and non-carbon 1D, 2D, and 3D materials. For instance, metal oxide nanotubes and sheets including beryllium oxide (BeO), titanium oxide (TiO\textsubscript{2}), and zinc oxide (ZnO) [12–15], nitride-based sheets or tubular structures such as boron nitride (BN), gallium nitride (GaN),
and aluminum nitride (AlN) [16–18], nanobuds [19–21], nanopeapods [22–24], etc., are worth citing. Among these structures, nitrides have great potential in various applications according to the reports provided by numerous studies. In a molecular dynamics (MD) study, Cong et al. studied the mechanical properties of BN-Al nanotubes/metal matrix nanocomposites. They found that the Young’s modulus, yield stress, and yield strain of the composites increased with the nanotubes diameter [25]. Ghorbanzadeh et al. [16] used the density functional theory (DFT) to examine the mechanical properties of single and multi-layer graphene-like sheets based on group III nitrides and showed that adding layers to the studied surfaces could increase the elastic modulus of AlN and BN sheets, but not GaN. Albooye et al. [26] used a MD method to consider the mechanical properties of boron nitride nanotubes (BNNTs) with point defects and doped by carbon atoms. They found that the concentration of vacancies could reduce their mechanical properties, and armchair BNNTs had a higher Young’s modulus than zigzag BNNTs. Besides, carbon-doped BNNTs had lower mechanical properties than pristine BNNTs in either zigzag or armchair configuration [26].

Another nitride-based nanostructure that has been much studied recently is 2D carbon nitride (C$_3$N). This structure can form during the CNT synthesis. This nanostructure has been the subject of many research works in recent years and has been used in a variety of applications such as energy storage, adsorption of CO$_2$, NO$_2$ and H$_2$S, electrocatalysis, and photocatalysis [27–35]. In this regard, Sadeghzadeh used MD simulation to design C$_3$N nanosheets and investigate the effect of holes on their tensile properties. He reported a considerable reduction in Young’s modulus, yield stress, and yield strain of the C$_3$N nanosheets when the diameter of the holes increased [36]. Shirazi et al. [32] used MD simulation to study the mechanical behavior of C$_3$N sheets under critical defects such as line cracks and notches, and found a lower mechanical strength of C$_3$N when the crack line or notch diameter increased. A research based on density functional theory (DFT) was developed by Ma et al. to understand the ability of pristine and B-doped C$_3$N to adsorb NO$_2$. They demonstrated that pristine C$_3$N has a high sensitivity to NO$_2$ and that doping with B atoms considerably increases this sensitivity [34]. In another article, Faye et al. used pristine and defective C$_3$N sheets for the adsorption of H$_2$S and NH$_3$. Their results revealed that the weak interaction between pristine C$_3$N and NH$_3$ or H$_2$S in the gas phase was considerably strengthened once a single N or C defect was created on the surface of C$_3$N [35]. The mechanical behavior of C$_3$N sheets was investigated by Mortazavi in a combined DFT-MD research [30]. He reported 341 GPa for the elastic modulus from the DFT calculation, which was only 3% different from the MD estimates. Mortazavi also predicted a thermal conductivity of about 815 W m$^{-1}$ K$^{-1}$ [30] for free-standing C$_3$N. He therefore proposed this nanostructure as a potential candidate for new applications such as reinforcement of polymer-based nanocomposites.

As discussed above, the structure and various properties of 2D C$_3$N materials have been investigated in depth. However, less attention has been devoted to exploring the properties of C$_3$N nanotubes (C$_3$NNTs), i.e., 1D structures. To the best of the authors’ knowledge, no research has been developed so far to study the mechanical properties of pristine and defective C$_3$N nanotubes as well as the 3D nanostructures that they can form, such as nanobuds. Such studies include chirality, tube dimension, number of walls, and the effect of temperature.

On the one hand, the structural defects that form during the process of nanotube synthesis play a crucial role in the mechanical performance of nanostructures, in particular at high temperatures. On the other hand, 3D nanostructures such as nanobuds have shown great potential for being widely used in various industrial applications. It is therefore necessary to study the new carbon nanostructures from the point of view of their mechanical properties, as this could open up a new perspective for future developments in nanotechnology.

The main goal of this article is therefore to use MD simulation to investigate the effect of chirality, tube diameter, number of walls, and temperature on elastic modulus, failure stress, and failure strain of flawless and defective C$_3$NNTs, as well as C$_3$N nanobuds. Since no research has been conducted so far to evaluate the properties of C$_3$NNTs, we modeled and tested carbon nanotubes with the same chirality under the same loading condition to validate the results. The obtained results will be fully discussed and compared in the following sections.
2. Computational Method

In this study, MD simulation was performed with large-scale atomic/molecular massively parallel simulator (LAMMPS) for modeling the mechanical properties of C3NNTs under uniaxial tensile loading. In order to determine the interaction between carbon atoms, the optimized Tersoff potential presented by Lindsay and Broido [37] was used. Besides, the Tersoff potential parameters developed by Kinaci et al. [38] were used for determining the interaction between C and N atoms. C3NNTs with an approximate length of 50 Å were modeled in armchair or zigzag chirality, and the obtained results were compared to the properties of carbon nanotubes (CNTs). MD simulations were carried out in two steps: first, the stress-free structures at the simulation temperature were obtained with the isothermal-isobaric (NPT) ensemble operating at 50 ps. Then, at an initial constant velocity, the simulation box was stretched along the loading axial direction. The simulations were carried out for nanotubes with various conditions such as chirality (zigzag or armchair), temperature (from 300 to 900 K), number of walls (from 1 to 3), and various defects (attachment of fullerene and point defects) to evaluate their impact on elastic modulus, failure stress, and failure strain.

3. Results

3.1. Geometrical Design

As mentioned above, the main objective of this study was to determine the mechanical behavior of C3N nanotubes and nanobuds as a function of diameter, chirality, number of walls, and temperature as input variables. For that purpose, armchair and zigzag C3NNTs with one, two, and three walls were modeled using the MD simulation method. Schematic views of the modeled C3NNTs along with the data of their chirality and stoichiometry are given in Figure 1 and in Table 1. Next, all samples were subjected to uniaxial tensile loading, as shown in Figure 2, with a strain rate of 0.001 ps\(^{-1}\) at a constant temperature of 300 K to calculate Young’s modulus, failure stress, and failure strain from the corresponding stress–strain plots.

| Chirality of SWC3NNTs | Number of Atoms | Chirality of MWC3NNTs | 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           |

3.2. Mechanical Properties of Single-Walled C3NNTs

The Young’s modulus of each SWC3NNT was determined as follows. After plotting the stress–strain (σ–ε) curves, a second-order polynomial was fitted to the linear part of the curves, and the Young’s modulus was calculated using Equation (1) [39,40]:

\[
\text{Young's modulus} = \frac{\text{Slope of linear part}}{\text{Area under the curve}}
\]
\[ \sigma = \frac{\partial U}{\partial \varepsilon} = D \varepsilon^2 + E \varepsilon + C \]  

where \( D, E, \) and \( C \) are the third-order elastic modulus, the Young's modulus, and the residual stress of the nanotubes, respectively. The stress–strain curve of a \((6,6)\) armchair \( \text{C}_3\text{NNT} \) at 300 K displayed in Figure 3a,b shows a zoom of the linear part used for the second-order polynomial fit.

**Figure 1.** Schematic (side and cross-sectional) views of the modeled \( \text{C}_3\text{N} \) nanotubes (\( \text{C}_3\text{NNTs} \)): (a) \((8,0)\) zigzag single-walled \( \text{C}_3\text{NNTs} \) (SWC\text{C}_3\text{NNT}), (b) \((4,4)\) armchair SWC\text{C}_3\text{NNT}, (c) \((8,0),(12,0)\) zigzag double-walled (DWC\text{C}_3\text{NNT}), (d) \((4,4),(8,8)\) armchair DWC\text{C}_3\text{NNT}, (e) \((8,0),(12,0),(20,0)\) zigzag triple-walled (TWC\text{C}_3\text{NNT}), and (f) \((4,4),(8,8),(12,12)\) armchair TWC\text{C}_3\text{NNT}. 


According to Figure 3a, the highest stress obtained is observed at a strain of about 40%. Then, the stress drops to a considerably lower amplitude, therefore the coordinates of this point correspond to the values of failure stress and failure strain. We repeated these steps for all SWC:NNTs and then for SWCNTs to compare and validate our results. The plots of Young’s modulus, failure stress, and failure strain are displayed in Figure 4. This figure shows that the variation of all the studied properties as a function of the radius of the nanotubes is rather limited. Indeed, as seen in Figure 4a, by increasing the radius of the nanotubes, the Young’s modulus of armchair SWC:NNTs increases by about 24 GPa, passing from 951.6 GPa in structure (4,4) to 975.5 GPa in structure (10,10), and then drops to 970.8 GPa in structure (12,12). Similarly, an upward behavior is observed in the Young’s modulus of armchair CNTs, except for the thickest ones where the values tend to stabilize, rising from 983.3 GPa in structure (4,4) to 1085.4 GPa in structure (12,12).

We observed the same behavior by comparing the Young’s modulus of zigzag and armchair SWC:NNTs. The Young’s modulus of zigzag SWC:NNTs increases slightly, from 903.8 GPa in (8,0) to 935.2 GPa in (20,0), similar to the upward trend of armchair SWC:NNTs. A general comparison between the modulus of SWC:NNTs and SWCNTs reveals that the values obtained for SWC:NNTs are much lower than for the corresponding SWCNTs at any chirality or radius considered. The higher mechanical behavior of CNTs compared to C:NNTs is caused by the length of the C-C bond, which is about 1.445 Å in the ideal structure of CNTs, while the length of the C-N bond in C:NNTs is about 1.468 Å. The shorter bond length between the elements of the nanostructures leads to higher mechanical properties as demonstrated by Ghorbanzadeh et al. [16]. As mentioned earlier, we modeled CNTs in the present paper to have the possibility of validating our simulation and obtaining results for C:NNTs. The Young’s modulus that we calculated for SWCNTs is around 1000 GPa, which is close to what has already been reported in previous theoretical articles, ranging from 0.5 to 1.5 TPa [41–45], as well as in experimental reports [46–48]. For instance, Treacy et al. reported a value of around
2 TPa for the elastic modulus of individual SWCNTs of different diameters and lengths [46], and Yu et al. reported an average modulus of 1002 GPa for 8 SWCNT ropes using atomic force microscopy (AFM) [48]. These results demonstrate the accuracy of our simulation and therefore also of our results for C₃NNTs.

Figure 4. (a) Young’s modulus, (b) failure stress, and (c) failure strain of SWC₃NNTs and SWCNTs under uniaxial tensile tests at 300 K, as a function of their radius.

Furthermore, from Figure 4b,c, we can see that the failure stress and failure strain of zigzag SWC₃NNTs and SWCNTs increase with the radius of the nanotubes, while those of armchair SWC₃NNTs and SWCNTs decrease under the same conditions. The highest failure stress and failure strain, equal to 282.6 GPa and 0.44%, respectively, were found for armchair (6,6) and (4,4) C₃NNTs, respectively. In an MD-case study, Shirazi et al. reported the ultimate tensile strength of armchair and zigzag C₃N sheets at 300 K, equal to 128 GPa and 125 GPa, which are both lower than what we
obtained for our strongest structures (250.21 GPa for armchair and 138.29 for zigzag) [32]. The results calculated for the mechanical properties of armchair and zigzag SWC:C3NNTs and SWCNTs are listed in Tables 2 and 3.

To take the effect of temperature into account, (10,10) and (18,0) single-walled C3NNTs and the CNTs with the closest dimensions were modeled and subjected to a uniaxial tensile loading while the temperature increased from 300 to 900 K. The calculated results are shown in Figure 5.

Table 2. Mechanical properties of armchair SWC:C3NNTs and SWCNTs under uniaxial tensile tests at 300 K.

| Nanotube | Properties | Chirality |
|----------|------------|-----------|
| C3NNTs   | Young’s Modulus (GPa) | (4,4) | (6,6) | (8,8) | (10,10) | (12,12) |
|          | Failure Stress (GPa)   | 951.6 | 964.7 | 972.6 | 975.5 | 970.8 |
|          | Failure Strain (%)     | 282.54 | 282.64 | 272.73 | 266.62 | 250.21 |
| CNTs     | Young’s Modulus (GPa)  | 983.3 | 1043.5 | 1080.1 | 1084.8 | 1085.1 |
|          | Failure Stress (GPa)   | 270.25 | 280.83 | 266.41 | 241.85 | 223.41 |
|          | Failure Strain (%)     | 0.395 | 0.395 | 0.388 | 0.387 | 0.384 |

Table 3. Same as Table 2, but for zigzag SWC:C3NNTs and SWCNTs.

| Nanotube | Properties | Chirality |
|----------|------------|-----------|
| C3NNTs   | Young’s Modulus (GPa) | (8,0) | (10,0) | (12,0) | (14,0) | (16,0) | (18,0) | (20,0) |
|          | Failure Strain (%)     | 903.8 | 910.4 | 917.3 | 924.5 | 930.3 | 933.8 | 935.1 |
|          | Failure Strain (%)     | 112.94 | 117.48 | 121.54 | 128.96 | 131.84 | 132.52 | 138.29 |
| CNTs     | Young’s Modulus (GPa)  | 1066.4 | 1064.7 | 1061.3 | 1059.4 | 1058.1 | 1056.3 | 1055.4 |
|          | Failure Strain (%)     | 126.15 | 131.52 | 135.32 | 139.46 | 142.03 | 149.71 | 155.41 |
|          | Failure Strain (%)     | 0.290 | 0.253 | 0.212 | 0.213 | 0.205 | 0.216 | 0.218 |

All the aforementioned mechanical properties decreased with temperature, whether for CNTs or for C3NNTs. Thus, the highest values for all tested samples were obtained at 300 K and the lowest values at 900 K. The (10,10) armchair C3NNT had a higher elastic modulus at any temperature compared to the (18,0) zigzag structure, and the C3NNTs showed a lower modulus than the CNTs. The Young’s modulus of (18,0) and (10,10) C3NNTs were respectively 2% and 5% lower than that at 900 K than at 300 K. Likewise, the failure stress and failure strain of all the samples decreased when the temperature increased. However, although the failure stress of zigzag and armchair C3NNTs was lower than those of the corresponding CNTs at most temperatures, these structures generally failed at a higher strain rate than those of CNTs. The same observations were reported by Shirazi et al. [32]. They noted a total decrease of 36% for the stress at failure of C3N sheets at 900 K compared to 200 K, in accordance with our own finding.

3.3. Mechanical Properties of Double-Walled C3NNTs

At this point, to probe the effect of adding walls to C3NNTs on their mechanical properties, we modeled and tested four zigzag and six armchair double-walled C3NNTs (DWC3NNTs) as well as the corresponding DWCNTs. It should be mentioned that there are some limitations to the modeling of multi-walled nanotubes, in particular regarding the interlayer distances. If the interlayer distance exceeds a certain value, no van der Waals interaction occurs between layers and the structure does not form. On the other hand, if the distance were less than a specific value, the structure would collapse because of instability. Therefore, to have an armchair and zigzag structures with the closest dimensions enabling reasonable comparisons to be made, we selected the distances according to the
schematic views displayed in Figure 6. Thus, we could model stable structures with close and comparable dimensions.

Figure 5. (a) Young’s modulus, (b) failure stress, and (c) failure strain of (10,10) and (18,0) SWC3NNTs and SWCNTs under uniaxial tensile tests, as a function of temperature.
After testing all the modeled samples under uniaxial tensile loading at a constant temperature of 300 K, the mechanical properties were plotted in Figure 7. As seen in Figure 7a, by increasing the interlayer distance, the Young’s modulus of all samples first increased and then constantly decreased to slightly lower values. Unlike single-walled nanotubes, the Young’s modulus of zigzag DWC3NNTs and SWCNTs was higher than that of armchair DWC3NNTs of similar radius, while DWC3NNTs had a lower elastic modulus compared to DWCNTs, as already observed for single-walled nanotubes. The results of double-walled armchair and zigzag C3NNTs and CNTs are collected in Tables 4 and 5, respectively. The highest values obtained for DWC3NNTs occurred in structures (8,0),(16,0) and (4,4),(8,8), 1448.7 GPa and 1418.6 GPa, respectively, and this property was about 10% lower in the weakest structure with respect to the strongest one, whatever the chirality.

**Figure 6.** Cross-sectional view of the structure of studied C3NNTs nanotubes: (a) armchair DWC3NNTs, and (b) zigzag DWC3NNTs.
Besides, making comparisons between the results of single and double-walled C\textsubscript{3}NNTs reveals that adding a wall to these nanotubes increased the elastic modulus so that DWC\textsubscript{3}NNTs have a considerably higher elastic modulus than SWC\textsubscript{3}NNTs. In addition, and just like SWCNTs, DWCNTs showed a higher Young’s modulus than DWC\textsubscript{3}NNTs regardless of the chirality. The Young’s modulus of DWCNTs was higher than that of SWCNTs, just like for C\textsubscript{3}NNTs. The highest Young’s modulus of DWCNTs found in the zigzag structure (8,0),(16,0), 1553.3 GPa, is close to that reported earlier [49,50], further supporting the accuracy of our simulation and the results calculated for DWC\textsubscript{3}NNTs.

Figure 7. (a) Young’s modulus, (b) failure stress, and (c) failure strain of DWC\textsubscript{3}NNTs and DWCNTs under uniaxial tensile tests as a function of interlayer distance.
Table 4. Mechanical properties of armchair DWC₃NNTs and DWCNTs under uniaxial tensile tests at 300 K.

| Nanotube | Properties             | Chirality       |
|----------|------------------------|-----------------|
|          |                        | (4,4),(7,7) (4,4),(8,8) (4,4),(9,9) (4,4),(10,10) (4,4),(11,11) (4,4),(12,12) |
| C₃NNTs  | Young’s Modulus (GPa)  | 1323.2          |
|         | Failure Stress (GPa)   | 351.68          |
|         | Failure Strain (%)     | 0.422           |
| CNTs    | Young’s Modulus (GPa)  | 1459.6          |
|         | Failure Stress (GPa)   | 365.26          |
|         | Failure Strain (%)     | 0.412           |

Table 5. Same as Table 4, but for zigzag DWC₃NNTs and DWCNTs.

| Nanotube | Properties             | Chirality       |
|----------|------------------------|-----------------|
|          |                        | (8,0),(14,0) (8,0),(16,0) (8,0),(18,0) (8,0),(20,0) |
| C₃NNTs  | Young’s Modulus (GPa)  | 1364.7          |
|         | Failure Stress (GPa)   | 180.24          |
|         | Failure Strain (%)     | 0.203           |
| CNTs    | Young’s Modulus (GPa)  | 1514.7          |
|         | Failure Stress (GPa)   | 208.72          |
|         | Failure Strain (%)     | 0.295           |

Finally, considering Figure 7b,c, we found that failure stress and failure strain of zigzag DWC₃NNTs were nearly two times lower than those of armchair DWC₃NNTs having a close radius. No chirality showed a significant trend by increasing the radius, and a similar trend was observed for DWCNTs. We obtained the highest failure stress and failure strain of DWC₃NNTs in the (4,4),(8,8) armchair: 374.4 GPa and 0.435%, respectively.

3.4. Mechanical Properties of Triple-Walled C₃NNTs (TWC₃NNTs)

In this section, we added one more wall to DWC₃NNTs to compare the mechanical behavior of TWC₃NNTs to that of SWC₃NNTs and DWC₃NNTs. For that purpose, we modeled and tested one zigzag and one armchair TWC₃NNT of structures (8,0),(14,0),(20,0) and (4,4),(8,8),(12,12), respectively, and the corresponding TWCNTs. A schematic view of the modeled structures is displayed in Figure 8, and the obtained results are presented in Table 6.

By examining this table, we found a significant growth in the Young’s modulus of TWC₃NNTs compared to double- or single-walled nanotubes, whether CNTs or C₃NNTs, and regardless of chirality. The Young’s modulus of armchair TWC₃NNT (1850.4 GPa) was higher than that of zigzag TWC₃NNT (1760.7 GPa), unlike what we had obtained for DWC₃NNTs. In addition, the Young’s modulus of TWC₃NNTs was lower than that of TWCNTs with the same structure, as for single-walled C₃NNTs and CNTs. Besides, the failure stresses of armchair TWC₃NNT and TWCNTs were not only
higher than for zigzag TWC\textsubscript{3}NNTs and TWCNTs, but also higher than for double- and single-walled nanotubes.

Table 6. Mechanical properties of zigzag and armchair TWC\textsubscript{3}NNTs and TWCNTs under uniaxial tensile tests at 300 K.

| Properties         | Chirality                  |
|--------------------|----------------------------|
|                    | (4,4),(8,8),(12,12) | (8,0),(14,0),(20,0) | (4,4),(8,8),(12,12) | (8,0),(14,0),(20,0) |
| Young’s Modulus (GPa) | 1850.4                 | 1760.7                | 2050.1                | 1886.9                |
| Failure Stress (GPa)   | 510.25                  | 388.30                 | 500.01                 | 355.18                 |
| Failure Strain (%)     | 0.419                    | 0.423                   | 0.414                   | 0.490                   |

Moreover, we compared the mechanical properties of single-walled (4,4) and (8,0) C\textsubscript{3}NNTs with double- and triple-walled C\textsubscript{3}NNTs made up of these two basic structures in Figure 9. From this figure, it can be observed that the addition of walls to the single-walled nanotubes had a remarkable impact on the Young’s modulus of both C\textsubscript{3}NNTs and CNTs, regardless of the chirality. By increasing the radius following the addition of one then two more walls to the SWC\textsubscript{3}NNTs, the modulus of (4,4) single-wall armchair C\textsubscript{3}NNT increased by 32% and 48%, respectively, in structures (4,4),(8,8) and (4,4),(8,8),(12,12), respectively. Similarly, the modulus of (8,0),(14,0) and (8,0),(14,0),(20,0) zigzag structures were respectively 33% and 46% higher than that of the (8,0) SWC\textsubscript{3}NNT. The same behavior is observed in TWCNTs compared to their corresponding double and single-walled counterparts.

Figure 9. Young’s modulus as a function of nanotube radius for different types of single-, double-, and triple-walled chiral C\textsubscript{3}NNTs.

3.5. Mechanical Properties of C\textsubscript{6}N Nanobuds

Nanobuds are 3D nanostructures that form when a fullerene or nanocage is randomly attached to the outer surface of nanotubes or graphenic structures in the synthesis process. The specific features of nanocages and fullerenes, including their porous shells and nanometric thickness, make them an appropriate choice for developing novel 3D nanostructures [51]. In the present work, we attached randomly one, two, three, and four C\textsubscript{60} fullerene molecules to the outer surface of zigzag and armchair SWC\textsubscript{3}NNTs to form C\textsubscript{6}N nanobuds. One armchair and one zigzag C\textsubscript{3}NNTs with the closest dimension of structures (10,10) and (18,0) were modeled and tested. The plots of the mechanical properties of armchair and zigzag SWC\textsubscript{3}NNTs after attaching one, two, three, and four C\textsubscript{60} to their surface are given in Figure 10.
Similar to what we had seen above for SWC\textsubscript{3}NNTs, the mechanical properties of armchair nanobuds were higher than zigzag nanobuds, and all the studied properties decreased constantly as the number of C\textsubscript{60} increased. This could be due to first, the increase in the effective surface area of the nanobuds with the number of attached fullerenes, and second to the associated increase in stress concentration, a higher number of attached fullerenes implying a higher stress concentration. In addition, the properties of C\textsubscript{3}N nanobuds were lower than for simple SWC\textsubscript{3}NNTs, either in zigzag or armchair structures. The highest elastic modulus was calculated for structures (10,10)-1C\textsubscript{60}: 874.5 GPa, and (18,0)-1C\textsubscript{60}: 865.8 GPa, i.e., was 10\% and 7\% lower than (10,10) and (18,0) SWC\textsubscript{3}NNTs, respectively. With four C\textsubscript{60} attached to armchair and zigzag nanobuds, the modulus was reduced by almost 20\% compared to those with only one C\textsubscript{60}. The same kind of results have been reported by other studies on other types of nanobuds. Mashhadzadeh et al. in their DFT-based research, reported that the Young’s modulus of

![Figure 10. (a) Young’s modulus, (b) failure stress, and (c) failure strain of C\textsubscript{3}N nanobuds under uniaxial tensile tests at 300 K.](image-url)
graphene-like BeO reduced considerably by increasing the number of attached nanocages [20]. Ghorbanzadeh et al. used DFT calculations to compare the mechanical properties of simple CNTs with CNT nanobuds. They found a reduction in Young’s modulus of armchair and zigzag CNTs after attaching a C₆₀ molecule to their surface. The values obtained for the mechanical properties of C₃N nanobuds are presented in Table 7.

Table 7. Mechanical properties of C₃N nanobuds under uniaxial tensile tests at 300 K.

| Chirality | Properties            | Number of Attached Fullerenes |
|-----------|-----------------------|------------------------------|
|           |                       | 1   | 2   | 3   | 4   |
| armchair  | Young’s Modulus (GPa) | 874.8 | 812.4 | 754.3 | 710.1 |
|          | Failure Stress (GPa)  | 141.77 | 135.84 | 115.92 | 96.67 |
|          | Failure Strain (%)    | 0.274 | 0.286 | 0.248 | 0.207 |
| zigzag   | Young’s Modulus (GPa) | 865.8 | 774.9 | 731.8 | 680.5 |
|          | Failure Stress (GPa)  | 122.7 | 114.5 | 105.08 | 91.82 |
|          | Failure Strain (%)    | 0.225 | 0.221 | 0.214 | 0.195 |

Figure 11 shows a snapshot of the failure process of a (18,0)-1C₆₀ SWC₃NNT. It can be seen that, as expected, the failure started around the region where the fullerene was placed on the nanotube surface. This is due to the higher stress concentration existing around this region, which facilitates the formation and propagation of cracks.

Figure 11. Snapshot of the failure process of a (18,0)-1C₆₀ C₃N nanobud.
3.6. Mechanical Properties of Defective C₃NNTs

In the end, we examined the effect of point defects on the mechanical properties of SWC₃NNTs. (10,10) armchair and (18,0) C₃NNTs were selected and we modeled the defective samples with one and two vacancies as well as Stone–Wales defects. All the designed samples are presented in Figure 12, where the two types of Stone–Wales defects can be seen. Type one (STW-1) forms when a horizontal C-N (or C-C) bond rotates 90 degrees, and type 2 (STW-2) forms once a skewed C-N (or C-C) bond rotates 90 degrees.

![Diagram of C₃NNTs with defects](image)

**Figure 12.** (A) Embedded defects in (10,10) armchair C₃NNT: (a) one carbon atom vacancy, (b) one nitrogen atom vacancy, (c) and (d) two carbon atoms vacancy, (e) and (f) one-carbon and one-nitrogen vacancy, (g) and (i) Stone-wales type 1, (h) and (j) Stone-wales type 2. (B) Same as (A) but for (18,0) armchair C₃NNT.

After having implemented tensile tests at a constant temperature of 300 K and at constant strain rate $\varepsilon$ of $10^6$ s⁻¹, the results are presented as bar graph in Figure 13. According to this figure, creating defects on the surface of armchair and zigzag C₃NNTs resulted in a reduction of all mechanical
properties compared to pristine SWC3NNTs. The Young’s modulus of different defected zigzag and armchair C3NNTs are close to each other (with higher values for most types of armchair), with very little differences and no significant trend. However, the failure stress and failure strain of defective armchair C3NNTs are considerably higher than the corresponding zigzag C3NNTs. The results obtained for each property are collected in Table 8 for each type of defect.

![Graphs showing Young's modulus, failure stress, and failure strain of defective C3NNTs at 300 K](image)

Figure 13. (a) Young’s modulus, (b) failure stress, and (c) failure strain of defective C3NNTs at 300 K

This table shows that the highest reduction in all properties occurred when two atoms were removed from the surface of zigzag and armchair SWC3NNTs. In contrast, defects of types STW-1 and STW-2 resulted in the lowest reduction in properties compared to pristine SWC3NNTs. The lowest Young’s modulus, failure stress, and failure strain, 900.3 GPa, 122.68 GPa, and 0.182%, respectively, were about 7%, 9%, and 15% lower than for the corresponding pristine SWC3NNTs. These values corresponded to two-atom vacancy C3NNTs, including armchair structure defect type c (2-C), zigzag structure defect type d (2-C), and zigzag structure defect type e (1-C, 1-N), respectively. The same kind of results have been reported by previous researches. Shirazi et al. provided the same results for C3N nanosheets with crack-type defects [32]. They showed that increasing the crack length could significantly decrease the mechanical response of the defective sheets. However, Sadeghzadeh et al. observed different results for their C3N sheet depending on the vacancy concentration [31]. They demonstrated that defective C3N had higher elastic modulus and failure strain than the defect-free sheets, which is different from the findings of Shirazi’s and ours. In another article, an adverse effect of point defects on the mechanical properties of graphene-like ZnO structures was reported by Ghorbanzade et al. [15]. In a MD-based study, Albooye et al. also reported that increasing the number
of missing atoms reduced the Young’s modulus of defective BNNTs so that the highest modulus was obtained in pristine structures, and the lowest modulus was observed in those containing three-atom vacancies [26]. In another MD studies, Gupta et al. investigated Young’s modulus, failure stress, and failure strain of hybrid single-layer graphene; they reported a reduction in the behavior of all properties with respect to non-defective graphene monolayers by imposing Stone–Wales and nanopore defects [52].

Table 8. Mechanical properties of defective SWCNTs.

| chirality | Properties | Defect Type |
|-----------|------------|-------------|
|           | none       | a           | b           | c           | d           | e           | f           | g           | h           | i           | j           |
| armchair  | Young’s Modulus (GPa) | 975.5 | 935.3 | 943.1 | 900.3 | 927.4 | 901.4 | 918.5 | 959.6 | 959.3 | 957.5 | 952.1 |
|           | Failure Stress (GPa)   | 266.62 | 155.18 | 138.30 | 182.47 | 174.23 | 138.07 | 231.59 | 266.62 | 221.62 | 209.37 | 209.35 |
|           | Failure Strain (%)     | 0.399  | 0.388  | 0.365  | 0.326  | 0.306  | 0.378  | 0.280  | 0.37  | 0.37  | 0.39  | 0.39  |
|           | Young’s modulus (GPa)  | 933.8  | 925.1  | 924.6  | 927.9  | 924.4  | 914.6  | 916.7  | 902.24 | 933.32 | 929.31 |
|           | Failure Stress (GPa)   | 135.52 | 126.74 | 127.41 | 124.87 | 122.68 | 124.93 | 123.98 | 130.29 | 132.09 | 132.11 | 131.50 |
|           | Failure Strain (%)     | 0.213  | 0.193  | 0.204  | 0.197  | 0.204  | 0.182  | 0.189  | 0.20  | 0.21  | 0.20  | 0.20  |
| zigzag    | Young’s Modulus (GPa)  | 975.5  | 935.3  | 943.1  | 900.3  | 927.4  | 901.4  | 918.5  | 959.6 | 959.3 | 957.5 | 952.1 |
|           | Failure Stress (GPa)   | 266.62 | 155.18 | 138.30 | 182.47 | 174.23 | 138.07 | 231.59 | 266.62 | 221.62 | 209.37 | 209.35 |
|           | Failure Strain (%)     | 0.399  | 0.388  | 0.365  | 0.326  | 0.306  | 0.378  | 0.280  | 0.37  | 0.37  | 0.39  | 0.39  |
|           | Young’s modulus (GPa)  | 933.8  | 925.1  | 924.6  | 927.9  | 924.4  | 914.6  | 916.7  | 902.24 | 933.32 | 929.31 |
|           | Failure Stress (GPa)   | 135.52 | 126.74 | 127.41 | 124.87 | 122.68 | 124.93 | 123.98 | 130.29 | 132.09 | 132.11 | 131.50 |
|           | Failure Strain (%)     | 0.213  | 0.193  | 0.204  | 0.197  | 0.204  | 0.182  | 0.189  | 0.20  | 0.21  | 0.20  | 0.20  |

Furthermore, a snapshot of the failure process of a (10,10) armchair SWCNT including a two-atom vacancy defect is presented in Figure 14. Similar to what happens in nanobuds, the failure of defective C3NNT begins from the defective region due to its higher stress concentration, and then the cracks propagate until the complete rupture of the structure.

![Figure 14. Snapshot of the failure process of a (10,10) armchair C3NNT with a two-atom vacancy defect.](image-url)
4. Conclusions

Molecular dynamics simulation has been used in the present work to determine the impact of parameters such as nanotube radius, number of walls, number of attached fullerenes, defect type, and temperature on the mechanical properties of single-, double-, triple-walled C₃NNTs, defective C₃N nanobuds, and C₃N nanobuds. The results revealed that adding walls to SWC₃NNTs improved the mechanical behavior whether in zigzag or armchair chirality. The properties of armchair nanotubes were higher than zigzag ones, and were negatively affected by the temperature. Besides, the elastic properties were improved by increasing the number of walls. The highest moduli of armchair and zigzag SWC₃NNTs, 975.5 GPa and 935.1 GPa, respectively, were obtained in structures (10,10) and (20,0), respectively. Those of armchair and zigzag (10,10) and (18,0) TWC₃NNTs were 1850.4 GPa and 1760.7 GPa, respectively, i.e., nearly 47% higher than the corresponding SWC₃NNTs. Furthermore, the failure properties generally decreased by increasing the radius of the nanotubes. The Young’s modulus, failure stress, and failure strain of armchair SWC₃NNTs and DWC₃NNTs were higher than zigzag ones, and these properties increased by adding walls to the nanotubes. Additionally, we considered C₃N nanobuds and found that their mechanical properties were lower than pristine C₃NNTs. This was especially the case when more fullerenes were attached to them, so that the Young’s modulus of a nanobud with four C₆₀ was 20% less than for a nanobud with only one C₆₀, whatever the chirality. Finally, we imposed vacancies and Stone–Wales defects to SWC₃NNTs. Our results demonstrated that two-atom vacancies and Stone–Wales defects resulted in the highest and smallest drop, respectively, in Young’s modulus, failure stress, and failure strain, whatever the chirality. The minimum Young’s modulus of armchair and zigzag C₃NNTs occurred with defects type c (2C removed): 900.3 GPa, and type e (1C and 1N removed): 914.6 GPa. Overall, the outcomes of the present article offer a new perspective for developing new carbon-based nanotubes for broad industrial applications.

Author Contributions: A.H.M. designed the case study and wrote the LAMMPS code of the present article. Z.K. carried out the computational measurements and designed the figures and tables. A.S. analyzed and rechecked the results for correctness and wrote the original draft of article. M.R.S. analyzed the data and discussed the results. V.F. and A.C. reviewed and edited the article to give it its final form. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Conflicts of Interest: The authors declare no conflict of interest.

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