Mechanical properties of SWNT X-Junctions through molecular dynamics simulation

B.A. Stormer, N.M. Piper, X.M. Yang*, J. Tao, Y. Fu, M. Kirca and A.C. To**

Department of Mechanical Engineering and Materials Science & Department of Civil and Environmental Engineering, University of Pittsburgh, Pittsburgh, PA, USA

(Received 12 August 2011; final version received 8 November 2011)

The mechanical behavior of seven different carbon nanotube (CNT) X-junctions with a varying number of bonds was investigated through molecular dynamics simulations. The X-junctions are composed of two (6,0) single-walled carbon nanotubes (SWNTs) created via vibration-assisted heat welding. The junctions, containing anywhere between one and seven bonds, are subject to uniaxial tensile, shear and torsional strain, and then the stiffness values are determined for each case. When subjected to tensile and shear strain, both the arrangement and orientation of bonds are found to affect the stiffness of junctions more substantially than the number of bonds, bond length or bond order. Surprisingly, anisotropic shear behavior is observed in the X-junctions, which can be attributed to the junction’s bond orientation. Also, the stiffness of X-junctions tested under an applied torque (torsion) differs from the stiffness under tensile and shear strain, however, in that it is more substantially affected by the number of bonds present in the junction than by any other property.

Keywords: carbon nanotube; molecular dynamics; X-junction; stiffness

1. Introduction

Carbon nanotubes (CNTs) have been studied extensively since their discovery in 1991 by Iijima [1]. Over the past 20 years, the excellent electrical, mechanical and thermal properties of CNTs have attracted researchers because these properties present the potential that CNTs could successfully be incorporated into random CNT networks.

Carbon nanotube junctions have been regarded as promising candidates for building blocks of nanoelectronic devices. In recent years, many studies have been performed to investigate methods of joining single-walled carbon nanotubes (SWNTs) to form multi-terminal junctions, such as ‘Y’, ‘T’ or ‘X’ junctions [2–11]. Proposed techniques include electron beam irradiation [2–4] or ion irradiation [5,6], mechanical manipulation with atomic force microscopes [7,8], nanotube soldering [2], chemical functionalization [9] and heat welding [10–13]. Moreover, due to the superior mechanical properties of CNTs, CNT junctions may potentially be used as reinforcing components in polymer composites [14]. These promising applications enhance the importance of studying the physical and mechanical behaviors of CNT junctions.
The CNT junction structure is more complex than that of an individual CNT. For instance, there are far more investigations concerning the physical and mechanical properties of individual CNTs than studies specifically focusing on the CNT junction. The tensile deformation behavior of ultrathin SWNTs along the axial direction has been studied in detail using molecular dynamics (MD) simulations by Meng and co-workers [15–18] for the heat-welded CNT X-junction. Sinnott and co-workers illustrated the change in energy as a function of strain during deformation in tension and compression for the irradiation-welded CNT X-junction [4]. Another type of CNT junction which is comprised of three portions – two segments of CNTs with different diameters and a conical part connecting the two CNTs – has also been investigated [19]. In that work [19], MD simulations were performed to study the mechanical properties of single-walled to four-walled carbon nanotubes with intramolecular junctions under uniaxial tension. To legitimately characterize the mechanical behaviors of the three-dimensional (3D) X-junction CNT structure, mechanical properties, such as the radial tensile, torsional and shear properties, were investigated in this work via MD simulations. In contrast to previous studies [15–18], loading is applied to deform the junction only instead of deforming the junction together with CNTs composing the junction. This allows the direct study of the mechanical properties of the junction only.

The paper is organized as follows. Section 2 discusses the details of the simulations and the junctions in each deformation mode. This is followed by the presentation of the results from the simulations as well as a detailed discussion of the results in Section 3. Conclusions are then drawn from the investigation in Section 4.

2. Computational method and simulation setup

The simulations discussed herein are initially composed of two pristine (6,0) SWNTs placed perpendicularly one on top of the other, with one tube extending in the z-direction while the other tube extends in the x-direction, so as to form an X-junction. The two nanotubes have been bonded together using vibration-assisted heat welding with the initial unbonded shell-to-shell distance between tubes being either 1.5 or 2.5 Å [20]. Seven separate systems are examined; each of the systems contains between one and seven bonds working in unison to join the CNTs. Table 1 shows the number of bonds contained in each system, as well as the initial distance separating the tubes before bonding. A cutoff distance of 1.6 Å was employed to determine the formation of covalent bonds between carbon atoms.

| CNT system | Number of bonds | Initial distance (Å) |
|------------|-----------------|----------------------|
| 1          | 1               | 1.5                  |
| 2          | 4               | 1.5                  |
| 3          | 4               | 2.5                  |
| 4          | 4               | 2.5                  |
| 5          | 4               | 2.5                  |
| 6          | 6               | 2.5                  |
| 7          | 7               | 1.5                  |
The seven systems are each subjected to three different types of uniaxial testing in order to gain insight into the mechanical behavior, primarily the stiffness, of each system. Additionally, the adaptive intermolecular reactive empirical bond order (AI-REBO) interatomic potential is employed to accurately model interactions between the carbon atoms [21]. The AI-REBO interatomic potential takes the following form where the total interaction energy, \( E \), is represented by a sum over pairwise interactions, including covalent bonding (REBO) interactions, LJ terms and torsion interactions [22]:

\[
E = \frac{1}{2} \sum_i \sum_{j \neq i} \left[ E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i,j} \sum_{l \neq i,j,k} E_{ijkl}^{Tors} \right].
\]

A cutoff distance of 2.5 Å for the AI-REBO potential was employed in this work. At the start of all simulations, the system’s energy is minimized by the conjugate-gradient method to ensure a result representative of the carbon atoms’ natural interactions. All of the MD simulations in this work were carried out using the LAMMPS software [23].

2.1. Tensile loading

When performing the tensile loading simulations, the CNTs are divided into four regions, depicted in Figure 1, that are assigned different functions. The top region of the upper CNT, indicated as region (1), is fixed against movement while region (4) is displaced in the negative \( y \)-direction only so as to apply a purely axial load on the bond(s). This configuration assures that the bond and the regions of the CNTs associated with the bond are free to move naturally. Hence, a displacement increment of 0.0025 Å is applied to the atoms in region (4) at a time step size of 0.001 fs to minimize the dynamical effects on the force response. The atoms in region (2) have a Langevin thermostat applied to ensure that the system remains at the assigned temperature of 300 K throughout the simulation. Region (2) does not include the junction itself so as to ensure that the junctions’ mechanical properties remain unaffected by the thermostat. Necessary information for obtaining the force–displacement curves, such as the atomic coordinates and force values in region (3), are recorded at the end of each strain increment throughout the simulation.

![Figure 1. Schematic illustration of typical SWNT system at the beginning of the simulation. Region (1) is fixed while region (4) is displaced to create the desired deformation mode. A Langevin thermostat is applied to region (2) and necessary data are collected from the atoms located in region (3).](image-url)
Note that in all the simulations performed in this work, a displacement is used as opposed to applying a force to create the desired deformation mode. Displacing the atoms ascertained more reliable results in this type of simulation than applying a force since it creates a uniform strain increment at each time step. For this reason, displacements are used throughout the study. However, because force data is required to calculate the stiffness values, the incremental force accumulated throughout each time-step is output to a data file during all simulations. The incremental force values obtained are then summed to determine the resulting force during the period of interest.

2.2. Torsional loading
The different regions of the system illustrated in Figure 1 and boundary conditions applied for the tensile loading simulations are identical to those utilized in the torsional loading simulations with one important alteration. Instead of region (4) being pulled away from the upper CNT, as is the case in the tensile simulations, this region remains in its plane and is simply rotated about the bond. In each simulation, a torsional increment of 0.02° is applied to the atoms in region (4) and each increment is held for 0.001 fs. This rotation results in a torque being applied to the bond, which allows for the observation of junction properties and failure mechanisms under torsional strain.

2.3. Shear loading
The methods discussed thus far have only displayed how to carry out simulations for examining mechanical properties in two of the four planar directions. For the completeness of this study, shear simulations are carried out in the x-direction as well as the z-direction (see Figure 1) to assure that junction characteristics in each of the four planar directions are observed and documented. Shear testing in two directions also allows for the observation of anisotropic behavior in this type of junction, if it should be present.

Region designations used in the two aforementioned testing methods have again been duplicated and implemented in this method. Region (4) is once again the mobile section; however, the shear simulations dictate that the lower CNT remain in its plane while being pushed in either the x- or z-direction. Hence, a displacement increment of 0.001 Å is applied to the atoms in region (4) and each displacement increment is held for 0.001 fs.

3. Results and discussion
During the course of this work, a large number of MD simulations were carried out under different constraints and conditions to determine the accuracy, dependability and repeatability of results obtained. Each simulation was analyzed, and then numerically, as well as visually, compared to its counterparts to verify the authenticity of the results. Due to the substantial quantity of simulations amassed, it has been determined that the presentation of the entire collection of results in this report would be quite cumbersome. Therefore, a handful of representative simulations are selected for discussion which are believed to most conservatively represent the collection of data as a whole while retaining general trends affected by items such as bond orientation and configuration. These simulations have become the basis of this paper and the source of all data presented below.
3.1. **Tensile loading**

To begin, the method for determining the hybridization of the bonds in the junctions was based on an empirical equation, fitted to DFT calculations, for C–C bonds where BO$_{ij}$ is the bond order and $r_{ij}$ is the bond length in Å between atom $i$ and $j$ [24]:

$$BO_{ij} = \exp \left[-0.097 \cdot \left(\frac{r_{ij}}{1.399}\right)^{6.38}\right] + \exp \left[-0.26 \cdot \left(\frac{r_{ij}}{1.266}\right)^{9.37}\right] + \exp \left[-0.391 \cdot \left(\frac{r_{ij}}{1.236}\right)^{16.87}\right].$$  

(1)

The basic information for all seven systems employed for all three loading conditions computed using Equation (1) has been tabulated in Table 2. Additionally, the stiffness values collected from the tensile simulations are displayed in Table 3. All stiffness values were obtained from a least-squares fit line on the initial straight-line portion of the force versus displacement plot for each simulation. The initial straight-line portion of each force versus displacement plot is taken up to 3.5 Å in all tensile and shear simulations. Because the system energy is minimized before each simulation is initiated, the $y$-intercept for every case is zero. The force–displacement plot for the single-bond system is presented in Figure 2 and shows the typical trend found for all tensile simulations.

As can be seen from Tables 2 and 3, the single-bond system has a bond order of 0.99 and a stiffness of 27.21 N/m. This value presents an excellent baseline for the comparison of remaining simulations, but one must be mindful that the bond length of this system is slightly longer than the majority of the other systems. When reviewing Table 3, the reader is likely to notice the inconsistencies in the stiffness values of the four-bond systems as well as the markedly low stiffness of the seven-bond system. While one may think that

Table 2. Bond length and bond order of the bonds in the SWNT junction.

| CNT system | Bonds | Bond lengths, (Å) | Bond orders |
|------------|-------|------------------|-------------|
| 1          | 1     | 1.577            | 0.99        |
| 2          | 4     | 1.473 1.417 1.411 1.406 | 1.21 1.39 1.42 1.44 |
| 3          | 4     | 1.564 1.542 1.541 1.530 | 0.97 1.03 1.03 1.06 |
| 4          | 4     | 1.550 1.520 1.453 1.404 | 1.01 1.08 1.27 1.08 |
| 5          | 4     | 1.455 1.419 1.412 1.411 | 1.27 1.40 1.41 1.42 |
| 6          | 6     | 1.528 1.492 1.449 1.441 1.387 1.385 | 1.06 1.16 1.29 1.31 1.52 1.53 |
| 7          | 7     | 1.641 1.608 1.524 1.425 1.425 1.392 1.387 0.82 0.88 1.07 1.37 1.37 1.50 1.52 |

Table 3. Stiffness values collected for tensile simulations.

| CNT system | Number of bonds | Stiffness (N/m) |
|------------|----------------|-----------------|
| 1          | 1              | 27.21           |
| 2          | 4              | 41.28           |
| 3          | 4              | 54.67           |
| 4          | 4              | 58.08           |
| 5          | 4              | 44.18           |
| 6          | 6              | 81.41           |
| 7          | 7              | 62.20           |
the stiffness values of the four-, six- and seven-bond junctions would be approximately equal to four, six or seven times the stiffness value for the single-bond junction, this is not the case. To explain this behavior, we will begin by discussing the lower-than-expected stiffness values, as well as the large inconsistencies, for the four-bond junctions.

By observing Table 3, it is evident that systems 2 and 5 have similar stiffness values; likewise, systems 3 and 4 have nearly the same stiffness. This behavior would be expected upon referencing Table 2 because each system contains four bonds with nearly identical bond lengths and comparable bond orders. However, the stronger set containing systems 3 and 4, with respective stiffness values of 54.67 N/m and 58.08 N/m as compared to values of 41.28 N/m and 44.18 N/m for systems 2 and 5, has bond orders that are generally lower than the weaker pair of systems. This behavior is counterintuitive, since a higher bond order should result in a larger stiffness value, so we must turn to the physical properties of the junctions themselves. Upon observation, it is evident that the junctions of systems 2 and 5 bond in nearly identical fashion despite being bonded under two separate circumstances. Table 1 shows the initial unbonded distances for systems 2 and 5 to be 1.5 and 2.5 Å, respectively, yet the bonds in both simulations are of approximately equal length. The bonds in these two systems have formed at the center of the top tube, but towards the edge of the bottom tube along its diameter which has caused the shell of this tube to bow slightly outward, as shown in Figure 3a. Moreover, the bonds have formed in a square arrangement with multiple hexagon rings on each CNT breaking to accommodate this bonding.

The second set of four-bond systems – those with high stiffness values – possess junctions that are each unique. In system 3, the bonds have arranged themselves in a diamond configuration that is centered along the diameter of the top tube and spans the entire width
of the bottom tube. This arrangement has resulted in a bond that is thick along the \(x\)-axis and thin along the \(z\)-axis, as shown in Figures 3b and 3c, respectively. Meanwhile, only two hexagon rings have been broken on the CNTs during bonding which has allowed the nanotubes to remain almost entirely intact with few deformations. System 4 contains the same square bond configuration as the first two systems that were discussed, but this junction has formed in a more compact arrangement, so less bowing of the bottom tubes shell has occurred. Additionally, fewer hexagon rings have been broken than in the other two junctions with the square-shaped bond configuration, so the CNTs comprising the X-junction contain fewer voids. The bond structure for system 4 can be viewed in Figure 3d.

The stiffness values are affected by not only the configuration of the bonds and defects incurred during bonding, but also by the orientation of the bonds themselves. The lower than anticipated stiffness values in the more highly-bonded junctions are attributed to the fact that the single bond of system 1 lies almost perfectly along the \(y\)-axis, making it perpendicular to the tubes which lie in the \(x-z\) plane. As a result, the single bond undergoes pure axial loading as the tubes are displaced in the \(y\)-direction. Conversely, the multi-bond systems contain bonds that are angled to the \(y\)-axis and are therefore subject to strain in more than one direction, unlike the single-bond system. This also explains the varied stiffness values collected from the four-bond junctions, since systems 2 and 5 are found to...
contain no bonds that are perpendicular to the CNTs. On the other hand, system 3 is found to have two bonds aligned with the axis of displacement, and all of the bonds contained in system 4 are nearly aligned with this axis. Therefore, the result of these differing bond orientations is observed in the form of varied stiffness values in Table 3 with the systems containing more bonds lying along the axis of displacement attaining a higher stiffness.

The junction observed in the six-bond system has a stiffness value of 81.41 N/m, which is higher than any of the tensile simulations. This junction has formed in the shape of a rectangle, with three bonds to a side, which is situated in the center of the bottom tube and slightly to the edge of the top tube. As a result of the rectangular configuration, this bond is wider along the x-axis than the z-axis, much like system 3, as shown in Figures 4a and 4b. Additionally, only two hexagons on the tubes are broken during bonding and negligible deformation of either CNT has occurred. Despite displaying such a high stiffness value, no bonds in this junction have formed along the axis of displacement. This detail suggests that the six-bond arrangement witnessed in this system is an optimal configuration for the creation of an X-junction with high stiffness.

In the final seven-bond tensile simulation, the stiffness value is found to be curiously low at 62.20 N/m – only slightly higher than that of the four-bond systems. A portion of this subpar stiffness can be attributed to the lower than average bond orders found in Table 2; however such a dramatic decrease in stiffness cannot be explained by this alone. After examining the bonds, it is apparent that the junction contains several defects which are indicative of low stiffness in previous simulations. Four of the bonds have attached to the edge of the bottom CNT and caused the bowing of the tube’s shell as has previously been witnessed; however, previous simulations have had no more than two bonds attached in this manner. Additionally, two of the bonds extending from the top CNT have merged and attached to a single site on the bottom CNT, causing four bonds to be joined with a single carbon atom; this defect is illustrated in Figure 5. Multiple hexagons have been broken during bonding which has severely compromised the strength of the junction by creating large voids in the CNTs around the bond site. Finally, the bonds in this situation have formed at angles much greater than that of bonds observed in any of the previous simulations, providing further validation that the degree to which bonds are aligned with the axis of displacement is paramount to the tensile strength of the junction.

3.2. Torsional loading

The second round of simulations was aimed at determining how junctions performed under an applied torsion. Table 4 shows the data collected from these runs, and again the results are surprising. The reader may notice that in this case, data for only six systems is presented. The data collected from system 5 is omitted because this system produced nonphysical results, so it is excluded from consideration. Nonphysical results, in this study, entail the simulations behaving in an unnatural manner once a bond breaks. The reason for this behavior is that a large amount of energy is released after a bond breaks and occasionally the simulations are unable to recover quickly.

Figure 6 shows a typical plot collected in the torsion simulations and the stiffness values in this case are calculated from the initial slopes of the lines composing the oscillations. Looking at the stiffness information in Table 4, one may note that the values generally decrease as the number of bonds contained in the junction increases, in contrast to the trend observed under tensile loading. Because the bonds in the torsional simulations tend to break and re-form continually throughout the simulation, this unique behavior is thought
Figure 4. Structure of the six-bond junction observed in system 6 as viewed from (a) the thick side and (b) the thin side.
Figure 5. Structure of the seven-bond junction observed in system 7 with the defect of four bonds joining a single carbon atom clearly visible.

Table 4. Stiffness values collected for torsion simulations.

| CNT system | Number of bonds | Stiffness (J/degree) \(10^{-17}\) |
|------------|----------------|-----------------------------------|
| 1          | 1              | 8.41                              |
| 2          | 4              | 7.88                              |
| 3          | 4              | 14.30                             |
| 4          | 4              | 5.82                              |
| 5          | 4              | –                                 |
| 6          | 6              | 2.29                              |
| 7          | 7              | 5.86                              |

to be a function of the number of bonds and the number of sites available on either CNT for re-bonding.

As the bottom CNT is rotated, bonds begin to break and leave their initial bond site available. If another bond is in close proximity to this site, it will generally break and re-form there. When fewer sites are available for re-bonding, the bonds remain at their initial bonding sites and exert a force against the applied torsion until their strength is overcome and break. On the other hand, having multiple sites continuously available for re-bonding will allow the bonds to break and re-form more easily, lowering the resistance of the junction against the applied torsion. For discrepancies found to counter the general trend, such as systems 3 and 7, bond orientation and bond order are thought to be the cause.

3.3. Shear loading

In the final set of simulations, the behavior of the junctions was investigated under shear strain. The results of these simulations are displayed in Table 5 with stiffness values shown for an applied displacement in both the \(x\)- and \(z\)-direction. As expected, the single-bond
system shows very close stiffness values in the two cases since anisotropic behavior is unlikely with only one bond. However, even the nearly identical four-bond junction of systems 2 and 5 show slight differences in the stiffness values in both the \(x\)- and \(z\)-direction shearing tests. This slight difference is likely due to errors when estimating the stiffness from the force versus displacement plots because, as Figure 7 shows, the typical graph obtained from the shear simulations does not have a well-defined initial straight line portion as previous tests have.

In systems 2 and 5, the difference in \(x\)-direction and \(z\)-direction shearing stiffness is in good agreement once error is taken into account. This difference, as well as the difference displayed by a majority of the other systems, shows that CNT X-junctions are anisotropic in nature. In these two systems, since the bonds are nearly identical, the decrease in stiffness from the \(x\)-displacement to the \(z\)-displacement cases is caused by the bond placement and
orientation. In the $x$-displacement case, many of the bonds are angled against the direction of motion and, since the bonds are formed on the well-braced and un-deformed side of the bottom CNT, the entire side of the tube flexes and resists motion when sheared. Conversely, in the $z$-displacement case, only one bond is angled against motion and it is connected to the bottom tube in such a manner that provides very little support. Additionally, the bonds in this case break very quickly because the CNT does not flex to provide reinforcement as it did when sheared in the $x$-direction.

Recalling the diamond-shaped bond from system 3, this arrangement is discovered to be thicker in the $x$-direction. Consequently, when the tubes are sheared in the $x$-direction, the bonds are aligned parallel with the direction of motion and a higher stiffness is observed than when shear is applied in the $z$-direction with the bonds being aligned perpendicular to the direction of motion. This concept is also observed to produce higher $x$-direction stiffness in system 6 which contains the same type of bond which is thicker in one dimension than the other.

The only multi-bond junction that does not display anisotropic behavior is observed in system 4 with stiffness values of 87.77 N/m and 89.66 N/m in the $x$- and $z$-directions, respectively. As mentioned earlier, the bonds in this junction have formed in a nearly perfect square arrangement. Upon further investigation it is noted that two bonds, each at opposite corners of the square along its diagonal, are oriented against motion in the $x$-direction while the remaining two bonds are oriented against motion in the $z$-direction. The symmetry observed in this system in both the $x$- and $z$-direction has resulted in a junction that behaves in an isotropic manner when subject to shear strain.

Referring to Table 5, the seven-bond junction of system 7 is shown to display remarkably similar stiffness values to that of system 6 despite being substantially weaker in the

Figure 7. Typical force–displacement plot collected during testing under shear strain.
tensile simulations. The extreme bonding angles of system 7 which made the junction weak under tension actually allow it to behave more favorably in the shear simulations. It is believed that a bond with a greater angle (i.e. more parallel to the CNTs instead of perpendicular to them) will provide more resistance to shearing and result in a stiffer junction. The seven-bond junction may be expected to be stronger than the six-bond junction because it contains more bonds at greater angles, but the defects contained in the seven-bond junctions result in a lowered stiffness value. Additionally, it may be observed from Table 2 that system 7 contains bonds with much lower bond orders than that of system 6, yet the junctions display similar stiffness properties. This holds true for many of the simulations, with the strongest systems generally containing bonds with lower bond orders. Moreover, this aspect provides evidence that the geometry of the bond and the orientation of the bonds have a greater influence on the junction strength than the bond length or bond order.

4. Conclusion
The mechanical properties, primarily the stiffness properties, of CNT X-junctions were studied using molecular dynamics simulations. Seven different junctions created by vibration-assisted heat welding were studied, with each junction containing between one and seven bonds. These junctions were subjected to three different forms of uniaxial testing in order to analyze their behavior in each case.

It has been found that the characteristics of junctions undergoing tensile or shear strain are primarily affected by the arrangement and orientation of bonds. The number of bonds also determines the stiffness of these X-junctions but may negatively affect the mechanical properties if bonds form in such a manner that has resulted in deformation of the tubes composing the junction. Anisotropic behavior is also observed in this type of junction under shear loading with the orientation of bonds being the primary cause.

The stiffness of X-junctions subject to torsion is found to be highly influenced by the number of bonds present within the junction. In this case, competition between the number of bonds and number of sites available for re-bonding determines the stiffness. In a junction with few initial bonds, there will be limited opportunities for the bonds to break and re-form at a new site and a higher stiffness will be observed. In the case that the junction contains a large number of bonds, these bonds will be able to readily re-form at a new site and provide little resistance to motion, resulting in low stiffness.

The simulations presented in this report are highly repeatable. All simulations were carried out on a single Intel Xeon E7450 processor using a Linux operating system, with each simulation requiring a duration of approximately 5 h to complete.

Acknowledgments
This work was supported by NSF REU through grants (CMMI-0928094 and BRIGE-EEC-0926885) and the Swanson School of Engineering at the University of Pittsburgh.

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