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To cite this article: Ahmad Y. Al-Maharma et al 2021 IOP Conf. Ser.: Mater. Sci. Eng. 1190 012026

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Molecular Dynamics Investigation on the Effect of MWCNTs on Thermo-Mechanical Properties of Amorphous Cellulose Reinforced with Silicon Carbide Nanotubes

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Abstract. Cellulose is a biopolymer frequently implemented as fibers and membranes to fabricate high-performance and multi-functional composites. In this study, the molecular dynamics simulation is used to investigate the effect of CNTs on elastic modulus, ultimate strength, and toughness properties of silicon carbide nanotubes (SiCNTs) reinforced cellulose nanocomposite. Based on the simulation results, the temperature of the surrounding environment controls the stress transfer at the nanotube-cellulose interface. As the cellulose expands with increasing temperature creating more void regions at the filler-matrix interface, the load transfer from cellulose to nanotubes is reduced, leading to a noticeable reduction in tensile properties of cellulose composite. This behavior critically affects the tensile strength of cellulose composite reinforced with multi-walled CNTs (MWCNTs). The single-walled CNT with a high aspect ratio increases the cellulose composite's tensile strength and toughness, while the MWCNT introduces the most significant increase in cellulose stiffness. The difference in polarity between MWCNT and cellulose, along with the low aspect ratio of the external nanotube, would limit the capability of MWCNT in improving the tensile strength and toughness of cellulose. The single-walled SiCNTs are structurally unstable, and their stiffness degrades rapidly at high temperatures. Therefore, they are hybridized with CNTs to improve their stiffness and structural stability. SiCNT, which is hybridized with two CNTs, exhibits the best structural performance at 100, 300, and 500 K temperatures.

1. Introduction

Polymers synthesized from natural materials received a large portion of interest in recently published research due to the depletion of petroleum resources and the associated harmful impacts of the materials synthesized from these resources on climate change. The main objective of this study is to improve the tensile properties of amorphous cellulose under varying thermal environments. The stiffness, strength, and toughness are characterized at three different temperatures: 100, 300, and 500 K. To the best of the authors’ knowledge, none of the previously published literature characterizes the mechanical properties of amorphous cellulose reinforced with either MWCNTs or hybrid multi-walled CNT/SiCNT in varying thermal environments. The available molecular dynamics (MD) studies in the published literature investigate the effect of single-walled CNTs [1] and double-walled CNTs [2] on cellulose properties. Improving cellulose properties through chemical treatments such as functionalization would compromise its properties such as strength and fracture toughness. Therefore, using mechanically high-
performance nano-fillers is the optimum technique to preserve the original structure of cellulose while its properties are improved.

With increasing cellulose content, the mechanical properties of natural fibers are increased [3]. Due to attractive aspects of natural fibers of biodegradability, high specific strength, and moderate mechanical properties, plant fibers can be used in many applications of automotive and aerospace industries [4]. SiCNTs and CNTs can be used to reinforce cellulose to improve its thermal stability and material properties. Carbonous nano-fillers can increase cellulose's bulk, elastic, and shear moduli by 25.6%, 30%, and 32.9%, respectively. These improvements can be attributed to increased intermolecular hydrogen bonds and cohesive energy density [5].

SiCNTs have distinct properties of good chemical inertness, excellent electronic properties, and high thermal stability [6]. Moreover, cellulose nanocomposites reinforced with SiC have tensile properties and thermal stability higher than the neat cellulose polymer [7]. There is a need to hybridize SiCNTs with CNTs to improve their properties as the elastic modulus of SiCNT is evaluated to be half that of CNT with about 0.61 TPa [8]. The chemical modifications applied to the structure of cellulose and SiC nanofillers could compromise their material properties. For instance, applying functionalization based on amines like (-NH₂) and oxidation to modify the surface of SiC reinforcements could further improve their reinforcing effect up to a specific extent [9]. However, based on the results of MD simulation conducted on oxidized single-walled SiCNTs (SWSiCNT), the stiffness, strength, and toughness of the functionalized SiCNTs are decreased with increasing degrees of functionalization [10].

CNTs can improve cellulose's mechanical properties and hygro-thermal aging behavior since they have a high aspect ratio and good moisture resistance [11]. When these nanofillers reinforce polymers, they can significantly improve their properties so the resulting nanocomposites can be implemented in broad practical applications such as drug delivery systems and infiltrating membranes [12]. The ideal arrangements of carbon-carbon covalent bonds oriented along the axis of CNTs make them very strong with a remarkable strength-to-weight ratio. They exhibit very high tensile strength and Young’s modulus values of 50-500 GPa and 1.50 TPa, respectively [13]. The combination of carbon and cellulose materials can improve the aspects of composite, such as tensile strength (23.1-277.5 MPa) and Young’s modulus (1.14-16.6 GPa) [14]. The composite materials that combine CNTs and SiC show high stiffness values, superb thermal stability at extreme temperatures, and excellent heat resistance [15].

This research is organized as follows: first, details of the material configurations and their properties, along with their computational analyses, are described in Section 2. Then, simulation results on the mechanical properties of the cellulose composite are discussed in Section 3, along with a comparison to the neat cellulose polymer. Finally, conclusions are given in the last section.

2. Materials and test methods
MD simulation is used in this study to understand how the nano-fillers such as CNTs and SiCNTs can provide the structural reinforcing effect to cellulose polymer and comprehend the process of load transfer between cellulose and nanotubes at various temperatures. At the first stage of this research, composite models are designed with details discussed in Section 2.1. Then, the recent variant of all atoms force fields (OPLS 4) coupled with Desmond GPU solver described in Section 2.2 is used to characterize the tensile behavior of cellulose at three different temperatures of 100, 300, and 500 K.

2.1. Cellulose composite models
The cellulose matrix synthesized of linear D-beta-glucose polymer is first prepared according to the procedures discussed in [16]. Both MWCNT and multi-walled SiCNT (MWSiCNT) have three walls, and the first inner wall has a chiral index of (6,6). The inner separation space between the walls of MWCNT is determined to be 0.335 nm, while the distance among the walls of MWSiCNT is taken as
0.435 nm. MWSiCNT and MWCNT have armchair structures with lengths of 73.13 and 73.53 Angstrom and diameters of 21.62 and 27.41 Angstrom, respectively. The MWSiCNT is hybridized by replacing the first and second inner tubes with CNTs. To increase the specific mechanical properties of cellulose composites, the MWSiCNT, MWCNT, and their hybrid are arranged in rope-like structures to improve the load transfer between them and the cellulosic matrix. The SiCNT-rope is hybridized by substituting the two adjacent single-walled SiCNT with minor diameters with two SWCNTs at similar sizes. It is noteworthy that the geometry of the nanotube plays a critical role in affecting the properties of the final nanocomposite. The increasing aspect ratio of SiCNTs decreases the critical compressive forces of nanotubes. By fixing the side length of nanotubes, SiCNTs with smaller radii have more structural stability and less tendency toward buckling [17]. The material models are classified into two groups to understand the effect of aspect ratio and orientation of the nanotubes on the final properties of cellulose composites: (i) unidirectional (UD) CNTs and SiCNTs with periodic terminal atoms aligned along Y-axis; (ii) short length nano-fillers with hydrogen terminal atoms randomly positioned within the cellulosic polymer.

The essential elements used to generate the MD models of cellulose composites are shown in figure 1. Increasing the content of MWCNTs in cellulose composite reinforced with MWSiCNTs would make the material stiffer and increasing its density to the highest extent. Table 1 shows how the arrangements of MWSiCNT and MWCNT, in addition to their molecular weights, affect the overall density of cellulose composites. Hybridizing SiCNTs with CNTs has a trivial effect on the density of cellulose. It can be inferred from the table data that the rope-like structure of nanotubes creates a larger void space inside the cellulose composites relative to the traditional form of the multi-walled nanotubes (MWNTs) reducing the overall composite density.

Figure 1. The fundamental elements used to construct the cellulose composite models: (a) amorphous cellulose, (b) MWCNT, and (c) MWSiCNT.

2.2. The setup of MD simulation
The OPLS force field defines the charges and positions of atoms, the optimum bond lengths, and dihedral angles distribution [18]. Energy minimization should be conducted before equilibrating the MD models using NPT and NVT ensembles to eliminate undesirable interactions, including clashes between atoms. The steepest descent (SD) and limited memory Broyden- Fletcher- Goldfarb- Shanno (L-BFGS) minimization methods are used to efficiently minimize large MD models' energy. The dihedral angles of the cellulose polymers are distributed in the unit cell so that minimum clashes among atoms can be guaranteed. The SD algorithm is superior to the conjugate gradient if the starting MD system is some way from the minimum energy [19]. NPT ensemble is then applied for 60 nanoseconds (ns) at 2 femtoseconds (fs) time step to relax the MD system and to increase its density based on Martyna Tobias
Klein barostat method [20]. To improve the distribution of cellulose polymers and to further increase the density of the MD models to the highest possible level, NVT ensemble is applied for 5 ns with 2 fs time step at T= 350 K. The latter ensemble is followed by another NVT ensemble for 3.36 ns with 1 fs time step at T= 500 K. The equilibration of MD models based on NVT ensemble is conducted based on Noose-Hoover thermostat as cellulose is flexible material [21]. The tensile properties are characterized under three different temperatures: 100 K, 300 K, and 500 K. NPT ensemble is used to expand the unit cell for 10 picoseconds (ps) with a time step of 2 fs.

Table 1. The effect of nanotubes' molecular weights and arrangements on the density of cellulose.

| Material               | Molecular weight (wt.%) | Average density (g/cm³³) |
|------------------------|-------------------------|--------------------------|
|                        | Cellulose | SiC | CNT | Traditional | Rope |
| Cellulose/short-MWCNT  | 100       | 0   | 0   | 1.41        | -    |
| Cellulose/short-MWSiCNT| 82.64     | -   | 17.36 | 1.46 | 1.33 |
| Cellulose/short-MWCNT  | 78.25     | 21.75 | -  | 1.42 | 1.30 |
| Cellulose/short-MWSiCNT| 79.01     | 17.97 | 3.02 | 1.39 | 1.27 |
| Cellulose/short-MWCNT  | 80.46     | 10.84 | 8.70 | 1.38 | 1.26 |
| Cellulose/short-MWSiCNT| 82.36     | -   | 17.64 | 1.48 | 1.35 |
| Cellulose/short-MWSiCNT| 77.84     | 22.16 | -  | 1.45 | 1.38 |
| Cellulose/short-MWSiCNT| 78.63     | 18.38 | 3.06 | 1.44 | 1.39 |
| Cellulose/short-MWSiCNT| 80.10     | 11.06 | 8.84 | 1.44 | 1.41 |
| Cellulose/short-MWSiCNT| 66.72     | 18.99 | 14.29 | 1.48 | -    |

3. Results and discussions
The cellulose's structure contains voids that provide to its composite's high capability to attenuate the damaging effect of loads. Without nano-fillers, there is a need to apply more pressure and heat on neat cellulose to increase its stiffness at the expense of fracture toughness. This treatment would remove a large part of air pores making cellulose stiffer material. The stiffness values of multi-walled and rope-like arrangements of SiCNTs and CNTs are characterized in Section 3.1, whereas strength and fracture toughness properties for shot length nanotubes of SiCNTs and CNTs reinforced cellulose are studied in Section 3.2.

3.1. Aligned unidirectional nanotubes reinforced cellulose
The magnitude of improvement achieved on the stiffness of cellulose composites is controlled by the aspect ratio and the number of nanotubes placed in the direction of the load. As the values in figure 2 can tell, all arrangements of CNTs and SiCNTs increase the stiffness of cellulose, which is evaluated as 9.48 GPa agreeing well with the determined value in the literature of 9.37 GPa [16]. It can be noted from the same figure that cellulose composites reinforced with CNTs have higher stiffness relative to the ones reinforced only with SiCNTs. All nanotubes' arrangements can improve the cellulose stiffness as the MWSiCNT and MWCNT can increase the stiffness up to around 2 and 10 times of pure cellulose, respectively. The MWNTs are thick structures showing a higher resistance to the applied tensile load than single-walled nanotubes composing the rope-like structure, as can be concluded from the deformed cellulose composites shown in figure 3.

3.2. Short length nanotubes reinforced cellulose
The conventional method used to optimize the material properties of most bio-composites is simply the incorporation of MWNTs into their structures. However, the addition of MWNTs to MWSiCNT reinforced cellulose will displace more elastic cellulose from the matrix replacing it with stiff carbon atoms. Therefore, the stiffness of cellulose composite is significantly increased relative to neat cellulose, as demonstrated by the values listed in table 2. However, the strength of MWCNT-MWSiCNT reinforced cellulose is severely reduced even below that of pure cellulose at 100 K since the MWCNT has an incompatible interface with hydrophilic cellulose matrix and the CNT that has direct contact with
cellulose has a lower aspect ratio relative to the internal tubes. This incompatibility in terms of polarity becomes more dominant and apparent at high temperatures, as shown in figure 4.

![Figure 2](image2.png)

**Figure 2.** The effect of nanotubes arrangements on the stiffness of cellulose composites, which is characterized at T=100 K: (a) stress-strain relationships, (b) Young's modulus values.

![Figure 3](image3.png)

**Figure 3.** The cross-sections of deformed cellulose composites under tensile loading at T=100 K, which are reinforced with the following nanotubes: (a) UD-MWCNT, (b) UD-MWSiCNT, (c) UD-SiC-SiC-CNT, (d) UD-SiC-CNT-CNT, (e) UD-CNTs-rope, (f) UD-SiCNTs-rope, (g) UD-SiC-SiC-CNT-rope, and (h) UD-SiC-CNT-CNT-rope.
### Table 2. The effect of temperature on tensile properties of cellulose/SiC-CNT hybrid composites.

| Material                          | T= 100 K |                     | T= 300 K |                     | T= 500 K |                     |
|-----------------------------------|----------|---------------------|----------|---------------------|----------|---------------------|
|                                   | $E$ (GPa) | $S$ (MPa) | $G$ (MJ/m$^3$) | $E$ (GPa) | $S$ (MPa) | $G$ (MJ/m$^3$) | $E$ (GPa) | $S$ (MPa) | $G$ (MJ/m$^3$) |
| Cellulose                        | 9.48     | 643.73              | 165.98   | 6.74                | 420.89   | 108.76            | 4.86      | 302.62   | 64.28            |
| Cellulose/MWCNT                  | 12.72    | 671.5              | 187      | 10                  | 533.63   | 138.86            | 8.31      | 347.98   | 82.3             |
| Cellulose/MWSiCNT                | 12.03    | 735.9              | 178.54   | 9.83                | 493.28   | 121.19            | 5.07      | 298.22   | 78.28            |
| Cellulose/MWCNT-MWSiCNT          | 12.21    | 592.89             | 172.03   | 10.22               | 451.2    | 121.68            | 5.81      | 312.89   | 74.14            |
| Cellulose/SiC-SiC-CNT            | 10.09    | 720.83             | 178.18   | 8.62                | 545.96   | 134.04            | 4.87      | 327.57   | 80.14            |
| Cellulose/SiC-SiC-CNT-CNT        | 11.25    | 703.41             | 182.82   | 9.70                | 526.89   | 136.89            | 7.21      | 357.97   | 92.06            |
| Cellulose/CNTs-rope              | 11.60    | 710.69             | 197.62   | 8.66                | 499.54   | 132.66            | 8.29      | 360.82   | 90.35            |
| Cellulose/SiC-SiC-CNT-rope       | 10.62    | 500.08             | 144.91   | 7.90                | 328.72   | 100.95            | 6.15      | 253.24   | 61.91            |
| Cellulose/SiC-SiC-CNT-rope       | 11.23    | 665.2              | 161.47   | 9.43                | 397.56   | 111.07            | 5.19      | 312.22   | 76.14            |
| Cellulose/MWCNT-SiC-CNT-rope     | 12.44    | 700.88             | 191.91   | 11.84               | 602.24   | 144.5             | 8.41      | 396.22   | 86.04            |

**Figure 4.** The generating of interfacial voids between MWCNT and cellulose with increasing temperatures: (a) 100 K, (b) 300 K, and (c) 500 K.

The rope-like structures shown in figure 5 prove that the single-walled SiCNTs are structurally unstable. Through hybridizing SiCNTs withCNTs, we will ensure that the hybrid nanotubes will have good interlocking with cellulose (needed for strength), more void spaces are generated as the CNTs with
small diameters will replace larger internal tubes of SiCNTs (needed for toughness), and the high aspect ratio stiff CNTs placed in the tube core will improve the tube capability to resist loads (needed for stiffness). The hybrid nanotube of SiC-SiC-CNT has a thick external wall with the capability to transfer load from cellulose. It functions perfectly to improve cellulose's strength and toughness at low to moderate temperatures (100-300 K), but its stiffness degrades rapidly at high temperatures (T= 500 K). The hybrid nanotube of SiC-CNT-CNT has a thin external wall with good interlocking with cellulose at low temperatures (T= 100 K), but it becomes structurally unstable with increasing temperatures (T= 300 and 500 K). Nevertheless, this configuration has a stable stiffness at all temperatures due to its stiff core.

Figure 5. The deformed cellulose composites reinforced with short nanotubes at T=100 K: (a) MWCNT, (b) MWSiCNT, (c) SiCNT-SiCNT-CNT, (d) SiCNT-CNT-CNT, (e) CNTs-rope, (f) SiCNTs-rope, (g) SiC-SiC-CNT-rope, and (h) SiC-CNT-CNT-rope.

The stress-strain curves characterized at low and high temperatures of cellulose composites reinforced with CNTs and SiCNTs are shown in figure 6. It is confirmed from the results shown in figure 6.a that CNTs play a critical role in improving the strength and fracture toughness of cellulose reinforced with rope-like configurations of nanotubes. The highest strength peaks are noticed at cellulose reinforced with CNT-rope since all CNTs, especially those with high aspect ratio, have direct contact with cellulose matrix at T=100 K. At room temperature of T=300 K, the only configuration that shows remarkable poor performance is SiCNT-rope reinforced cellulose as shown in figure 6.b since the low aspect ratio, thin, and single-walled SiCNT is structurally unstable with increasing temperatures. The rope-like configuration, modified with two high aspect ratio CNTs, exhibits the highest tensile strength. Figure 6.c shows that the tensile properties of SWSiCNT are reduced significantly at 500 K, and these tubes play a damaging role in the cellulose structure. It can be concluded from the previous discussion that the hybridization of SiCNTs with CNTs would improve the values of stiffness and toughness at all temperature ranges. The stiffness and toughness values of cellulose reinforced with only CNTs (CNT-rope & MWCNT) are stable at all temperatures (100, 300, and 500 K) and do not experience any severe degradation. Furthermore, the SiCNTs have effective interlocking with cellulose matrix at low and high temperatures, as shown in figure 6.d increasing the tensile strength of cellulose composite.
Figure 6. The effect of SiCNT/CNTs on tensile behavior of cellulose at three different temperatures: (a) 100 K, (b) 300 K, and (c) 500 K, and (d) effective interlocking of thick SiCNT wall with cellulose at 100 K (left) to 500 K (right).

4. Conclusions

CNTs are high mechanical performance nanofillers with competitive stiffness and strength values. However, these nanofillers have poor compatibility with biomaterials like cellulose due to the difference in polarity. SiCNTs have an effective interlocking with hosting cellulose matrix. However, their stiffness is degraded fast with increasing temperatures. Additionally, the SWSiCNT is structurally unstable and cannot be used as standalone reinforcements in varying thermal environments. Incorporating MWCNT directly into MWSiCNT/ cellulose composite without hybridization would increase the stiffness of the composite at the expense of strength and toughness properties. Therefore, CNTs are used to hybridize SiCNTs to improve cellulose composites’ stiffness, strength, and toughness properties. Two models of
hybrid MWNTs are considered. The first model has a thick external wall of double-walled SiCNTs, while the other has SWSiCNT. The hybrid MWNT of SiCNT-SiCNT-CNT shows superb strength and fracture toughness values with a moderate increase in stiffness at 100 and 300 K. This can be justified to the large void space created inside the core of MWNT after substituting SiCNT with high aspect ratio CNT and good interlocking of the thick external wall of SiCNT with cellulose. At 500 K, the stiffness of SiCNT-SiCNT-CNT is degraded, and the composite shows the stiffness of neat cellulose. Therefore, additional SiCNT is replaced with CNT to improve the stiffness, strength, and toughness at high temperatures.

The results of the MD simulation confirm that at a low temperature of 100 K, the cellulose polymers are adequately compressed to the nanotubes leading to effective load transfer from cellulose to fillers. To improve the tensile properties of cellulose composites at higher temperatures of 300 and 500 K, chemical functionalization is needed at nanotube- matrix interface, but care must be taken during this process to avoid compromising the structural aspects of cellulose.

Acknowledgment

The first author would like to acknowledge the financial support provided by the German Academic Exchange Service (DAAD) to accomplish this research.

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