Study of Mechanical Properties of Polyethylene/CNT Nanocomposites: Experimental, FEM and MD

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Abstract—Designing and developing a new material can be challenging due to several aspects that require consideration. Material behavior, material properties (physical or chemical), and other material characteristics are the factors to consider when developing new materials. In this work, polymer-based nanocomposite material is developed using High-Density Polyethylene (HDPE) as a matrix, Single-walled Carbon Nanotube (SWCNTs) as the reinforcing particles. Moreover, the mechanical properties of the produced HDPE/SWCNT nanocomposites, such as elastic modulus, were investigated at different weight fractions of SWCNTs. The investigation was conducted using numerical (Molecular Dynamics MD), theoretical (Finite Element Method FEM), and experimental approaches. The major aim of this study was to validate the accuracy of the developed MD model and the theoretical FEM with the experimental results. The obtained elastic modulus results from the MD and FEM were compared to see which method produced the results correlating with the experimental results. The compared results showed that MD results were consistent with the experimental results, even though they are not accurate, though the model can be improved. However, the FEM results do not correlate with the experimental results, hence the FEM model developed is not better for the prediction of the elastic modulus of HDPE/SWCNTs nanocomposites.

Keywords—Polyethylene, Carbon Nanotubes, Elastic Modulus, Nanocomposite, Molecular Dynamics

I. INTRODUCTION

Plastics are among the first artificial materials with their structure based on chemical elements such as carbon, hydrogen, oxygen, nitrogen, chlorine, and sulfur. These elements are found in air, coal, gas, water, oil, and even living plants. They turn to produce numerous and endless strands of different chemical compositions when mixed in various chemical reactions. Some of these chemical reactions include polymerization of hydrocarbon chains to produce polymers. It is generally thought that plastics are to be emerging materials, but in fact, they are part of a more prominent family of polymers, an essential element in the life of animals and plants. A polymer is a pure material resulting from a polymeric reaction that has long molecules and a chain of species, including even elastics. Polymers are high-molecular synthetic molecules composed of and joined together by thousands of small molecular units called monomers. The polymer structure has very long-chain molecular molecules that are entirely different from the metal structure. The method of bonding molecules to each other is called polymerization, and the number of these tiny molecular units in the long chain is called the degree of polymerization.

Polymers have received significant interest in the last few decades and are extensively utilized in advanced engineering applications such as automotive parts, electronic and food packaging, various optical components, semiconducting materials, liquid crystal displays, insulating, and vibration damping [1]. Polymer combinations are a practical and economical way to produce materials with various properties and broader applications. The advantage of mixing the polymer with other nanoparticles is to produce materials with desired specifications at a low cost and to expand applications of engineered polymers (polymer-based nanocomposites).

Given the ultimate application of polymer nanocomposites, there are issues concerning their production, enhancements, mechanical properties and other related aspects. However, several studies have been carried out on polymer-based nanocomposites, some of which are described here. One of the early studies of polymer/CNT composites was done by Ajayan et al. [2]. In their research, they mixed Multi-Wall Carbon Nanotubes (MWN Ts) with liquid epoxy resin through mechanical mixing. Their results showed advancement in the mechanical properties of epoxy resin.
After that, many other publications have addressed the fact that combining a small percentage of Carbon Nanotubes (CNTs) by weight into polymer matrices could enhance the mechanical [3-16], and electrical [17, 18], properties of polymer composites. Han and Elliott [19] conducted a computational study using classical molecular dynamics (MD) simulations to model polymer/CNT composites by embedding SWCNTs into two various amorphous polymer matrices at different volume fractions. Their investigation demonstrated improvement in the mechanical properties of the composite. Fu et al. [20], presented an acceptable theoretical approach based on the modified rule of mixtures that successfully determined the CNT strength and polymer/CNT interfacial strength. Xiao et al. [21], investigated the mechanical and rheological properties of a Low-Density Polyethylene (LDPE) matrix reinforced with MWNTs. Their study showed an increase in the tensile strength and the Young’s modulus of the composites. Kulkarni et al. [22], performed the numerical prediction on the elastic behavior of reinforced polymers. The numerical results of Nano-reinforced laminated composite were validated with the experimental results and found to be correlated. Zeng et al. [23], presented a review that summarizes the latest advances in the fundamental understanding of polymer-based nanocomposites reinforced with Nanofillers, which actuate further research in this area. Their review paper recommended computational approaches that have been applied to assist in the study and development of polymer-based nanocomposites. This includes molecular scale, microscale to mesoscale and macroscale. They further discussed the detailed applications of the mentioned methods in different aspects of polymer-based nanocomposites. They also discussed the importance of multiscale simulation strategies in the predictive capabilities and understanding of polymer-based nanocomposites, in which few studies have been reported. The present study focuses on predicting the tensile properties of HDPE/SWCNT nanocomposites at different weight fractions of SWCNTs nanoparticles through the numerical (MD) model and the theoretical (FEM) model. The prediction models are developed to reduce the time and costs required to execute experimental analysis of the polymer-based nanocomposites’ tensile properties at various nanofillers weight fractions. The numerical and theoretical results are authenticated with the experimental results regarding elongation. This is done to determine which model is suitable for the prediction of the tensile properties of the HDPE/SWCNTs nanocomposites. The paper outlines the theoretical FEM model approach in section II A, numerical MD approach in section II B, the experimental approach in section II C, the results and discussions in section III, the comparison of the results in section IV, and the conclusion in section V.

II. METHODOLOGY

A. Theoretical FEM Approach

This section demonstrates the model of a Representative Volume Element (RVE) adopted from the test segment of a reinforced tensile test sample. The test region of the represented tensile test sample in Figure 1, was assumed to contain the randomly distributed SWCNTs nanofillers through the HDPE matrix. The selected RVE at that region plays a major role in demonstrating the physics and the mechanics of random heterogeneous materials in computing and understanding their effective properties [24]. The RVE of HDPE/SWCNT nanocomposites is used to determine the tensile properties of the presented specimen through analytical modelling utilizing the Finite Element Method (FEM).

FEM is a techniques applied to solve physics, mathematical and engineering problems such as structural analysis, fluid flow or heat transfer, and others through analytical and numerical approaches [25, 26]. However, in this study, structural analysis of the HDPE/SWCNT nanocomposites, RVE, is determined using an analytical FEM approach. The assumptions made for the FEM model of the RVE are that the forces applied to the tensile test samples in Figure 1 are the same as those applied to the RVE. Figure 2 shows the RVE with the forces applied to it. The RVE in Figure 2 is assumed to contain the HDPE matrix, SWCNT nanoparticle, and the intermediate phase with the properties presented in Table 1.
The dimensions and properties of the RVE in Table 1 were used according to the methods used in Fattahi et al., [27] and Tebeta et al., [28] to determine the x parameter of the RVE as presented in Figure 3. The x parameter was calculated based on the weight fractions of SWCNT nanoparticles. The obtained values of the x parameter and the dimensions of each RVE at a given weight fraction of SWCNTs nanoparticles are summarized in Table 2.

![Image of RVE dimensions and the x parameter](image)

**Fig. 3. RVE dimensions and the x parameter**

<table>
<thead>
<tr>
<th>SWCNTs weight fractions [wt%]</th>
<th>Parameter x [nm]</th>
<th>RVE Width [nm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11636.73</td>
<td>23444.26</td>
</tr>
<tr>
<td>2</td>
<td>7854.19</td>
<td>15739.18</td>
</tr>
<tr>
<td>3</td>
<td>6181.17</td>
<td>12393.14</td>
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<tr>
<td>4</td>
<td>5190.48</td>
<td>10411.76</td>
</tr>
<tr>
<td>5</td>
<td>4518.80</td>
<td>9068.40</td>
</tr>
</tbody>
</table>

**TABLE II. CALCULATED X PARAMETERS OF THE RVE.**

The FEM was used to predict the strain of the RVE according to the applied loads and the boundary conditions. This was achieved using the obtained dimensions and the properties of RVE for each weight fraction of SWCNT in Tables 1 and 2. The RVE strain was determined in terms of the displacements occurring during the tensile load application on the presented geometry of the RVE. The Finite Element Analysis (FEA) approach of [29] was applied to determine the unknown values of the change in the height of the RVE. For the application of FEA, the RVE was divided into units called elements which are connected by the nodes. Figure 4 shows the elemental and nodal representation of the RVE of zero-weight fractions of SWCNT.

The elemental and nodal representation of RVE together with the concept of the 1-dimensional (1D) spring were used to generate the general solution of the displacement of the RVE according to Eq. (1).

$$ F = k \Delta u $$  \hspace{1cm} (1)

Where $F$ is the applied force, $\Delta u$ is the displacement, and $k$ is the spring stiffness. Eq. (1) was converted into vector forms according to Eq. (2) for better determination of the RVE displacement and the resulting force.

$$ \{ F \} = [K] \{ u \} $$  \hspace{1cm} (2)

Where, $\{ F \}$ is a vector of applied forces at the nodes, $[K]$ is the stiffness matrix, and $\{ u \}$ is the vector of the unknown displacements at the nodes. Eq. (2) was applied in the determination of the maximum displacement of the RVE according to Figure 4.

![Image of RVE and nodes](image)

**Fig. 4. (a) RVE of pure HDPE, (b) 1-dimensional elemental and nodal representation of pure HDPE RVE**

**TABLE III. INITIAL AND FINAL NODES OF ELEMENT 1 FOR PURE HDPE RVE.**

<table>
<thead>
<tr>
<th>Element</th>
<th>i-node</th>
<th>j-node</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

For the determination of the stiffness matrix of element (1) in Figure 4 (b) for pure HDPE RVE, the stiffness matrix in Eq. (2) was resolved according to Eq. (3) as:

$$ [K] = \frac{A_{HD}}{B_H} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} $$  \hspace{1cm} (3)

Where $A_{HD}$ is the cross-sectional area of the matrix/HDPE RVE, $E_{HD}$ is the elastic modulus of HDPE, and $B_H$ is the height of the HDPE RVE presented in Figure 3.

Since the cross-sectional area of the RVE varies with parameter $x$, then the RVE diameter of 1 wt% in Table 3 was used to determine the cross-sectional area of pure HDPE RVE as $A_{HD} = 1.359 \times 10^{-4} \text{mm}^2$. The height used for pure HDPE was $B_H = 2 \times 10^7 \text{nm}$.

By letting $\frac{A_{HD}}{B_H} = C$ from Eq. (3), we then have the stiffness matrix of element 1 in Figure 4 (b) reduced to:

$$ [K] = \begin{bmatrix} C_{11} & -C_{12} \\ -C_{12} & C_{22} \end{bmatrix} $$  \hspace{1cm} (4)

Note that $C_{11} = C_{12} = C_{21} = C_{22} = C$  \hspace{1cm} (5)
Where $C$ is the term of each element. Eq. (4) present the stiffness matrix in terms of $C$.

For the global force vector, the nodal force is:

$$\{F\}^T = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix}$$

(6)

Where $F$ is the applied force at node 2. The global displacement of the RVE at nodes 1 and 2 is represented by Eq. (7) as:

$$\{U\}^T = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

(7)

Where $U$ is the deflection per node.

The final system equation for pure HDPE RVE is presented by substituting Eq. (4), the transpose of Eq. (6) and Eq. (7) into Eq. (2), which results in Eq. (8) as:

$$\{F\} = \begin{bmatrix} \begin{bmatrix} C_{11} & -C_{12} \\ -C_{12} & C_{12} \end{bmatrix} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

(8)

For the boundary constraints/conditions applied to pure HDPE RVE in Figure 4, stating that the RVE is fixed at node point 1, therefore, $u_1 = 0$, reaction force should exist at point node 1 which is represented as $R_1$. Then by substituting the boundary conditions into Eq. (8), the general system is presented according to Eq. (9):

$$\begin{bmatrix} R_1 \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} C_{11} & -C_{12} \\ -C_{12} & C_{12} \end{bmatrix} \end{bmatrix} \begin{bmatrix} 0 \\ u_2 \end{bmatrix}$$

(9)

The general system solution of Eq. (9) yields the displacement of the pure HDPE RVE at node point 2 which is the maximum displacement and the reaction force at node point 1 according to Eqs. (10) and (11), respectively.

$$u_2 = \frac{F}{C_{12}}$$

(10)

$$R_1 = (-C_{12}) \frac{F}{C_{12}} = -F$$

(11)

Eq. (10) and the boundary condition are used to calculate the strain on the pure HDPE RVE according to Eq. (12).

$$\varepsilon = \frac{(-u_2 + u_2)}{L_{SWCNT}}$$

(12)

The same approach used to determine the strain of pure HDPE RVE is applied to determine the strain of the reinforced RVE at given weight fractions. However, the procedure is slightly different and presented according to Figure 5.

Figure (a) represents the applied forces and the possible displacement that may result in the HDPE/SWCNTs nanocomposites RVE. Figure 5 (b) presents the nodes and elements generated from Figure 5 (a). It shows that the RVE of reinforced HDPE has 2 nodes and 3 elements. According to the assumptions made in Figure 5 (b), element (1) is the HDPE matrix, element (2) is the intermediate phase, and element (3) is the SWCNT fibre. Elements (1), (2), and (3) are situated between nodes 1 and 2. Force $F$ is applied to node 2 and the result is along with node 1. The element’s initial and final nodes of Figure 5 (b) are summarized in Table 4.

Since HDPE/SWCNT nanocomposites RVE in Figure 5 are presented by three elements and two nodes, as shown in Table 4, then the resulting system equation will contain stiffness matrices which are: $[K^{(1)}]$, $[K^{(2)}]$, and $[K^{(3)}]$ for each element.

Element (1) represents the HDPE matrix of the RVE, which is characterized by the stiffness matrix $[K^{(1)}]$, and it is presented by Eq. (13) as:

$$[K^{(1)}] = \begin{bmatrix} \frac{E_{SWCNT}A_{SWCNT}}{L_{SWCNT}} & 1 \\ 1 & -1 \end{bmatrix}$$

(13)

Where $A_{SWCNT}$ is the cross-sectional area of the HDPE matrix in the reinforced RVE at element (1) depending on the calculated $x$ parameter in terms of the given weight fraction, $E_{SWCNT}$ is the elastic modulus of HDPE and $h_{SWCNT}$ is the height of the HDPE/SWCNTs nanocomposites RVE.

By letting $\frac{E_{SWCNT}A_{SWCNT}}{L_{SWCNT}} = C^{(1)}$, form Eq. (13), then the stiffness matrix of element (1) can be decreased to Eq. (14).

$$[K^{(1)}] = \begin{bmatrix} C^{(1)}_{11} & -C^{(1)}_{12} \\ -C^{(1)}_{12} & C^{(1)}_{22} \end{bmatrix}$$

(14)

Where $C^{(1)}_{11} = C^{(1)}_{13} = C^{(1)}_{13} = C^{(1)}_{22} = C^{(1)}_{33}$ (15)

The stiffness matrix for element (2), which represents the intermediate phase, is demonstrated by Eq. (16).

$$[K^{(2)}] = \begin{bmatrix} \frac{E_{inter}A_{inter}}{L_{inter}} & 1 \\ 1 & -1 \end{bmatrix}$$

(16)

Where $A_{inter}$ is the cross-sectional area of the intermediate phase in HDPE/SWCNTs nanocomposites RVE, $E_{inter}$ is the elastic modulus of the intermediate phase, and $h_{inter}$ is the height of the intermediate phase.
By letting \( \mathbf{C}^{(2)} \mathbf{e}^{(2)} = \mathbf{C}^{(2)} \) from Eq. (16). Then the stiffness matrix of element (2) is presented through Eq. (17) as:

\[
\begin{bmatrix}
C_{11}^{(2)} & -C_{12}^{(2)} \\
-C_{12}^{(2)} & C_{22}^{(2)}
\end{bmatrix}
\]  
(17)

Where \( C_{11}^{(2)} = C_{11}^{(2)} = C_{12}^{(2)} = C_{22}^{(2)} \) (18)

The stiffness matrix for an element number (3) is determined by Eq. (19).

\[
\begin{bmatrix}
\mathbf{K}^{(3)}
\end{bmatrix} = \frac{\mathbf{A}_f^{(3)}}{H_f} \begin{bmatrix}
1 & -1 \\
-1 & 1
\end{bmatrix}
\]  
(19)

Where \( \mathbf{A}_f^{(3)} \) is the cross-sectional area fibre (SWCNT) in HDPE/SWCNTs nanocomposites RVE, \( E_f^{(3)} \) is the elastic modulus of MWCNT, and \( H_f \) is the height of SWCNT.

By letting \( \mathbf{f}_r^{(3)} \mathbf{d}^{(3)} = \mathbf{C}^{(3)} \) form Eq. (19). Then the stiffness matrix for element (3) can be reduced to Eq. (20).

\[
\begin{bmatrix}
\mathbf{K}^{(3)}
\end{bmatrix} = \begin{bmatrix}
C_{11}^{(3)} & -C_{12}^{(3)} \\
-C_{12}^{(3)} & C_{22}^{(3)}
\end{bmatrix}
\]  
(20)

Where \( C_{11}^{(3)} = C_{11}^{(3)} = C_{12}^{(3)} = C_{22}^{(3)} \) (21)

Figure 5 shows that the HDPE matrix, intermediate phase, and SWCNT have the same height \( H_{RVE} = H_{IC} = H_{t} = H_{f} \).

To solve the general system equation of the reinforced RVE, first, we look at the elements that have common nodes. Table 5 shows that elements (1), (2), and (3) have the same i-nodes and j-nodes which are node 1 and node 2. To generate the general solution, we add the stiffness matrix for elements (1), (2), and (3) since they have common nodes.

The stiffness matrix for elements with the same notes is calculated as:

\[
\sum \mathbf{K}^{(1,2,3)} = \mathbf{K}^{(1)} + \mathbf{K}^{(2)} + \mathbf{K}^{(3)}
\]  
(22)

\[
\sum \mathbf{K}^{(1,2,3)} = \begin{bmatrix}
C_{11}^{(1)} & -C_{12}^{(1)} \\
-C_{12}^{(1)} & C_{22}^{(1)}
\end{bmatrix} + \begin{bmatrix}
C_{11}^{(2)} & -C_{12}^{(2)} \\
-C_{12}^{(2)} & C_{22}^{(2)}
\end{bmatrix} + \begin{bmatrix}
C_{11}^{(3)} & -C_{12}^{(3)} \\
-C_{12}^{(3)} & C_{22}^{(3)}
\end{bmatrix}
\]  
(23)

Where,

\[
\sum C_{11}^{(1,2,3)} = C_{11}^{(1)} + C_{11}^{(2)} + C_{11}^{(3)}
\]  
(24)

\[
-\sum C_{12}^{(1,2,3)} = -C_{12}^{(1)} - C_{12}^{(2)} - C_{12}^{(3)}
\]  
(25)

\[
-\sum C_{22}^{(1,2,3)} = -C_{22}^{(1)} - C_{22}^{(2)} - C_{22}^{(3)}
\]  
(26)

\[
\sum C_{22}^{(1,2,3)} = C_{22}^{(1)} + C_{22}^{(2)} + C_{22}^{(3)}
\]  
(27)

We then have

\[
\sum C_{ij}^{(1,2,3)} = \sum C_{ij}^{(1,2,3)} = \sum C_{ij}^{(1,2,3)} = \sum C_{ij}^{(1,2,3)}
\]  
(28)

The resulting sum of the stiffness matrix of elements (1), (2), and (3) is presented in Eq. (29).

\[
\sum \mathbf{K}^{(1,2,3)} = \begin{bmatrix}
\sum C_{11}^{(1,2,3)} & -\sum C_{12}^{(1,2,3)} \\
-\sum C_{12}^{(1,2,3)} & \sum C_{22}^{(1,2,3)}
\end{bmatrix}
\]  
(29)

Therefore, the stiffness matrix \( \mathbf{K} \) in Eq. (29) is substituted in Eq. (2) together with the boundary conditions of reinforced HDPE RVE stating that, \( \mathbf{u}_1 = \mathbf{0} \), and the reaction force should exist at point node 1, which is represented as \( R_1 \). Then the general equation of HDPE/MWCNTs nanocomposites at various weight fractions of SWCNTs nanoparticles can be represented by Eq. (30).

\[
\left\{ \begin{bmatrix}
R_1 \\
F
\end{bmatrix} \right\} = \begin{bmatrix}
\sum C_{11}^{(1,2,3)} & -\sum C_{12}^{(1,2,3)} \\
-\sum C_{12}^{(1,2,3)} & \sum C_{22}^{(1,2,3)}
\end{bmatrix} \left\{ \begin{bmatrix}
\mathbf{u}_1 \\
\mathbf{u}_0
\end{bmatrix} \right\}
\]  
(30)

The maximum displacement of the reinforced HDPE RVE and the resulting force is determined using Eq. (31) and (32), respectively.

\[
\mathbf{u}_1 = \frac{F}{\sum C_{11}^{(1,2,3)}}
\]  
(31)

\[
R_1 = \left( -\sum C_{11}^{(1,2,3)} \right) \frac{F}{\sum C_{11}^{(1,2,3)}} = -F
\]  
(32)

Therefore, Eq. (31) is used to calculate the strain of the reinforced HDPE RVE according to Eq. (33).

\[
\varepsilon = \frac{\mathbf{u}_1 + \mathbf{u}_0}{H_{RVE}}
\]  
(33)

From the derived general solutions, the maximum displacements and strains of HDPE/SWCNTs nanocomposites were determined for each given weight fraction of SWCNTs nanoparticles, and their results are presented in Table 5.

B. Numerical (MD) Approach

Molecular Dynamics (DM) in this study is introduced through LAMMPS (Large scale Atomic/Molecular Massively Parallel Simulator) [30]. Atomic-scale modelling of an HDPE/SWCNTs nanocomposites system is somehow challenging due to many atoms involved at various scales [31]. However, the present MD simulation study is focusing on composite systems with a considerable SWCNT volume fraction. To cut down the total size of the model, the simulation is performed for HDPE/SWCNTs nanocube with 35.5x35.5x27 Å as a RVE. The SWCNT was arranged in the centre of a periodic simulation cell. Figures 6 and 7 show the modelled SWCNT.
Then HDPE molecules with various numbers of repeat units were then located haphazardly around the tube in non-overlapping positions. Figures 8 to Figure 10 show the representative HDPE/SWCNT nanocube simulated model.

To control the temperature, MD simulations were reorganized in terms of constant number of particles, volume, and temperature using a Nose-Hoover thermostat. The amount of time step was chosen as 0.001 ps. Firstly, simulations were performed to predict the equilibrium configuration of a three-dimensional HDPE/SWCNT nanocube at the temperature of 300 K.

One of the significant factors affecting the correctness of a MD simulation is the excellence of the potential function that is used to illustrate the interaction of particles in the system [32]. An HDPE/SWCNT nanocomposite has three distinguished components: HDPE matrix, SWCNT nanoparticles and interface. The REBO potential function is used in this study. REBO potential is so efficient for the simulation of materials with stronger intermolecular forces such as HDPE. This is due to its ability to reproduce most of its characteristics [33]. The non-bonded van der Waals interaction between the SWCNT and the HDPE, and within the HDPE itself is modelled with the 12-6 Lennard-Jones potential [34] given as:

$$E = 4\alpha \left( \frac{\xi}{r} \right)^{12} - \left( \frac{\xi}{r} \right)^6$$

(34)

where $E_{int}$ is the potential energy between a pair of atoms, $r$ is the distance between the pair of atoms, $\alpha$ is the potential well depth, and $\xi$ is the van der Waals separation distance.
The summary of the potential parameters of Lennard-Jones is shown in Table 5 [35].

**TABLE V. POTENTIAL PARAMETERS OF THE LENNARD-JONES**

<table>
<thead>
<tr>
<th>Element</th>
<th>( u ) (keal/mol)</th>
<th>( C_{ij} )</th>
<th>( B_{ij} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>C (sp2)</td>
<td>0.0859</td>
<td>0.046</td>
<td>0.0301</td>
</tr>
<tr>
<td></td>
<td>3.3997</td>
<td>2.958</td>
<td>2.42</td>
</tr>
<tr>
<td>q (e)</td>
<td>0</td>
<td>-0.115</td>
<td>0.115</td>
</tr>
</tbody>
</table>

These are some of the most prosperous experimental potentials which are preferable for systems consisting of many atoms. Other details of the present simulation are as follows: the axial elongation is applied along the axis of the cube; the rate of applied axial load is equal to 0.01 \( \text{A} / \mu \text{s} \); the entire energy of the system is minimized; the atoms at two ends of the cube are fixed to simulate clamped edge supports and the cut-off radius is 0.8 nm. The system temperature is checked by rescaling the atom velocities [37]. Figure 11 shows the direction of the applied axial load.

**Fig. 11.** Applied axial load in the direction of Z axes

**C. Experimental Approach**

The MD model and the theoretical FEM results were validated with the experimental tensile test results. For the conduction of the tensile test results, the HDPE/SWCNTs nanocomposites specimen were produced at various weight fractions of SWCNTs as follows:

HDPE was provided as white pellets and SWCNTs as back powder. The HDPE pellets were molten and mixed with SWCNTs at various weight fractions using twin screw extruder operations at the temperature of 170 – 190 °C, screw rotating speed of 250 RPM and a pressure of 120 MPa. To ensure consistency in the weight fractions of SWCNTs, the weighing method applied by [28] was used. 400 g of HDPE was measured and processed through the extruder, and the resulting strip was then ground into small pellets that were fed to the injection moulder to produce 0 wt% HDPE tensile samples. For 0.2 wt% HDPE/SWCNTs nanocomposite tensile test samples, 0.2 % of 400 g, which is 0.8 g of SWCNTs nanoparticles, was mixed with 399.2 g of HDPE to produce 0.2 wt% HDPE/SWCNTs nanocomposites. The same procedure was repeated for 0.4 wt%, 0.6 wt%, and 0.8 wt%. All the resulting HDPE/SWCNTs nanocomposites were processed at the injection pressure of 9 MPa, and the temperature of 175 – 200 °C to produce the tensile test samples according to the ASTM D638-14. The produced HDPE/SWCNTs nanocomposites tensile tests were tested according to the ASTM D638-14 and ISO 527-1. The obtained tensile test results of presents in Table 6.

**TABLE VI. EXPERIMENTAL TENSILE TEST RESULTS**

<table>
<thead>
<tr>
<th>Sample number</th>
<th>SWCNTs weight fractions [wt%]</th>
<th>Elastic modulus [MPa]</th>
<th>Average elastic modulus [MPa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test 1</td>
<td>Test 2</td>
<td>Test 3</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>340.3</td>
<td>271.11</td>
</tr>
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<td>6</td>
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</table>

### III. RESULTS AND DISCUSSION

The analytical FEM was performed using the Representative Volume Element (RVE) approach according to section II A. The strain results were obtained from the derived general solutions of the maximum displacement of HDPE/SWCNT nanocomposites RVE. The numerical investigation section analysed the HDPE/SWCNTs nanocomposite model through simulation by applying initial conditions, boundary conditions, and appropriate force field. Finally, the results of this test were obtained according to Figure 11 to Figure 15. The results of the two presented models were converted percentage elongation (strain %) so they can be compared to the percentage elongation results of the tensile test. The experimental tensile test results illustrate the relationship between the tensile stress applied to HDPE/SWCNTs nanocomposite polymer samples and the resulting strain at a constant temperature. The percentage elongation of the models and experimental tensile test results at various weight fractions are compared in Figure 16.
IV. COMPARISON OF THE RESULTS

The theoretical FEM, numerical MD, and the tensile test experimental, results are presented in Table 7 and Figure 16. The last two columns of Table 7 demonstrate the percentage deviation between the MD results and FEM results from the experimental results. The MD and experimental results contain the acceptable correlation whereas the FEM results show non acceptable correlation compared to the experimental tensile test results. The relationship between the theoretical FEM model, the MD model and the experimental results are summarized in Figure 16.

<table>
<thead>
<tr>
<th>SWCNT weight fractions [wt%]</th>
<th>Experimental Results</th>
<th>Molecular Dynamics Result</th>
<th>Analytical FEM Results</th>
<th>Error Between the Experiments and MD results [%]</th>
<th>Error Between the Experiments and FEM [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>11.36</td>
<td>7.41</td>
<td>16.50</td>
<td>58.31</td>
<td>45.25</td>
</tr>
<tr>
<td>1</td>
<td>10.88</td>
<td>6.29</td>
<td>15.05</td>
<td>72.97</td>
<td>38.33</td>
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<tr>
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<td>11.07</td>
<td>6.91</td>
<td>16.30</td>
<td>60.20</td>
<td>47.24</td>
</tr>
<tr>
<td>3</td>
<td>10.31</td>
<td>6.71</td>
<td>10.90</td>
<td>53.65</td>
<td>5.72</td>
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<td>4</td>
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<td>5.80</td>
<td>9.15</td>
<td>60.17</td>
<td>-1.51</td>
</tr>
<tr>
<td>5</td>
<td>9.04</td>
<td>5.76</td>
<td>9.10</td>
<td>56.94</td>
<td>0.66</td>
</tr>
</tbody>
</table>
Reinforced Polymers.

As shown in Figure 16, the addition of Single-Walled Carbon Nanotubes (SWCNTs) into the High-Density Polyethylene (HDPE) matrix, reduced the percentage elongation of HDPE/SWCNTs nanocomposites in both experimental results. This observation achieved:

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K. Yoshino, H. Kajii, H. Araki, T. Sonoda, H. Take and S. Lee, "Electrical and optical properties of conducting polymer-fullerene and


