MECHANICAL AND STRUCTURAL PROPERTIES OF CARBON NANOTUBES: A MOLECULAR DYNAMIC STUDY

N.H.J. Al Hasan

University of Basrah, College of Engineering, Department of Engineering Materials, Basrah, Iraq
nuha.jasim@uobasrah.edu.iq

Abstract- Carbon nanotubes (CNTs) have a wide variety of applications in many industries. It exists in different structures; among them are single-walled carbon nanotubes classified into the armchair, zigzag, and chiral. In this study, the mechanical properties of these structures are calculated according to Reuss-Voigt-Hill estimation by using Materials Studio. It is used in simulations to detect and discuss the properties of single-walled carbon nanotubes (SWNTs); zigzag (6,0), armchair (6,6), and chiral (6,4) in different tube diameters and five repeat units. The COMPASS force field describes the interatomic interactions of materials studio. The results show that chiral with (6,4) has the lowest mechanical properties among zigzag (6,0) and armchair (6,6).

Keywords: Materials Studio, Single Walled Carbon Nanotubes, Molecular Dynamics, Chiral, Zigzag, Armchair.

1. INTRODUCTION

A Molecular dynamic (MD) simulation is used in many studies to predict different prosperities such as surface tension [1] and dynamical structure factor [2] and compute many parameters as related to molecules under certain conditions; it is also investigated in order and disorder crystalline using nonequilibrium MD simulations suited to the study with the picture in a two-layered projection of a three-layered object [3]. Carbon nanotubes (CNTs) are used in a wide range of applications in drugs, proteins, and nucleic acids to result from functionalities with different biological molecules, which have many advantages for carbon nanotubes in biomedicine. Carbon nanotubes (CNTs) are used in a wide range of applications in drugs, proteins, and nucleic acids to result from functionalities with different biological molecules, which have many advantages for carbon nanotubes in biomedicine.

Carbon nanotubes (CNTs) exhibit exciting chemical and physical properties derived from rolled graphene planes [4, 5]. In 1993, Iijima initially observed only multi-wall carbon nanotubes with layers of 2 and 20. In subsequent research, he confirmed the presence of single-walled carbon nanotubes SWNTs and illustrated their structure [5].

Figure 1 is being drawn in the Material Studio. To describe such a principle of the nanotube characteristic, C_h and T are vectors; which rectangle defines the unit cell. The C_h is circumference vector on the tube surface which connects two carbon atoms equivalent [4], $C_h = n\hat{a}_1 + m\hat{a}_2$, where, $\hat{a}_1$ and $\hat{a}_2$ are two basis graphite vectors, n and m are indexes, which is determined the chiral angle θ [4]:

$$\theta = \tan^{-1}[\sqrt{3}(n/(2m+n))] \qquad (1)$$

Carbon nanotubes are classified according to electronic characterization into three differentiated classes: armchair (when, $n = m$, and $\theta = 30°$), zigzag (when, $m = 0$, $n > 0$, and $\theta = 0°$), and chiral (when, $0 < |m| < n$, and $\theta = 30°$), as shown in Figure 1, the diameter of a nanotube can be expressed as [4]:

$$d_t = \sqrt{3}[a_{c-c}\left(m^2 + mn + n^2\right)^{1/2}/\pi] = C_h/\pi \qquad (2)$$

The computation of the density of an individual SWNT can be determined when is rolled sheet honeycomb of diameter D_{SWNT}, and length L. The density of F_{SWNT} is [4]:

$$\rho_{SWNT} = \frac{m}{V} = \frac{N_c m_c}{L\pi \frac{D_{SWNT}^2}{4}} = \frac{\frac{\pi D_{SWNT} L}{D_2} \frac{D_2}{D_2}}{L\pi \frac{D_{SWNT}^2}{4}} Zu = \frac{4Zu}{D_{SWNT} D_2^2} \qquad (3)$$

where, $D_2 = 2.83$ Å; longest distance between carbon atoms in a single hexagonal lattice.

m: mass
V: volume
N_C: the number of carbon atoms
m_C: the mass of the carbon atoms
Z: atomic mass
$u = (1.6605 \times 10^{-27}$ kg) atomic mass unit, SWNT bundle density can be calculated as the size of the simulation cell, which was adjusted as shown in Table 1, such that the SWNTs density was 1.40 g/cm³.

Where the size of a unit cell changes as the number of repeat units increases, as shown in Table 1, the unit cell's size is equal in an armchair and zigzag nanotube; in the chiral nanotubes, the unit cell size differs by 0.1.
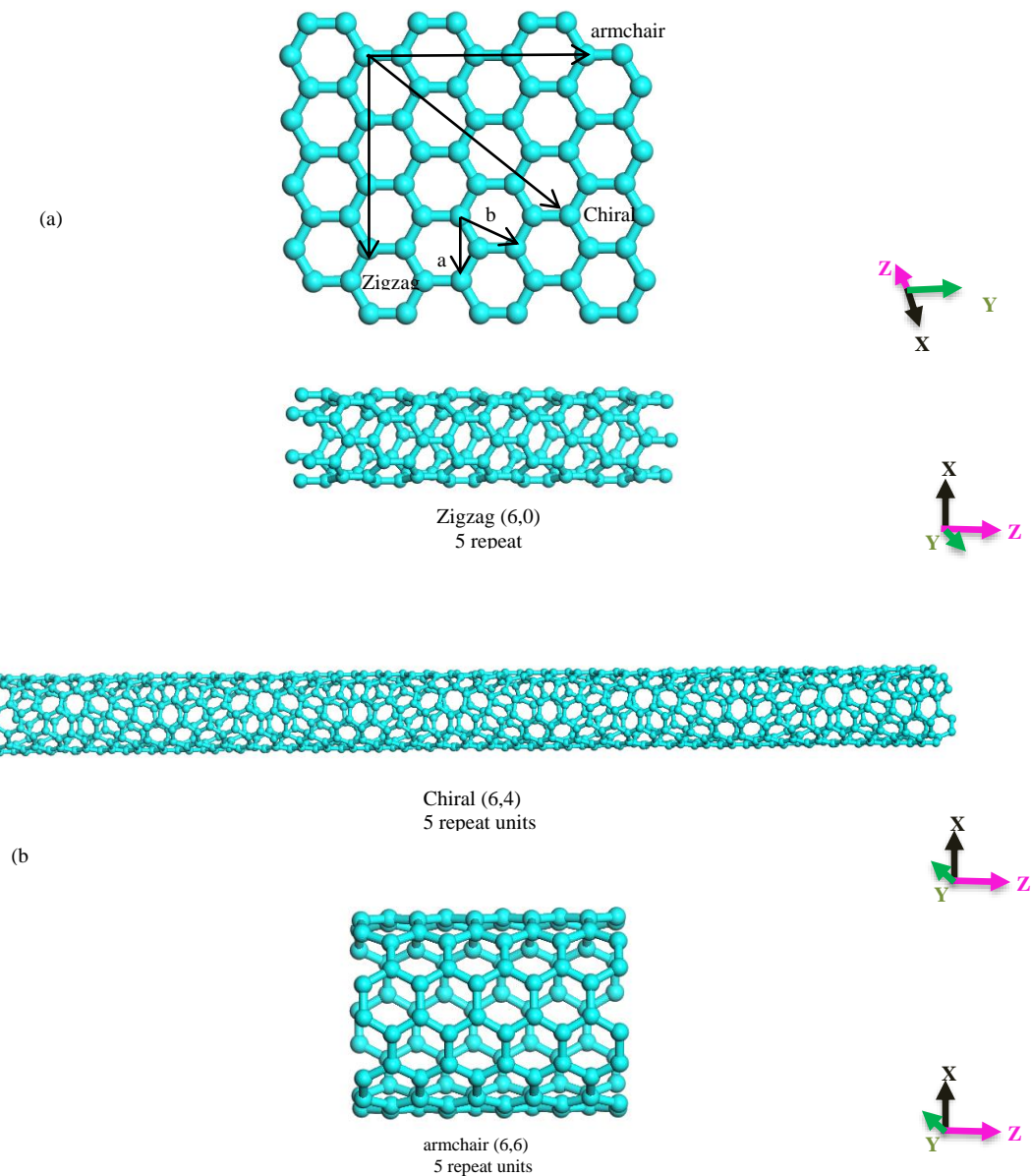
Figure 1. (a) roll-up vector of graphene lattice of a and b base vectors, (b) Sample a zigzag (6,0), chiral (6,4), and armchair (6,6) for 5 repeat units of each

Table 1. units cell size at 1.4 g/cm^3 density (units cell size used in this study)

repeat unit	unit cell size		
	zigzag (6,0)	chiral (6,4)	armchair (6,6)
1	7×7×7	12.9×12.9×12.9	7×7×7
2	8.8×8.8×8.8	16.3×16.3×16.3	8.8×8.8×8.8
3	10.1×10.1×10.1	18.7×18.7×18.7	10.1×10.1×10.1
4	11.1×11.1×11.1	20.5×20.5×20.5	11.1×11.1×11.1
5	12×12×12	22.1×22.1×22.1	12×12×12

X. Lei, et al., [6] developed a model to characterize the Poisson's ratio and Young's modulus of an armchair and zigzag SWCNTs; the outcomes reasoned that way to deal with research SWCNTs mechanical properties is a valid method and concise. It is considered destined to be a valuable strategy to advance on examination of this kind.

J. Ceponkus, et al., [7] studied functionalized nanotubes of single-walled carbon nanotubes by Fourier transform infrared (FTIR) at low temperatures. spectroscopic was viewed as delicate enough for the checking of nanotube functionalization and ID of the specific practical gatherings connected to the nanotubes.

S. Sharma, et al., [8] evaluated the elastic properties of single-wall carbon nanotubes by molecular dynamics simulation for armchair, zigzag, and chiral nanotubes. The analytical results concluded that Young's moduli of single-wall carbon nanotubes decrease as radius increases and increase as the volume fractions of carbon nanotubes and aspect ratios /diameter.

I.D. Muhammad, et al., [9] used the approach of finite element method for modeling young's modulus of single-walled zirconia nanotube which it is consider as beam elements, the simulated done by axial tensile strain apply on nanotube end, then computed the Young's modulus.

B.D. Jensen, et al., [10] used molecular dynamics for modeling arrangements of the single wall nanotube array, which is idealized by elastic deformations, yield, and fracture modeling.

There are many techniques for modeling molecular dynamics, examples of atomistic modeling techniques are molecular dynamics by using atomistic modeling for obtaining Young's modulus of CNTs, but it is limited time and length and needed high power; the methods of continuum modeling overcome these finite element methods is common approach utilizing continuum structures and coupled with the molecular mechanics, within the system of carbon nanotubes, the modeling of nanoscale continuum elements replaces the carbon to carbon bond [11].

2. SIMULATION

The steps of the molecular dynamics model and simulation process are as follows:

I. To construct the model of SWNTs from the menu bar, select File |built| built nanostructure |single-wall nanotube|. Set the all required then, click Build from the menu bar, and the SWNT model is achieved.

II. In the molecular dynamics simulation, the structure is optimized to avoid erroneous results in the subsequent simulation. So, geometry optimization is important; Select modules |for cite| calculation, then optimization geometry is selected to advance the underlying cell model and guarantee the steady low energy structure cell. The best savvy estimate for the reenactment and the time reproduction changed following the size of the design. The results involve the files of the cell size diagram, convergence, energy, and density curve.

III. The molecular dynamics simulation is necessary to obtain the actual density of materials; under the effect of external pressure, the cell density progressively increases external pressure. Then, the system can be increased the pressure via NPT simulation. The NPT option is selected from modules |for cite| calculation from more tab.

IV. The mechanical properties calculation by select for cite from model calculation to open the dialog, the relevant information of the initial parameters, the stiffness matrix, bulk, and shear modulus determined by Reuss Voigt and Hill formulas.

3. RESULT AND DISCUSION AND DISCUSION

In this work, simulations of molecular mechanics have been performed by using the commercial software 7.0 materials studio to study the properties of zigzag (6,0), chiral (6,4), and armchair (6,6) SWNTs with different repeat units so that different lengths result. The COMPASS force field performs the interatomic simulations. (Atomistic simulation studies mean condensed phased optimized molecular potential) [13, 14].

The simulations were at a temperature of 298 K. The thermal effect is considered under the conditions shown in Figure 2; it is the result of this study using Material Studio simulations. The force field model is an empirical model that can predict the mechanical properties of the covalent bond in a CNT [12].

The initial unit cell of (12×12×12) was prepared for each zigzag (6,0), chiral (6,4), and armchair (6,6) to satisfy the magnitude of density equal to 1.4 g/cm3 by NPT simulation at 1 atm with an integration step of 1 fs at 298 K room temperature.

It is noticed that the diameter and length change as the variations in the structure of SWCNTs and the number of unit cells shown in Table 2 and Figure 2. The length was increased as the number of unit cells increased. can show that the chiral size increased more than that in the armchair and zigzag, where the armchair length is the lowest.
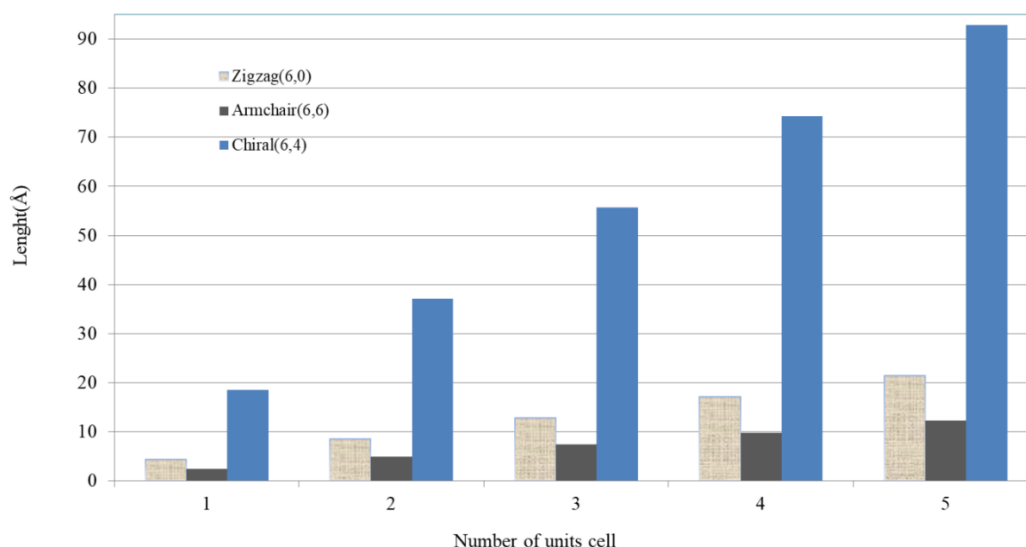
Figure 2. length of three different type of SWCNs structure with variation repeat units

Table 2. Variation of diameter of three different type of SWCNs structure

SWCNs structure	zigzag (6,0)	chiral (6,4)	armchair (6,6)
Diameter (Å)	4.7	6.83	8.41

The diameter of (6,0) SWNT is 4.7 Å with lengths of $L = 4.26, 8.52, 12.78, 17.04$, and 21.3. The diameter of (6,4) SWNT is 6.83 Å with lengths of $L = 18.57, 37.14, 55.71, 74.28$, and 92.84 Å.

The diameter of (6,6) SWNT is 8.41 Å with lengths of L = 2.46, 4.92, 7.38, 9.84, and 12.3 Å. After adjusting hydrogen in the structures, the properties were calculated, As in Figure 3 and Figure 4, the amorphous cells are shown in these figures for each system (zigzag, chiral, and armchair), adjusted with five repeat unit cells for the armchair (6,6) architecture, zigzag (6,0), and chiral (6,6).
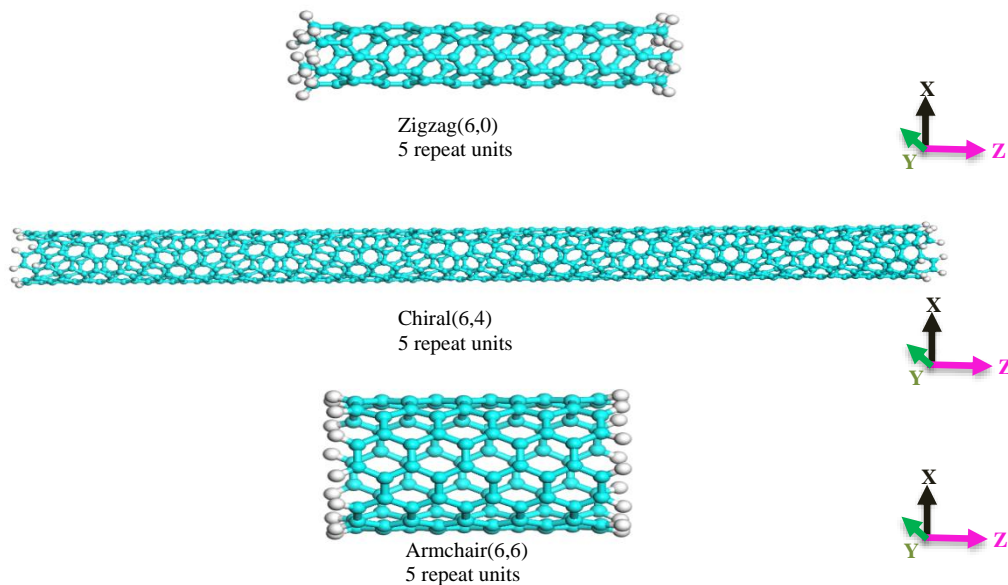

Zigzag(6,0)
5 repeat units

Chiral(6,4)
5 repeat units

Armchair(6,6)
5 repeat units

Figure 3. Hydrogen adjusts and clean structures, 5 repeated units of each structure

Chiral(6,4)
5 repeat units

Zigzag(6,0)
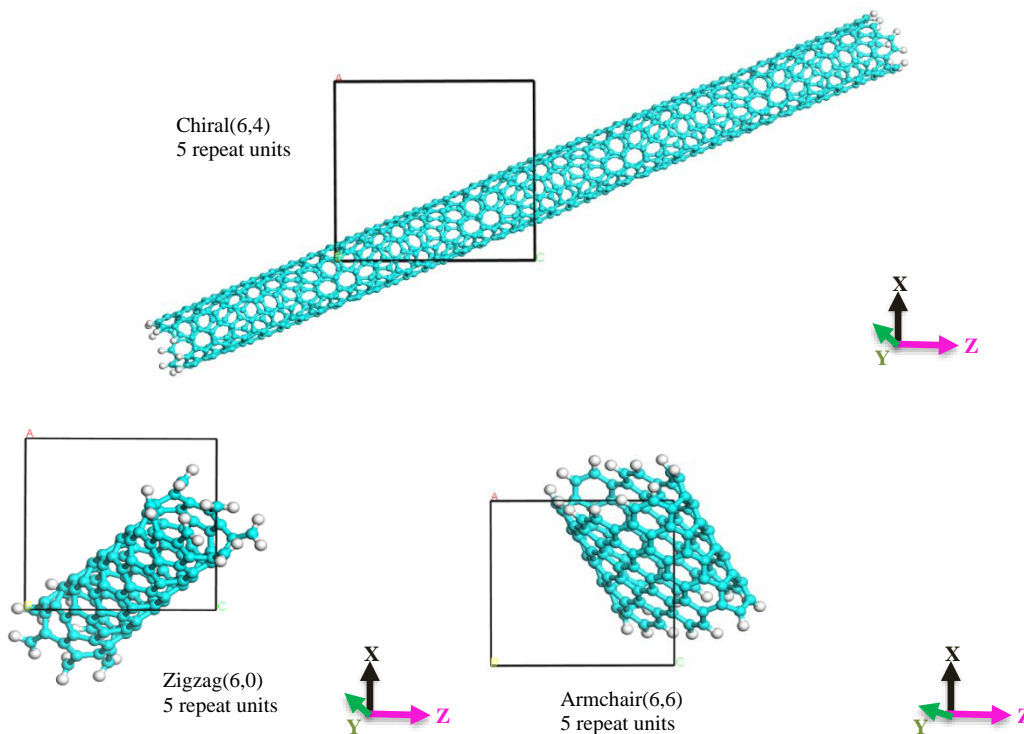5 repeat units

Armchair(6,6)
5 repeat units

Figure 4. The amorphous cell, 5 repeated units of each structure

The system was compressed when the pressure increased. At the same time, the NPT and the density increased, and the compressibility, bulk, and shear modulus of the unit cell of SWNTs can be calculated in a simulation of mechanical properties. First, the simulation results from the molecular dynamics calculations on the three different architectures in Table 2. are shown in Figure 5, where the curves of the cell density change with time. This figure can indicate the excellent density of the armchair (6,6) architecture in comparison to zigzag (6,0) and chiral (6,6).
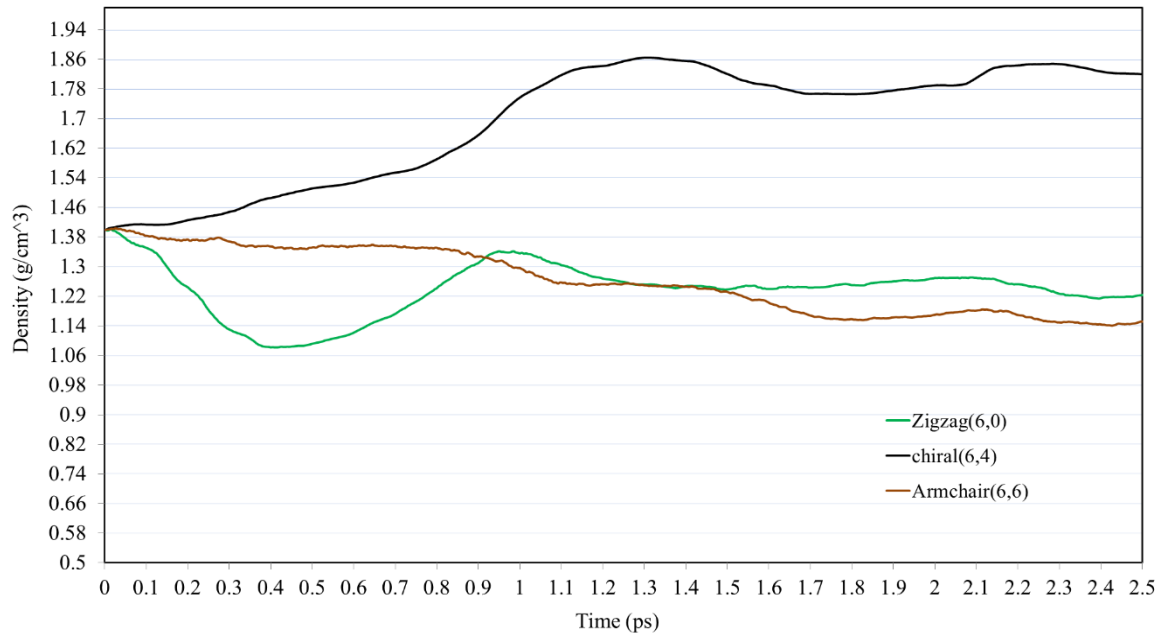
Figure 5. For cite dynamic density

The result of mechanical properties for each structure in 5 repeated units is illustrated in Table 3.

Table 3. Mechanical properties for structure

- Properties for zigzag (6,0), 5 repeat units:			
	Reuss	Voigt	Hill
Bulk modulus (GPa) =	31.0690	1.2329	16.1509
Shear modulus (GPa) =	4.2361	5.4985	4.8673
Compressibility (1/TPa) =	32.1864		
Young Modulus (GPa)	Poisson Ratios		
X = 6.1666	Exy = 0.7340	Exz =	0.3512
Y = 6.3076	Eyx = 0.7507	Eyz =	0.0832
Z = 11.1314	Ezx = 0.6340	Ezy =	0.1469
- Properties for chiral (6,4), 5 repeat units:			
	Reuss	Voigt	Hill
Bulk modulus (GPa) =	0.0000	-3.0460	-1.5230
Shear modulus (GPa) =	0.0000	-0.6332	-0.3166
Compressibility (1/TPa) =	-158.0851		
Young Modulus (GPa)	Poisson Ratios		
X = -7.5798	Exy = 0.0477	Exz =	-0.3329
Y = -24.3507	Eyx = 0.1532	Eyz =	-0.1011
Z = 10.1564	Ezx = 0.4460	Ezy =	0.0422
- Properties for armchair (6,6), 5 repeat units:			
	Reuss	Voigt	Hill
Bulk modulus (GPa) =	16.0116	28.8243	22.4179
Shear modulus (GPa) =	13.5886	24.3276	18.9581
Compressibility (1/TPa) =	62.4549		
Young Modulus (GPa)	Poisson Ratios		
X = 28.3537	Exy = 0.2802	Exz =	0.2928
Y = 19.7092	Eyx = 0.1947	Eyz =	0.3615
Z = 18.6772	Ezx = 0.1928	Ezy =	0.3426

From the results, the mechanical properties of the armchair (6,6) were significantly different compared with the zigzag (6,0) and chiral (6,4).

4. CONCLUSIONS

It essentially employs numerical approaches such as molecular dynamics (MD) to simulate CNTs structures and detect and evaluate mechanical properties via the physical properties of CNTs. By amorphous cell calculations, we can find the change in density as the unit cell parameters change for three different SWCNs, which increases with time for chiral (6,4).

At a density of 1.4g/cm3, the zigzag and armchair have the same unit cell parameter in all repeat units from 1 to 5. The chiral (6,4) has low mechanical properties compared with the zigzag (6,0) and armchair (6,6). The length of chiral (6,4) for five repeat units is more significant than zigzag (6,0) and armchair. For chiral CNTs, the Reuss method using MD simulations shows that the bulk modulus and shear modulus values are 31.0690 GPa and 4.2361 GPa, respectively. It can be higher than a zigzag and an armchair.

NOMENCLATURES

1. Acronyms
SWCNs   Single Walled Carbon Nanotubes
MWCNs   Multiple Walled Carbon Nanotubes
CNTs   Carbon nanotubes

2. Symbols / Parameters
V: volume
N_C: Number of the carbon atoms
m_C: Mass of the carbon atoms
Z: Atomic mass for a carbon atom
θ : Chiral angle

REFERENCES

[1] A. Shahzad, M.G. He, S. Ghani, M. Kashif, T. Munir, F. Yang, "Crystalline Order and Disorder in Dusty Plasmas Investigated by Nonequilibrium Molecular Dynamics Simulations", Chinese Physics B, Vol. 28, No. 5, p. 055201, 2019.
[2] A. Shahzad, M.A. Shakoori, M.G. He, F. Yang, "Dynamical Structure Factor of Complex Plasmas for Varying Wave Vectors", Physics of Plasmas, Vol. 26, No. 2, p. 023704, 2019.

[3] S. Jain, L. Qiao, "Molecular Dynamics Simulations of the Surface Tension of Oxygen-Supersaturated Water", AIP Advances, Vol. 7, No. 4, p. 04500, 2017.

[4] P. Pandey, M. Dahiya, "Carbon Nanotubes: Types, Methods of Preparation and Applications", International Journal of Pharmaceutical Science and Research, Vol. 1, No. 4, pp. 15-21, 2017.

[5] J. Michael, "Carbon Nanotubes Properties and Applications", Taylor and Francis Group, LLC, 2016.

[6] X. Lei, T. Natsuki, J. Shi, Q.Q. Ni, "Analysis of Carbon Nanotubes on the Mechanical Properties at Atomic Scale", Journal of Nanomaterials, p. 1, 2011.

[7] J. Ceponkus, A.P. Smilga, I. Rumskaite, I. Puodziute, V. Sablinskas, "Infrared Absorption Spectroscopy of Functionalized Single-Walled Carbon Nanotubes", Chemija, Vol. 24, No. 1, 2013.

[8] S. Sharma, R. Chandra, P. Kumar, N. Kumar, "Moulecular Dynamics Simulation of Carbon Nanotubes", Nanoscience and Technology: An International Journal, Vol. 24, No. 1, 2013.

[9] I.D. Muhammad, M. Awang, O. Mamat, K.Z.K. Shaari, "Estimating Young's Modulus of Single-Walled Zirconia Nanotubes Using Nonlinear Finite Element Modeling", Journal of Nanomaterials, Vol. 16, No. 1, p. 8, 2015.

[10] B.D. Jensen, K.E. Wise, G.M. Odegard, "Simulation of Mechanical Performance Limits and Failure of Carbon Nanotube Composites", Modelling and Simulation in Materials Science and Engineering, Vol. 24, No. 2, p. 025012, 2016.

[11] L. Perumal, L.T. Leng, C.P. Tso, "Nanoscale Continuum Modelling of Carbon Nanotubes by Polyhedral Finite Elements", Journal of Nanomaterials, 2016.

[12] M.E. Karagoz, I. Celik, "Investigation the Role of Carbon Nanotubes for High Resolution Visual Prostheses", International Journal on Technical and Physical Problems of Engineering (IJTPE), Issue 18, Vol. 6, No. 1, pp. 192-197, March 2014.

[13] R.S. Ruoff, D. Qian, W.K. Liu, "Mechanical Properties of Carbon Nanotubes: Theoretical Predictions and Experimental Measurements", Comptes Rendus Physique Journal, Vol. 4, pp. 993-1008, 2013.

[14] A.S. Abdinov, R.F. Babayeva. "Flexible Photocells Based on Layered A III B VI Semiconductor Compounds", International Journal on Technical and Physical Problems of Engineering (IJTPE), Issue 40, Vol. 11, No. 3, pp. 23-27, September 2019.

[15] Q. Lu, G. Keskar, R. Ciocan, R. Rao, R.B. Mathur, A.M. Rao, L.L. Larcom, "Determination of Carbon Nanotube Density by Gradient Sedimentation", J. Phys. Chem. B, Vol. 110, No. 48, pp. 24371-24376, 2006.

[16] Q. Wang, "Estimate of Material Property of Carbon Nanotubes via Nonlocal Elasticity", Adv. Theor. Appl. Mech., Vol. 1, No. 1, pp. 1-10, 2008.

BIOGRAPHY

Nuha Hadi Jasim Al Hasan was born in Basrah, Iraq, on April 18, 1981. She graduated from Department of Engineering Materials, College of Engineering, University of Basrah, Basrah, Iraq in 2003. She was a student of M.Sc. and Ph.D. in mechanical engineering at the same university. Her areas of interest are composite materials, selection design, corrosion, powder metallurgy, failures of engineering materials, and her publications in corrosion heat treatment.