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Investigation on Mechanical Properties of Polyoxymethylene Reinforced by Carbon Nanotube Using Molecular Dynamics

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ABSTRACT: Polyoxymethylene as a thermoplastic or soft plastic material, in addition to its acceptable mechanical strength, has a much lower density comparing to metals. Therefore, it can be a good alternative to non-ferrous metals in the industry. In this study, nanocomposites of this polymer with carbon nanotubes were used to enhance the strength and improve the mechanical properties of the polymer. Experimental analyses of the nanocomposites have limitations due to the high cost. Therefore, using microscopic scale simulation methods can be a good alternative to study the properties and behavior of these nanocomposites. In this study, the molecular dynamics method is used to simulate the mechanical properties of the nanocomposite. The simulation results obtained in this study show that the density and mechanical properties of the pure polymer such as Young's modulus, yield stress, and the ultimate stress are consistent with experimental values. Moreover, with temperature increase, these mechanical properties will be reduced. Also, these properties by reinforcing polymer with carbon nanotubes which functionalized with hydroxyl and fluoro groups in a nanocomposite structure can modulate Young's modulus from 41.31 to 44.6% and yield stress from 20 to 80% respectively.

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1. INTRODUCTION

Today, composites of polymer and nanomaterials such as graphene and Carbon Nanotube (CNT) have many applications. Researchers use many simulation methods to study the properties of nanocomposites such as Molecular Dynamics (MD) and Quantum Mechanics (QM) [1-4]. Investigation of the behavior and properties of nanocomposites was first started experimentally but the experimental method is limited due to its high cost. Therefore, the use of microscopic scale simulation techniques can be a good solution for studying the properties and behavior of nanocomposites. MD simulation is one of these efficient simulation methods which can be used to investigate the mechanical and thermal properties of nanostructures. MD simulation is a classical physics-based method based on solving Newton's dynamics equation for each particle and studying the time evolution of its system.

Several articles have investigated the properties of polymer nanocomposites reinforced with carbon nanostructures, including graphene and CNT using molecular dynamics simulation. Han and Elliott [5] used the MD technique to simulated the Polymethyl Methacrylate (PMMA) and Poly Metaphenylenevinylene (PmPV) polymer/CNT composites by using a single wall (10, 10) CNT. Their simulation results showed that the CNTs can mechanically reinforce a polymer matrix, especially in the longitudinal direction of the nanotube. Frankland et al. [6] investigated the effects of the CNT lengths and their discontinuities on the reinforcement of polymer matrix behaviors. The results showed that only the long CNTs could provide a clear reinforcement in the polymer matrix. Nayebi and Zaminpayma [7] studied the mechanical properties of graphene–polythiophene composite with Reax force field. They found that mechanical characters of tension along the zigzag orientation are higher than in the other directions. Also, by increasing the weight concentration of graphene in composite, Young's modulus and breaking strain increase. They showed that Young's modulus decreases with increasing temperature. Islam et al. [8] studied the mechanical properties of Polyoxymethylene (POM)/CNT composite. They considered only a simple CNT without any functionalized group in the center of the simulation box with a reactive force field. They found that CNT increases Young's modulus of the polymer.

The POM is one of the thermoplastic polymers used in precision parts requiring high stiffness, low friction. In this paper, we study the mechanical properties of POM and functionalized CNT such as hydroxyl (-OH) and fluoro (-F) groups.

2. SIMULATION METHOD

Molecular dynamics simulations were performed using LAMMPS software [9] with applying the Parents Circle

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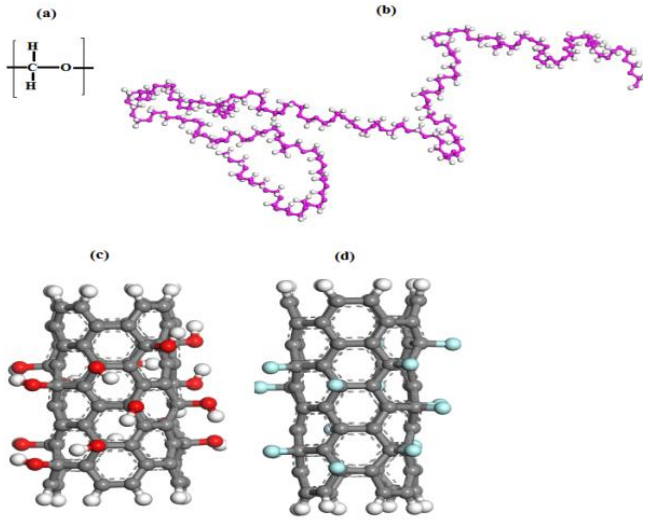

Fig. 1. Structures used in simulation

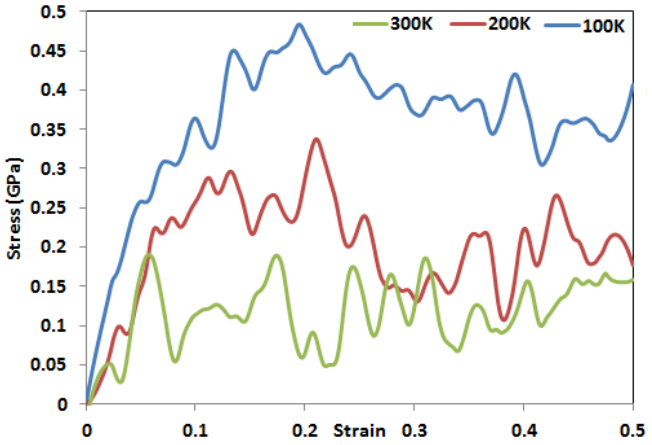

Fig. 2. Stress-strain curves of the polymer at three different temperatures 100, 200, and 300 K (rate of 10^9 s^{-1})

– Families Forum (PCFF) force field to investigate the mechanical properties of functionalized CNT reinforced POM nanocomposites. This force field, which is one of the compatible force fields, is often used for molecules with covalent bonds such as organic matter and polymers [10]. Energy statements in this field of energy include the sum of interconnected (valence), merged interactions (cross-term), and nonconnected (non-bond) as follow:

$$E_{total} = E_{valence} + E_{cross-term} + E_{non-bond} \quad (1)$$

The valence interactions are divided into four categories: bond, angle, torsion (dihedral), and out-of-plane angle as follow:

$$E_{valence} = E_{bond} + E_{angle} + E_{torsion} + E_{oop} \quad (2)$$

In order to prepare the structure of the composite, three functionalized CNT were inserted in the POM network in different directions. The boundary conditions of the simulation box were periodic. In the first stage, the structure is built at a very low density. In order to get the experimental density, the structure is pressed at 1 GPa and 300K for 1 nanosecond (the compression stage). Then, the system is heated up to 700K in 1 atm for 1 nanosecond (the heating phase). The compression-heating cycle is repeated five times and then relaxed for 1 nanosecond at 300K reaching the equilibrium at atmospheric pressure; in order to approach the density to experimental polymer density. The time step was 1 femtosecond and the temperature and pressure were controlled using a noise-hoover thermostat. To obtain the stress-strain curve, the loading mechanism in the simulation process was strain loading with a constant rate in one direction.

3. RESULTS AND DISCUSSION

Fig. 1 a,b,c,d show the POM monomer, POM chain with 100 monomers, CNT with –OH group, and CNT with –F group, respectively. Fig. 2 shows the stress-strain curve for pure POM at 100, 200, and 300K with a strain rate of 10^9 s^{-1}, the simulation box has 10 chains. Table 1 also shows the mechanical characteristics obtained from these graphs, including Young's modulus (slope of the graph in the linear region), yield stress (yield of linear end of the region), and ultimate stress.

As it can be seen, with temperature increase, the mechanical properties will be decreased; this can be due to the material softening as the temperature increases.

We added three functionalized CNT with hydroxyl (-OH) and fluoro (-F) groups to the simulation box and computed the stress-strain curves at 300 K and a rate of 10^9 s^{-1}. Table 2 also shows the mechanical characteristics obtained from these graphs. These results show that composites with functionalized CNT are stronger than those without any CNT. In addition, the Young's Modulus of –F group is higher than the –OH group because of the high electronegativity of the –F group related to the –OH group.

Table 1. Young's modulus, yield stress, and ultimate stress of POM polymer

Temperature (K)	Young's Modulus (GPa)	Yield Stress (GPa)	Maximum Stress (GPa)
100	6.68	0.16	0.48
200	3.37	0.10	0.35
300	3.92	0.05	0.19

Table 2. Young's modulus, yield stress and maximum stress composites with functionalized CNT and without CNT

Functionalized	Young's Modulus (GPa)	Yield Stress (GPa)	Ultimate Stress (GPa)
No-CNT	3.92	0.05	0.19
-OH	5.54	0.06	0.20
-F	5.67	0.09	0.19

4. CONCLUSIONS

In this paper, mechanical properties of POM/ functionalized-CNT by molecular dynamics simulation and applying PCFF force field are investigated. The results show that as the temperature increases, the mechanical properties such as Young's modulus, yield stress, and ultimate stress are decreased, which may be due to the softening of the material as the temperature increases. In addition, the Young's Modulus of –F group is higher than the –OH group because of the high electronegativity of the –F group related to the –OH group. The simulation results demonstrate that CNT with -OH and -F groups in a nanocomposite structure leads to increasing Young's modulus from 41.31 to 44.6% and yield stress from 20 to 80%.

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