EFFECT OF VACANCY DEFECTS ON THE MECHANICAL PROPERTIES OF CARBON NANOTUBE REINFORCED POLYPROPYLENE

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ABSTRACT

In this work, a study has been performed to explore the effect of vacancy defects on the single-walled carbon nanotubes reinforced polypropylene composites using molecular dynamics simulation. Polypropylene is a thermoplastic polymer consisting the high melting point compared to similarly weighted plastics which finds applications in toys, automobile products, laboratory equipment, loudspeakers and other important industry sectors. Two types of carbon nanotubes, one with perfect hexagonal lattice and another consisting 1, 3 and 5% vacancy defects, respectively used as fiber. A commercially available software package Materials Studio 8 has been used for all modeling and simulation purpose. Results show the decrease of 6.87%, 10% and 23.12% in young’s modulus with 1, 3 and 5% vacancy defects, respectively.

Key words: Carbon Nanotubes, Defects, Mechanical Properties, RDF, Compass, Young’s Modulus.

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1. INTRODUCTION

Defects play an important role in deciding the nature of materials for aerospace and defense industry. After the discovery of CNTs, it has been considered as one of the most important nanoscale fiber to manufacture the advanced composites. Many studies have been performed to obtain the defects behavior on CNTs and their composites.

In recent years, many experimental and theoretical approaches come in light to explore the behavior of carbon nanotubes as a form of fiber in composites. In theoretical the most
research conducted using molecular dynamics simulation technique because of complicated experimental setup and cost. Effect of weight and volume addition of multi-walled carbon nanotubes in polycarbonate matrix studies by Sharma et al.\textsuperscript{1} Their studies show the 2 weight % addition of multi-walled carbon nanotubes in polycarbonate matrix gives the 89% increase in young’s modulus. A molecular dynamics simulation technique, used by Sharma et al.\textsuperscript{2} to study the effect of CNF (carbon nanofiber) volume fraction and weight % addition on the mechanical properties of CNF-reinforced polypropylene composites. Their results show the 2% carbon nanofiber addition by volume in PP (polypropylene matrix) increases the longitudinal elastic modulus about 748%. Sharma et al.\textsuperscript{3} using a molecular dynamics simulation technique studied the Influence of single-walled carbon nanotube functionalization on the mechanical properties and load transfer mechanism in functionalized carbon nanotube-polypropylene composites.

CNTs and their composites show the extraordinary performance and strength as discussed above but the defects such as Stone-Wales, vacancies occur at the time of purification or chemical treatment which degrades its properties. There are many studies which have been performed to understand these phenomena, but every new approach gives a new idea to improve its performance. Effect of randomly occurring Stone-Wales and vacancy defects on the elastic properties of carbon nanotubes-polypropylene composites studied by Sharma et al.\textsuperscript{4} using molecular dynamics simulation with COMPASS force field. They used a commercially available software package Materials Studio which gives accurate results in comparison to experimental methods when proper simulation techniques used. The simulated results of their studies show that SW defect has more influence in reducing the mechanical properties as compared to that of vacancy defects. Sharma et al.\textsuperscript{5} studied the effect of volume fraction on the elastic modulus of (10,10) armchair reinforced PMMA (poly(methyl methacrylate)) and PmPV (poly{(m-phenylene-vinylene)-co-[{(2,5-dioctoxy-p-phenylene) vinylene}]} matrix using molecular dynamics simulation. They observed that with increasing volume fraction there is a significant increase in longitudinal Young’s modulus. There is also some work exploring the mechanical properties of composites made by graphene sheets. Sharma et al.\textsuperscript{6} used a molecular dynamics simulation technique to study the mechanical properties of single layer graphene, and CNT reinforced amorphous metallic glass. They have observed for same volume fraction Young’s modulus of long graphene/MG nanocomposite is more than the long CNT/MG composite. Mechanical properties of CNT-polymer composites strongly depends on their interfacial shear strength (ISS). The stronger interface between CNT and polymer will provide the more strength to the composites. Chawla and Sharma\textsuperscript{7}investigated the young’s modulus and interfacial shear strength (ISS) of a pristine carbon nanotube-polymer composites. Their studies show the 14.30% reduction in longitudinal young’s modulus (E33) when SWCNT pulled out 10Å from the polyethylene matrix. In addition, ISS was mainly distributed over first and final 10Å of pull-out. Chowdhuryet al.\textsuperscript{8}investigated the effect of vacancy defects on the interfacial shear strength (ISS) of carbon nanotubes in carbon nanotubes-polymer composites. Simulated results revealed that breakage in CNTs could occur during the pull-out process in the presence of large size vacancy defect.

The focus of this study is to explore the role of vacancy defects in degrading the mechanical properties of carbon nanotube reinforced polypropylene composites using a molecular dynamics simulation technique.

2. METHODOLOGY

Classical molecular dynamics of composite structures with COMPASS force field has been studied using Materials Studio. An (8,0) zigzag single-walled carbon nanotube of diameter 0.62nm and length of 5.94 nm has been generated and used as fiber. Three concentrations of
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1.3 and 5% vacancy defects has created on the pristine CNT structures. Ten chains of PP have been generated and used for packing at an initial density of 0.93. Figure 1 shows a single monomer of PP chain and figure 2 illustrates 10 repeat units.

![Figure 1 A Polypropylene monomer](image1)

Five types of systems have been developed including one pure polymer and 4 with CNTs. Percentage defects have been created with the idea of vacancy atoms/number of atoms in the CNTs. Figure 3 shows the pure propylene matrix with the cell dimension of 17.5×17.5×59.64Å³. Figure 4 shows the developed PP-CNT composite systems after relaxation.

![Figure 2 Ten repeats of Polypropylene monomer](image2)

"Amorphous cell" module of Materials Studio software with COMPASS® force field has been used for packing the molecules in the CNT cell. It allows the molecule to pack in the cell using MonteCarlo fashion. Simulation has been started with the geometry optimization then system put into an NVT ensemble at a temperature of 298K over 100 ps. Then a fine quality

![Figure 3 A pure Polypropylene Matrix](image3)

![Figure 4 A CNT- Polypropylene Composite](image4)
geometry optimization has been used and again applying 800K NVT ensemble over 50 ps system has been equilibrated. Finally, one more geometry optimization applied and system with proper density and less residual stresses have been obtained. Figure 5 shows the averaged density that has been obtained after relaxation of the pure PP system. Obtained density of 0.898 gm/cm$^3$ makes a good agreement with the experimental density of (0.895 to 0.92 gm/cm$^3$). Figure 6-7 shows the side view of the pristine and 5% vacancy defects nanocomposite system.

**Figure 5** Averaged density of CNT- Polypropylene Composite obtained after relaxation

**Figure 6** Side view of CNT- Polypropylene Composite

**Figure 7** Side view of the 5% vacancy defected polypropylene composite
4. RESULTS AND DISCUSSION
A constant strain minimization approach has been used to obtain the mechanical properties of CNT-PP composites. A small tensile strain of 0.003 has been applied to the system. The application of this strain is accomplished by expanding the dimensions of the simulation cell uniformly in the direction of deformation and re-scaling. In previous studies, it has been proven that this method can be used to calculate the mechanical properties of composite systems. Simulated results show Young’s modulus of 1.5GPa for the pure PP polymer which makes an excellent agreement with the experimental value of 1.3GPa to 1.8GPa. Figure 8 illustrates the variation in Young’s modulus with an increasing vacancy defects percentage. It has been observed that 1, 3 and 5% vacancy defects reduced the young’s modulus 6.87%, 10%, and 23.12%, respectively in comparison to pristine carbon nanotube composite. Simulated results show the same trend that has been obtained by Sharma et al. using COMPASS force field. By the Figure 8, it can be concluded that Young’s modulus of CNT-polymer decreases with increasing vacancy defect percentage in carbon nanotubes.

![Figure 8 Variation in Young's modulus with varying vacancy defect percentage](image)

5. CONCLUSIONS
Molecular dynamics simulation technique has been applied to study the mechanical properties of carbon nanotube reinforced polypropylene composites. A comparison has made, between composites made by pristine carbon nanotubes and with vacancy defects. Obtained results show the decrease in Young’s modulus of composites which has been reinforced by vacancy defected carbon nanotubes. From above results and discussions, it can be concluded that nanocomposites reinforced with vacancy defected carbon nanotubes consist less young’s modulus in comparison to the pristine ones.

REFERENCES


