Carbon Nano-tube Reinforced Nylon 6,6 Composites: A Molecular Dynamics Approach

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A R T I C L E I N F O	A B S T R A C T
	Composites prepared by Single Wall Carbon Nano-tube (SWCNT) as well as Nylon assume a vital part in practical applications as in ultrastrong lightweight materials, vehicle and flying machine parts. In the present work, the influence of aspect proportion (l/d) on the longitudinal Young's modulus (E_{11}) as well as transverse modulus (E_{22}) for the SWCNT/Nylon 66 composite have been critically analyzed through utilizing tools of Molecular Dynamics (MD) simulations. Materials Studio 8.0 simulation software utilized in the current study for finding Young modulus. Aspect proportion (l/d) of used CNT in the composite was ranged from l/d = 5 up to l/d = 30 while the fraction of volume (V_f) of the CNT had been kept constant at 8%. Results demonstrated however that the lengthwise Young's modulus for the current composite increment essentially by expanding the aspect ratio (l/d) of Nano-tube while the change in transverse modulus with fluctuating perspective proportion was not exceptionally noteworthy. The results of the simulation have been consequently matched with the Mori-Tanaka model as well as the Finegan model.

1. Introduction

Polymers of Nylon had observed noteworthy viable utilizations for fibbers, shapes of molded parts for engine components of automobiles and electrical equipment (Huang et al., 2003; Santella, 1994; Sugimoto, 1989). The initial case related to nylon 6,6 believed to be created on 1935 and the inventor was Wallace Carothers at DuPont's research centre (Kohan et al., 1986). It has also being used in carpet manufacturing and tire cords because of its excellent abrasion resistance, high melting point, compact molecular structure, and better weathering properties. Nylon widely believed as a nonspecific designation related to a group consists mainly of synthetic polymers, furthermore particularly semi-aromatic polyamides or aliphatic and Polynylon 6,6 created as a repetitive unit for the Nylon 6,6 monomer. Nylons are very promising as a matrix materials in composites, with reinforcing fibers like glass, carbon fiber and CNTs which will certainly have improved mechanical properties like higher density, higher Young's modulus, this makes it quite valuable if utilized for additive manufacturing, fused deposition modeling 3d printers, intake manifold parts of engine and in aircraft materials, etc. Among these reinforcements, CNTs are considered as the best reinforcement in polymer composites till now (Breuer at al., 2004; Sharma et al., 2015). The past studies show that if CNTs reinforced with polymer matrix, the obtained structures could be lightweight and stronger than conventional aluminium alloys and polymer composites

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made by reinforcing carbon fibre. It has also been suggested that new manufacturing techniques for CNT composites ought to be established as well as currently used techniques needs improvement for controlling the orientation and dispersion for the Nano-tubes inside the polymer. Right from the beginning, from the discovery of carbon Nano-tubes (CNTs) by Iijima et al., (1991), CNTs have gained a lot of research interest because of their interesting and remarkable properties, for example, high thermal and electrical conductivity (Ruoff et al., 1995; Ebbesen et al., 1996). CNTs believed as the stiffest and strongest materials discovered till now on the parameters of mechanical properties such as tensile strength as well as Young's modulus (Yu et al., 2000; Coleman et al., 2006). It has also been observed that Young's modulus for the carbon Nano-tubes (single-walled) reduced by increasing the radius of Nano-tube, however, it's valued increased by increasing the Carbon Nano-tube volume fraction and aspect ratio. The bulk modulus, shear modulus as well as Poisson's ratio shows decreasing trends with arise in the diameter of Single Wall Carbon Nano-tubes. Because of the wide applicability, it becomes necessary to study and analyze the need and properties of CNT/Nylon composite at different parameters. A lot of research has been conducted on experimental analysis of CNT/Nylon composite through commonly used polymerization and other techniques like In situ polymerization, Simple melt compounding and Continuous spinning (Haggenmueller et al., 2006; Gao et al., 2005; Liu et al., 2004). It has also been observed that amalgamation of the fewer amount of CNT along with polymer matrix could considerably enhance the hardness, strength, and modulus but no significant work has been found which investigates the effect of change of geometrical parameter on mechanical properties of composite through molecular modelling or simulation. By using molecular simulation, we can have a better insight into the behaviour of the nano-composites without consuming the physical resources in conducting the experiments. Molecular simulation considered as a microscopic investigation technique which is believed to be exceptionally helpful to understand the physical phenomena through the nuclear stage, and also extremely valuable for developing original and improved sort of materials (Satoh, 2010).

Molecules, as well as minute particles in the structure, were processed in a particular manner such that essential quantities especially microscopic were found through analyzing the behaviour of the concerned system (Frenkel et al., 2001). Molecular Dynamics (MD) and Monte Carlo (MC) are two widely used molecular simulation methods for molecular analysis. MC technique has the capability of inspecting thermodynamic symmetry; but the Monte Carlo technique not found suitable to examine dynamic phenomena (Anjana et al., 2016). The MD method is suited for thermodynamic symmetry and also for dynamic phenomena (Binder, 1995). In MD simulation, elements should be constructed for interacting in a specific period, however, the behaviour during the motion of particles is kept which is based on Newton's equation regarding the system's motion of molecules interacting to analyze the path of the molecules (Rapaport et al., 2004). This method is being used widely in diverse areas such as modeling of materials, chemical, and bio-molecules science (Karplus et al., 2002; Tang et al., 2010; Tuckerman et al., 1995). MD simulations are also widely used to analyze the properties of carbon Nano-tubes and Nano-composites (Sharma et al., 2013, 2014, 2015, 2016, 2018). Chawla et al. (2017) have also done a study to analyze the influence of carbon Nano-tube pullout in the polyethylene matrix for the mechanical properties of the composite made of Polyethylene and Carbon Nano-tube. Their results show that when the CNT removed from the polyethylene matrix by 10Å, the longitudinal modulus of composite reduced by 14.3% and increment in the volume fraction of (5,5) Single-Walled Carbon Nano-tube armchair-polyethylene Nano-composite system that leads to a lessening of the average energy growth.

The literature lacks any evidence about significant study done at the molecular stage that would demonstrate the effect of the geometrical parameter, for example, aspect ratio on the mechanical properties of Nylon/CNT Nano-composites. The aspect ratio is the essential geometrical parameter that influences the overall properties of composites made by CNT as the potency of carbon Nano-tubes as a material of reinforcement is not only because of their extraordinary high modulus but also likewise to the high aspect ratio (Martone et al., 2011). It has been also found that the influence of aspect ratio on transverse and longitudinal Young's modulus of SWCNT and poly-nylon 66 has not been addressed until now. It is thus necessary to investigate the effect of the aspect ratio of CNT on Young's modulus of

SWCNT/poly-nylon 6,6 composite. In the present work, Molecular Dynamics simulations with "Condensed phase optimized molecular potential for atomistic simulation studies" (COMPASS) force field has been applied for analysing any effect of aspect ratio (l/d) towards the lengthwise Young's modulus (E_{11}) as well as the transverse Young's modulus (E_{22}) for SWCNT/poly-nylon 6,6 composites.

2. Methodology Adopted

Molecular Dynamics (MD) was used for simulation and also for determining mechanical properties related to Poly-nylon reinforcement with SWCNT. Materials Studio 2017 atomic modelling simulation tool developed by Accelrys was utilized for executing the simulations. MD simulation contains resolving the standard multi-body statement in settings pertinent to analysing the matter at the molecular stage. Conventional equilibrium Molecular Dynamics related to the micro-canonical ensemble of statistical mechanics was applied, however in some situations; properties at fixed pressure or temperature are needed. Other methods are also there in MD to modify the motion equations for producing those systems. However, the distinct trajectory does not denote the result for Newton's equations of motion. Firstly, the carbon Nano-tube and the poly-nylon modelling is done by using "build nanostructure" and "build polymer" tool of Material Studio respectively. After that packing of composite has been done by using the amorphous module of Material Studio. Then Geometry optimization task has been performed by using the Forcite module of Material Studio. Afterward, dynamics run simulations have been conducted by using NVT (number of particles, temperature, and volume are constant) and NPT (number of particles, temperature, and pressure are constant) ensembles. Afterward, the Simulation of Mechanical properties has been conducted by using Materials Studio's Forcite module.

In the present work, simulations were executed utilizing the force field known as COMPASS that is "Common all-atom force field for atomic simulations" to perform simulations related to normal inorganic particles, polymers and organic particles, created by utilizing "state-of-the-art ab initio" and observed parameterization approaches. This force field along with MD simulations has previously been used to study the properties of CNTs, polymers, and composites. In the operational form of the COMPASS force field, there are 11 valence terms which include diagonal and off-diagonal cross-coupling terms plus also there are two non-bonding interaction terms i.e. Columb function and Lennard-Jones for electrostatic and van der Waals interactions respectively. COMPASS was the first force field that has been used for condensed phase properties and also the empirical data for molecules that are in isolation. Therefore, the COMPASS force field can be used for the exact prediction of structural, vibrational, thermal and physical properties for huge ranging particles that are in condensed and in isolation forms.

3. Modelling and Simulation

3.1 Modelling and Packing of Composite

Firstly, A single-walled armchair carbon Nano-tube (SWCNT) with a diameter of 5.42 Å has been generated with Build Nanostructure tool in Materials Studio (refer Fig. 1). Integer indices (n,m) of carbon Nano-tube was set at (4,4). A couple of integer indices (n, m) known as chirality, denotes the method by which the sheet of graphene is enclosed. The m and n define the value of unit vectors in the two-directional crystal framework of the graphene sheet. Thereafter, the length of the Nano-tube has been adjusted by changing the lattice parameters of Nano-tube and yellow colour has been selected for the carbon Nano-tube. Afterward, in the modelling of Polynylon 6,6 polymer chain was created by using 10 repeated units of Nylon 6,6 by utilizing the "Build Polymer" option in Materials Studio (Figs. 2 and 3). The classical Nomenclature of Polynylon 6,6 is [NH-$(CH_2)_6$-NH-CO-$(CH_2)_4$-CO]$_n$ constructed by adipic acid and hexamethylenediamine and here n represents the number of repeat units in the polymer. The tacticity used was isotactic and the orientation while making polymer was head-to-tail. Colour coding used while modelling of the monomer of Nylon 6,6 was according to the elements and is given in Table 1.
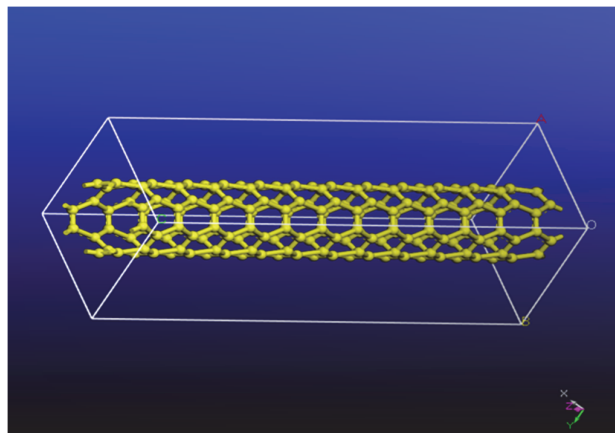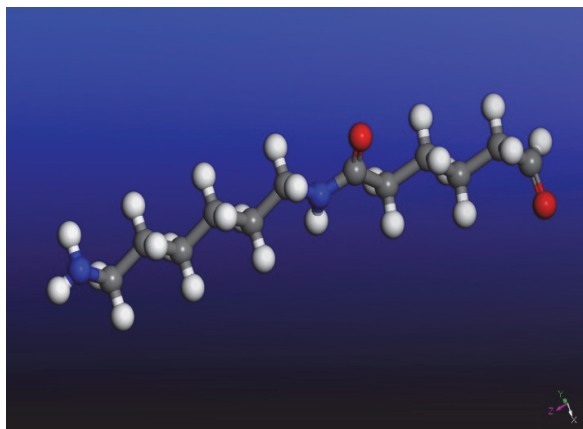
Fig. 1. Armchair (4,4) SWCNT with diameter 5.42 Å

Fig. 2. Nylon 6,6 monomer

Table 1. Colour coding shown while modeling of nylon 6,6

S.N.	Colour	Atom
1	White	Hydrogen
2	Red	Oxygen
3	Grey	Carbon
4	Blue	Nitrogen

After that, the amorphous module of Materials Studio 8.0 has been used for the packing of Polynylon 6,6 around single-walled carbon Nano-tube at an initial density of 1gm/cm³ (as shown in Fig. 4). The SMART algorithm has been utilized and structure packed in iso-surface surrounded volume in the current simulation. The temperature was 298K and the loading steps were 1000. The amorphous cell module is having a wide-ranging collection of tools to form a three-dimensional repetitive structure for polymeric systems and molecular liquids. The module constructs molecular structure within a cell through lowering close relations among particles, while confirming a feasible distribution of the torsional angles for the concerned utilized force field.
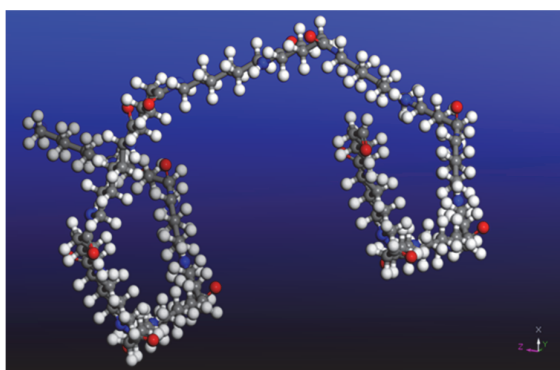

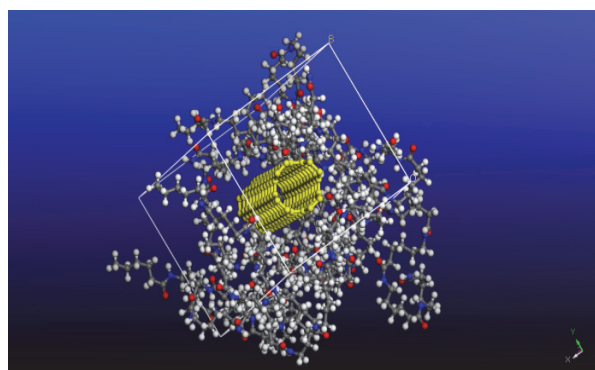**Fig. 3.** Polynylon 6,6 constructed by 10 repeated units of monomer Nylon 6,6

Fig. 4. Packing of SWCNT with Polynylon 6,6 by amorphous module

The structures made by this module serve as an initial input to modeling as well as simulation workflows related to the amorphous matters, such as annealing calculations, geometry optimization, dynamics run and quenching.

3.2 Simulation of Mechanical Properties

After packing, the initial step of the simulation was geometry optimization and this step enable refining the geometrical structure to the point when it fulfils certain particular benchmark. An iterative procedure is utilized to perform the geometrical optimization, where the related coordinates of the cell parameters and the atoms are balanced to the point when the overall energy related to the structure tends to lessened substantially, thereafter the structure which is optimized leads to the lowest value resulting towards potential energy surface. Geometrical optimization is focussed on decreasing the magnitude of the computed stresses and forces until the point when their value is lesser than definite convergence tolerances. "Smart Algorithm" utilized here and the set parameters are force convergence tolerance of 0.5 Kcal/mol/Å, displacement convergence tolerance of 0.015 Å, energy convergence tolerance of 0.001 Kcal/mol, and highest set value of iterations were 5000. Afterward, Dynamics run simulation has been conducted and this task in the Forcite module allows us to simulate the atomic structure which will vary under the influence of calculated forces. NVT and NPT ensembles were applied during the dynamics run of the composite. In the NVT ensemble, the dynamics of the structure are modified to allow the system to exchange heat with the environment at a measured temperature and in the NPT ensemble; a barostat is used to control the pressure. Forcite is an assemblage of tools in molecular mechanics and their utilization is to investigate the enormous range of molecular structures. The key finding mainly related to the potential energy surface, for which variation of atomic nuclei, is characterized through classical Forcefields which are formed by critically arranging data through experiments and advanced level quantum mechanical measurements. Intra and interatomic and molecular structural formations were defined through the "Condensed Phase Optimized Molecular Potential" (COMPASS) force field which is the first ab initio forcefield that allows simultaneous and accurate predictions of condensed phase properties as well as gas-phase properties for an extensive range for the polymers and molecules. Anderson thermostat has been used and simulations were conducted in the ranging interval of 1 femtosecond, thereafter the set total time was 50 picoseconds. After that, simulation of mechanical properties has been conducted by using the Forcite module. The constant strain method has been used which approximates the elastic constant matrix also called a stiffness matrix by a sequence of limited difference approximations. This method initiates through eliminating structural similarities within the current system, subsequently, an optional re-optimization has been conducted for the composite system, and thus the cell constraints can be altered. Elastic modulus has been computed by using the COMPASS force field. The process was repeated at different aspect ratios of SWCNT.

Table 2. Parameters used during simulation of mechanical properties

S. N.	Parameter for initiating the simulation	Value
1	Constant Strain	0.001
2	Pre Optimized Structure	Yes
3	Algorithm Applied	Smart
4	Highest Possible Iterations	5000
5	Force Field used	COMPASS

4. Results and Discussion

This section comprises of MD simulation comparison of results with mathematical models for the verification. The volume fraction related to single-walled carbon Nano-tube was kept constant at 0.08 and aspect ratio was varied in the range of 5 to 30. The energy plotting after dynamics run shows that potential energy generated is greater than kinetic energy and kinetic energy generated is greater than non-bond energy in the molecules for dynamics run (Fig. 5).
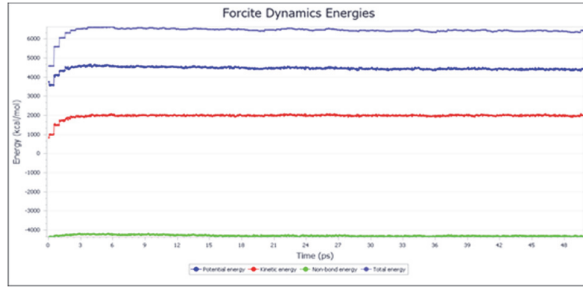
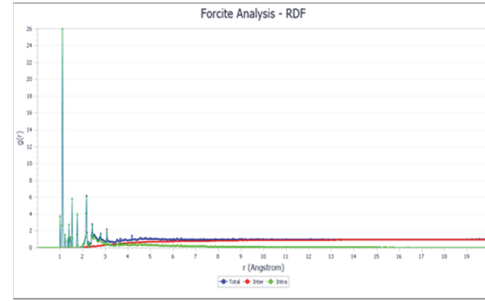**Fig. 5.** Energies obtained from composite after dynamics run

Fig. 6. Radial distribution function plot for CNT/Polynylon 6,6 composite

Radial distribution function (RDF) analysis has been done through the Forcite analysis module. The prime significance of Radial distribution function (RDF) analysis considered as the categorization for the molecular structures, however, it is also applied as a probability function to get a couple of atoms for the distance (r) from any other atom in a random atomic scattering system. The pair correlation function (also termed as Radial Distribution Function) has been helpful for applications in operational findings of both liquids as well as solid packing to study the definite interactions, for instance, hydrogen bonding, regarding factual mechanical theory for the mixtures as well as liquids. In a functional sense for solving the findings of Molecular simulations for artifacts that emerge because of the essential requirement for physically small systems while performing atomistic molecular simulations. Figure 6 shows the RDF between the atoms of the composite and plots are produced for an intermolecular component of RDF, intra-molecular RDF, and total RDF. The cut-off distance was 20 Å and the interval was of 0.02 Å. It has been found that initially the g(r) is having high values when the distance is less than 3 Å but later the g(r) almost till the cut-off distance of 20 Å. Fig. 6 signifies the difference of lengthwise Young's modulus for the fibre ratio of aspect i.e. (l/d) for a constant fraction of volume. When l/d varies in the range of (5-10), E_{11} (Longitudinal Young's modulus) increased from 6.355 GPa to 21.25 GPa. The increment in longitudinal modulus could also be co-related to the fact that along with arising for the aspect ratio, the area of surface for the Carbon Nano-tube arises, consequently will result in improving the transfer of load among poly-nylon 6,6 and Carbon Nano-tube.

Table 3. E_{11} at different aspect ratios of CNT for composite

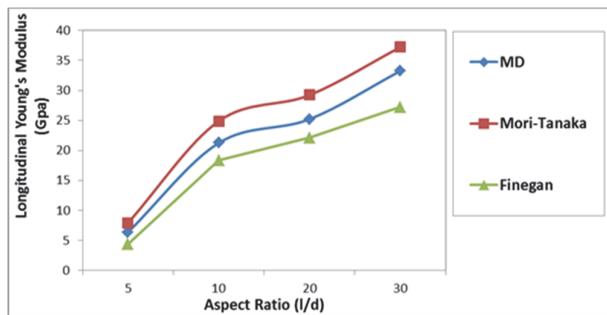| S. No.	Aspect Ratio (l/d)	MD Simulation Results (GPa)	Mori-Tanaka Model (GPa)	Finegan Model (GPa)
1	5	6.355	7.92	4.35
2	10	21.25	24.89	18.34
3	20	25.21	29.23	22.11
4	30	33.24	37.21	27.22

Fig. 7. Results comparison for longitudinal modulus of CNT/Polynylon 6,6 with varying aspect ratio (l/d) and volume fraction = 0.08
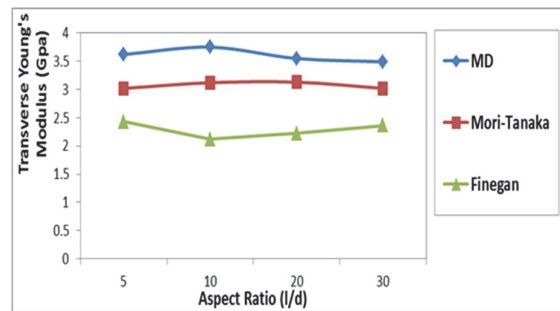

Fig. 8. Results comparison for transverse modulus of CNT/Polynylon 6,6 by changing ratio of aspect (l/d) and volume fraction i.e. 0.08

It can be seen that while l/d varies in the range of 5 to 10 then the E_{11} changes from 6.355 to 21.25 and the MD findings were in acceptable agreement when compared to theoretical models of Finegan and Mori-Tanaka (see Table 3 and Fig. 7).

Table 4. Results of E_{22} at different aspect ratios of CNT for composites

S. No.	Aspect Ratio (l/d)	MD simulation results (Gpa)	Mori-Tanaka (Gpa)	Finegan (Gpa)
1	5	3.62	3.02	2.43
2	10	3.75	3.12	2.12
3	20	3.55	3.13	2.22
4	30	3.49	3.02	2.36

It has been found from Table 4, that the transverse Young's modulus (E_{22}) of composite almost remains constant at every value of aspect ratio and it is in the range of 3 to 4 in GPa. The results from theoretical models are also confirming the pattern and the previous works of literature also suggest that the influence of aspect ratio (l/d) of carbon Nano-tube for the transverse modulus of the composite is not very significant. It has been observed that the effect of aspect ratio on E_{22} (Transverse Young's modulus) was not significant as the increase in aspect ratio from 5 to 10 leads to change in E_{22} from 3.62 to 3.75 only. Theoretical models also suggest that the effect of aspect ratio is not very much on the transverse modulus of the composite. Simulation results from MD were in good agreement by the Finegan model and Mori-Tanaka model which display the robustness of the paper's findings (see Figs. 7 and 8).

5. Conclusion

Simulations through Molecular Dynamics were conducted for investigating the influence of the Carbon Nano-tube aspect ratio (l/d) regarding the mechanical properties of Polynylon 6,6/CNT composites. The inter-atomic potential has been utilized through the force field of COMPASS. Constant strain reducing approach, however, has been referred with the constant strain of 0.001 to calculate Lengthwise as well as Transverse Young's modulus. Major deductions which were drawn on the basis of current work are specified below:

Increment in Carbon Nano-tube aspect ratio (l/d) from 5 to 10 initially rises the lengthwise Young's modulus up to (234%) and rise in aspect ratio from (20-30) consequently raise the lengthwise Young's modulus to (31.8%).The increase in CNT aspect ratio (l/d) from 5 to 20 did not show any significant effect on the transverse Young's modulus. It was also concluded that while dynamics run of 50 ps, potential energy is more than kinetic energy and non-bond energy was lowest out of these. From the Radial distribution function plot, it was concluded that the probability of pair correlation function i.e. g(r) fluctuates very much and shows very higher values also till 4 Å but afterward g(r) remains almost constant up to the cutoff distance of 20 Å. Effect of Nano-tube aspect ratio (l/d) on lengthwise Young's modulus is very important if matched with the transverse modulus. The findings of current work will surely be helpful for the researchers in designing and developing the CNT/Polynylon 6,6 composites with better mechanical properties.

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