

# Mechanical Interactions in Polymeric Materials with Carbon Nanotubes: a Brief Review

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## Abstract

This short review summarizes mechanical interactions occurring in polymer with carbon nanotubes. The work contains a detailed discussion of methods for improving the mechanical characteristics of polymer composites with carbon nanotubes, for which both experimental and computational work in this area are presented. The paper discusses in detail such methods of improving the connection between carbon nanotubes and the polymer as functionalization (covalent and non-covalent), enhancement by embedded nanoparticles and structural modification of the matrix. The review focuses on the molecular dynamics method as one of the promising methods for studying mechanical interactions in polymer composites with carbon nanotubes.

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*Keywords:* Nanocomposites; Carbon nanotubes; Polymers; CNT

## 1. INTRODUCTION

The combination of carbon nanotubes with polymer matrices (e.g., thermoplastics, epoxy resin) leads to the creation of nanocomposites with improved structural and functional properties due to the interaction between carbon nanotubes (CNTs) and the polymer matrix. Materials of this type have found applications in various fields such as electronics, automobiles, aerospace engineering, sporting goods, and so on [1–4].

Such nanocomposites have improved mechanical properties, in which nanotubes act as reinforcing fibers, increasing the tensile strength of the composite and its

stiffness, reducing its deformation under load, absorb impact energy, increasing the impact toughness of the composite [5]. In addition, these nanocomposites have improved thermal properties and electrical conductivity because carbon nanotubes themselves have high thermal/electrical conductivity [6,7]. Besides, carbon nanotubes delay the decomposition of the polymer matrix, increasing the thermal stability of the composite [8]. All these properties together explain the multifunctionality of such composites. Note that certainly dispersion, size of carbon nanotubes (their functionalization) in the composite, matrix composition have a significant influence on its properties.

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## 2. POLYMER COMPOSITE WITH CNTs AND MECHANICAL TESTING

Schematically, an example of a polymer nanocomposite based on carbon nanotubes is shown in Fig. 1. It should be noted the importance of the interfacial region between the carbon nanotube and the polymer [9,10].

The interface in polymer composites with CNTs consists of two nanolayers. The near layer (about 0.1–2 nm from the CNT surface) contains polymer chains, which are extremely immobile due to strong adhesion to the CNT surface. The far layer is thicker than the near layer and is formed at a distance of about 2–10 nm from the CNT surface. This layer contains polymer chains that are weakly bound to the CNTs. The thickness of the interfacial region depends on the type of polymer, the CNT surface (in some cases it can be functionalized), the volume fraction of fillers used, the particle size (and distribution) of fillers, and the quality of dispersion of fillers within the matrix [11–15]. The importance of considering the interface is that the mechanical properties of the material discussed below directly depend on it. It is worth noting that CNTs in the

composite can be located both inside the matrix and in the pores. Example of CNTs and silicone-based polymer with CNTs in section is shown in Fig. 2.

Consider for clarity the general influence of CNTs on mechanical characteristics. For this purpose, let us turn to the results of mechanical tests, which are important for evaluating the strength and durability of nanocomposite polymers with CNTs and at the same time reveal integral information about the mechanical changes occurring in the structure. Through these tests, quantitative data on properties such as elastic modulus, tensile strength and impact strength can be obtained. Different types of mechanical tests are used to test CNT nanocomposite polymers, both standard tensile/bending tests and less common ones such as dynamic tests [16]. Fig. 3 shows typical tensile curves obtained from tensile tests of pure polymer (epoxy resin) and nanocomposites containing 0.3, 0.5, 0.8 and 1.0% CNTs. Young's modulus, yield strength and tensile strength of the epoxy resin were significantly improved by the incorporation of CNTs [17–19]. The strain at break tended to decrease as the CNT content increased, indicating that the addition of CNTs made the nanocomposite

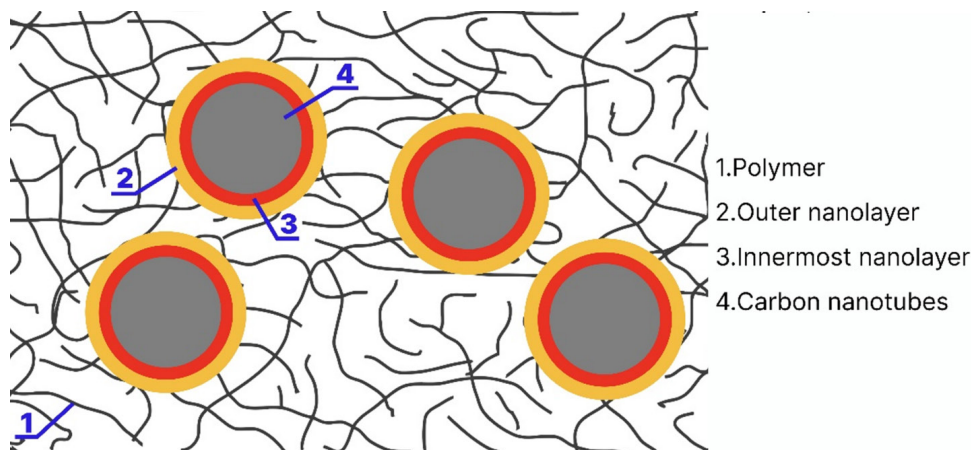


Fig.1. Polymer composite with carbon nanotubes in section.

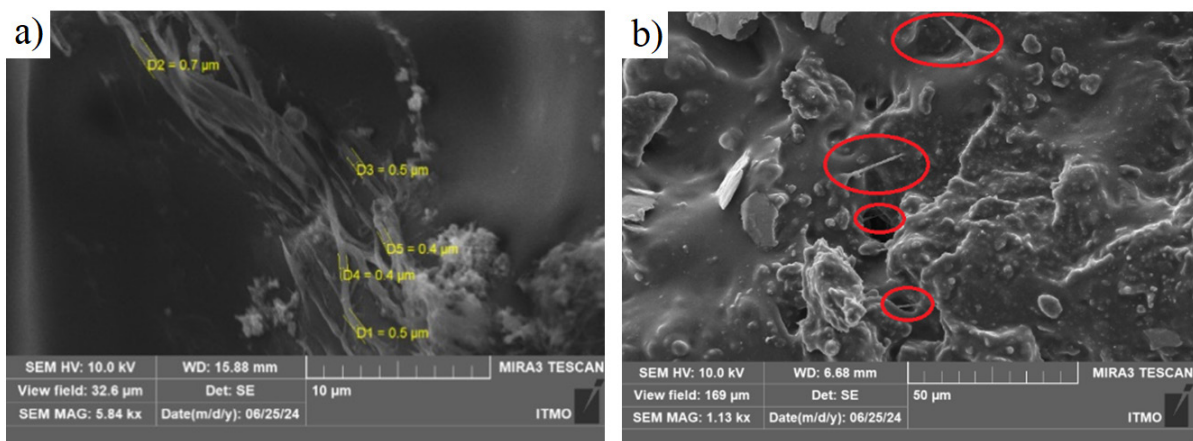


Fig. 2. CNT and nanocomposite: (a) bundle of CNTs, (b) CNTs in a polymer matrix

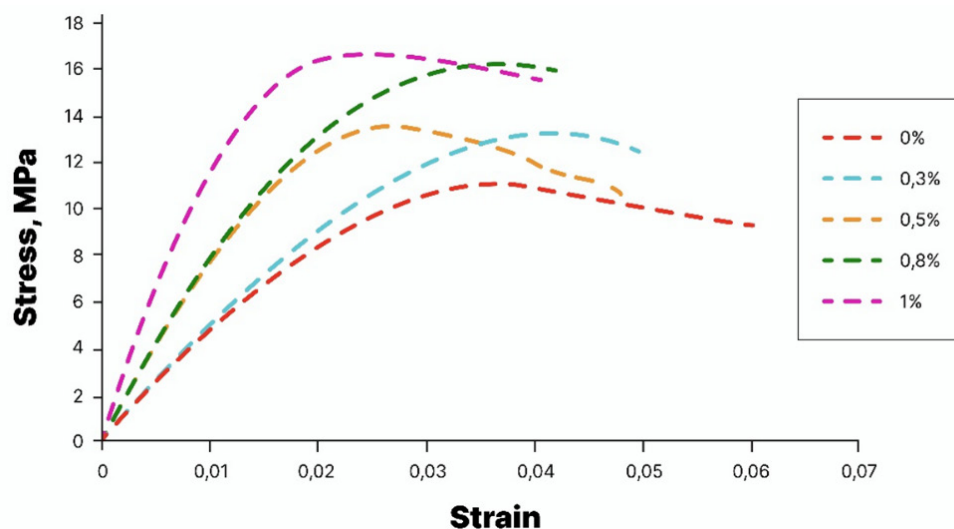


Fig. 3. Typical tensile curves obtained from tensile tests of nanocomposites with different CNT content. Adapted from Ref. [16].

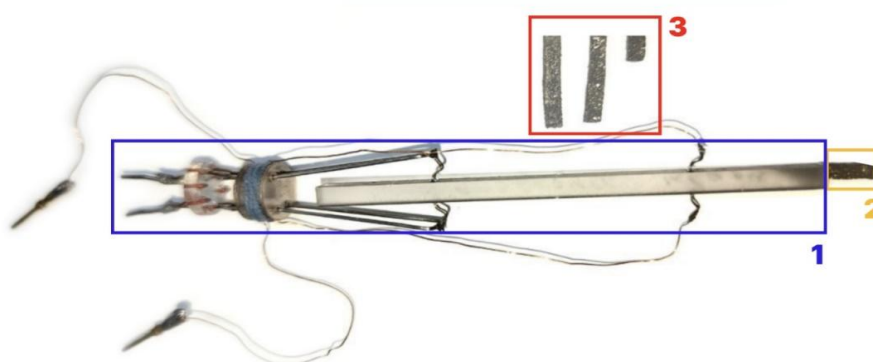


Fig. 4. Example of a dynamic testing device: (1) – the composite piezoelectric oscillator itself, (2) – a CNT nanocomposite sample fixed on the end, (3) – a set of CNT nanocomposite samples of different sizes.

stiffer and slightly more brittle compared to the pure epoxy resin. These results are typical of the polymer-CNT composite.

In addition to standard tensile/bending techniques, dynamic methods can be used for mechanical testing [20–22], such as the compound piezoelectric oscillator [23,24] shown in Fig. 4. In this device, Young's modulus is related to the resonant oscillation of a sound wave passing through the specimen. From the dynamic test, it can also be observed that the elastic modulus increased with increasing CNT loading due to polymer-CNT interaction (Fig. 5). As in the previous example at the molecular level, the adsorption of polymer chains on the CNT surface decreases the mobility of molecules, increasing the Young's modulus.

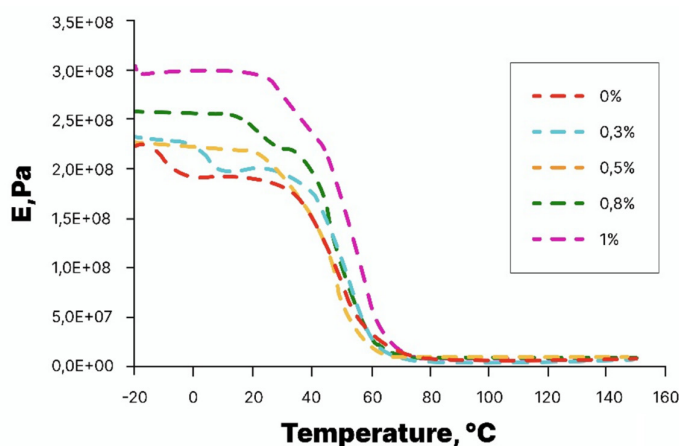
Despite the existence of quite a large number of experimental works based on mechanical testing, today molecular modeling methods are developing more rapidly and are successfully used to predict the mechanical properties of polymers with CNTs. In the next Section we will discuss these molecular dynamics (MD) simulations in more

detail, but first we will describe the mechanical interactions occurring between the polymer and CNTs.

### 3. LOAD TRANSFER MECHANISMS AND THEIR OPTIMIZATION TO IMPROVE THE MECHANICAL PROPERTIES OF POLYMER COMPOSITES WITH CNTs

To understand the mechanical interactions between the polymer and CNTs, as well as their influence on the strength characteristics, we will conditionally define three main mechanisms of load transfer in polymer composites with CNTs:

1. *Direct load transfer*. In direct load transfer, the load is transferred directly from the polymer matrix to the CNTs through their interface. This occurs when the CNTs are well distributed and have a strong bond with the matrix. Strong interfacial adhesion ensures efficient load transfer, resulting in significant improvement in the mechanical properties of the composite.



**Fig. 5.** Elastic modulus ( $E$ ) as a function of temperature for pure epoxy resin and nanocomposite with different CNT content. Adapted from Ref. [16].

2. *Shear load transfer.* Shear load transfer occurs when load is transferred from the matrix to the CNTs through mechanical adhesion or friction between them. This occurs when the interfacial bonding between the CNTs and the matrix is not ideal, or when the CNTs are not uniformly distributed. Shear load transfer is less effective than direct load transfer, but can still contribute to the overall reinforcement of the composite.

3. *Bridge load transfer.* Bridging load transfer occurs when polymer chains form bridges between neighboring CNTs. These bridges act as physical bonds, transferring load from one CNT to another. Bridging load transfer can be particularly important in composites with low CNT content, where the distance between CNTs is relatively large.

Now that we have understood the main load transfer mechanisms, let us determine the optimization of these mechanisms to achieve maximum reinforcement of polymer composites with carbon nanotubes. Direct load transfer is the most efficient method of load transfer. Consider how the mechanical properties can be improved by this method. One of the main problems deteriorating the mechanical properties of CNT nanocomposite polymers is the weak mechanical bonding between the matrix and CNTs due to the atomically smooth surface of the nanotubes. Although CNTs have some surface defects such as different diameters and bending/twisting due to defects, the mechanical bonding of CNTs to the polymer remains a problem.

To solve this problem, micromechanical interlocks that prevent the nanotubes from sliding under load are utilized. These structures can be created in several ways.

### 3.1. Covalent functionalization

The attachment of functional groups to the surface of nanotubes can create covalent bonds with the matrix and

prevent sliding. Thus the paper [25] discusses covalent functionalization of CNTs, where oxidation of CNTs leads to the formation of various functional groups such as carboxyl, hydroxyl and epoxy groups on their surface. Covalent functionalization can be performed by anchoring reactive groups on the surface of both the polymer and CNTs, followed by their interaction (the “attachment” method), or by placing chemical groups (initiators) on the surface of the nanotubes followed by polymerization of the monomer directly on their surface (the “growing” method). Another example is the work [26], where the use of the rare earth element  $\text{LaCl}_3$  to modify CNTs is considered, which also led to the creation of covalent bonds between CNTs and epoxy resin in composites and improved the mechanical properties of the nanocomposite.

Fasanella and Sundararaghavan [27] used functionalized single-walled carbon nanotube as a reinforcement material through molecular dynamics simulations. This work used a dendrimer approach (Fig. 6), in which a thermoset resin was modeled as a single monomer cross-linked with a second layer of monomers around it, and so on. With the addition of fluorinated single-walled CNTs, they found that there was a significant improvement in the elastic modulus, while a decrease in the coefficient of thermal expansion was observed as the temperature increased.

Park and Yun [28] used molecular dynamics simulations to determine the shear modulus at the interface by applying a shear strain model between epoxy resin and functionalized graphene. They performed pull-out calculations to characterize the interface properties between graphene and cured epoxy resin, as shown in Fig. 7. The key finding is that when graphene is functionalized, the pull-out force moderately increases and the interface shear modulus decreases significantly. Similar conclusions can be attributed to CNTs in polymer.

The effect of chemical cross-links between a single-layer nanotube and a polymer matrix on the matrix-

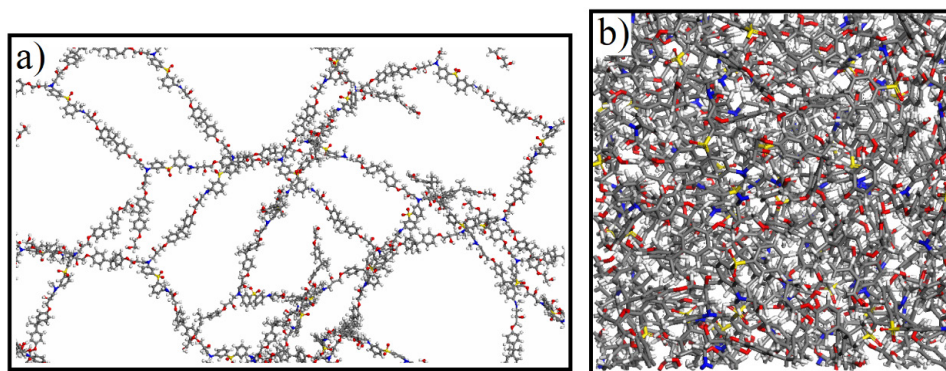


Fig. 6. The dendrimer structure before (a) and after (b) energy minimization. Adapted from Ref. [27].

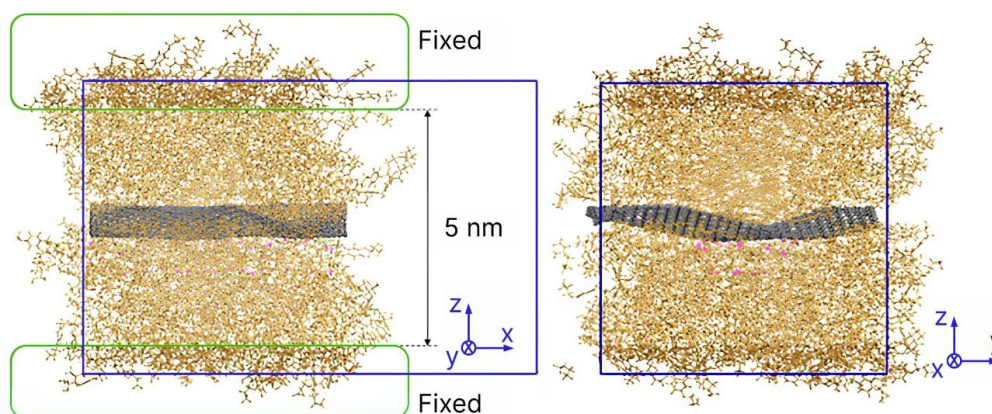


Fig. 7. Graphene/epoxy system for pull-out simulation. Adapted from Ref. [28].

nanotube shear strength was studied using molecular dynamics simulations [29]. A nanotube embedded in a crystalline or amorphous polyethylene matrix is used as a model for an unbonded interface (in the absence of cross-links). Modeling predicts that the shear strength and critical lengths required for load transfer can be increased and decreased, respectively, by more than an order of magnitude with the formation of cross-links involving less than 1% of the nanotube carbon atoms. At this level of chemical functionalization, calculations also predict that there is a negligible change in tensile elastic modulus for the nanotube.

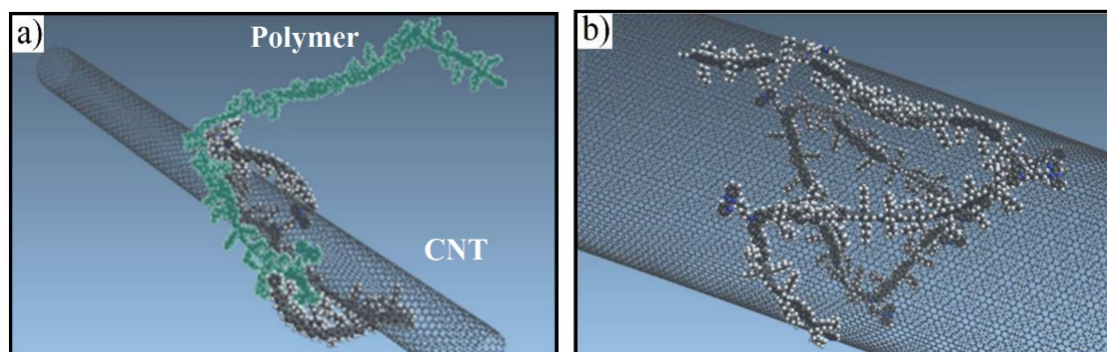
When synthesized nanotubes are used, composites often fail due to nanotube pulling out due to poor adhesion between the nanotube and the polymer matrix. However, chemically functionalized carbon nanotubes adhere more strongly to the polymer matrix due to efficient load transfer through the formation of chemical bonds between the polymer and nanotube. Hu et al. [30] investigated the chemical modification of carbon nanotube/polystyrene composites by polyatomic ion beam deposition using molecular dynamics simulations. Several composite structures and incident ion energies are considered. Simulation results show that modification by ion-beam deposition creates cross-links between otherwise unfunctionalized

nanotubes and polymer backbone chains, which serve to strengthen the composite. High incident ion energies and compact composite structures are predicted to be optimal for efficient chemical modification of the system.

### 3.2. Non-covalent functionalization

Molecules such as polymers or surfactants can adsorb on the surface of nanotubes and form physical interactions that prevent sliding. In Ref. [31], polyesters based on acetylenedicarboxylic acid were synthesized. In the study, the polyesters were used as a platform for copper-free cycloaddition reaction to introduce side functional groups (pyrene, pyrene/COOH, pyrene/OH and pyrene/C≡CH) using organic azides. These pyrene side groups interact non-covalently with the surface of multi-walled carbon nanotubes (MWCNTs) via  $\pi$ - $\pi$  stacking. The non-covalent functionalization via  $\pi$ - $\pi$  stacking improves the interaction between nanotubes and polymers, leading to improved mechanical properties.

The authors of Ref. [32] studied the interaction of polyfluorene and fluorene/carbazole copolymers containing various functional groups and side chains with small and large diameter—from 1.7 to 9 nm—CNTs in vacuum. Variable charge molecular dynamics simulations based on



**Fig. 8.** Adsorbed functional groups on the chain: (a) example of inter-chain steric hindrance for two polymers (initially on opposite sides relatively to the nanotube) on a 1.7 nm diameter, 20 nm long CNT, after 800,000 steps of 0.3 fs, i.e., 240 ps; (b) example of adsorbed geometry for the two same 30-monomers long P1 polymers (also initially on opposite sides relatively to the nanotube) on a 9 nm diameter, 20 nm long CNT, after 400,000 steps of 0.3 fs, i.e., 120 ps. Adapted from Ref. [32].

the ReaxFF reactive force field were used for the study. It was shown that the non-covalent functionalization of nanotubes is driven by  $\pi$ - $\pi$  interactions, effective for all polymers studied due to their conjugated main chain and independent of the presence of certain functional groups (Fig. 8). It is shown that adsorption of polymers on the nanotube sidewalls can be either complete—with the entire chain physisorbed—or partial—due to intra-chain torsion or inter-chain repulsion—depending on the initial geometry, the amount of polymers and the nanotube diameter. The ReaxFF force field and its available parameterization used for the simulations are validated through benchmarking and a review of higher-level quantum calculations—for simple interacting  $\pi$ - $\pi$  compounds consisting of polycyclic aromatic molecules adsorbed on a graphene sheet or bilayer graphene.

### 3.3. Embedded nanoparticles

The incorporation of nanoparticles such as aluminum oxide or boron nitride into the matrix can create obstacles for nanotube motion. Thus the effect of dispersion of aluminum oxide ( $\text{Al}_2\text{O}_3$ ) nanoparticles and graphene nanoplatelets (GNPs) on the mechanical properties of fiber and polymer reinforced composites (FRPs) has been recently investigated [33]. Both microstructural changes and mechanical behavior of the reinforced samples are investigated. This approach allows to confirm how the incorporation of nanoparticles into the matrix of FRPs can enhance the mechanical performance of composites. In Ref. [34], the use of hybrid nanocomposites based on MWCNTs and  $\text{Al}_2\text{O}_3$  to improve the mechanical properties of epoxy materials is discussed. It is especially observed that chemical hybridization of MWCNTs- $\text{Al}_2\text{O}_3$  via CVD process significantly improves the mechanical performance compared to physically mixed hybrid nanofillers. The effects of dispersion and agglomeration of nanoparticles on the mechanical properties of the composites

are also discussed in detail. This confirms that the inclusion of nanoparticles in the matrix (in this case MWCNTs and  $\text{Al}_2\text{O}_3$ ) can create barriers to the movement of nanotubes, affecting their dispersion and interaction in the composite. Despite the fact that experimental work has shown interesting results it is difficult to find works related to molecular dynamics on this topic, partly justified by the complexity of the computational process.

### 3.4. Structural modification of the matrix

Changing the morphology or structure of the matrix can result in the formation of mechanical interlocks, such as a porous structure or textured surface. However, most often, this is a parasitic phenomenon, but the chemical modification of polymers is of interest for practical applications.

Interesting work has been done using MD simulations of the interaction of a number of modified polymers (PS, PPA, PmPV and PPV) with CNTs in vacuum show that although all these polymers exhibit obvious attractive interactions with carbon nanotubes, the interaction between CNTs and the polymer is highly dependent on the specific structure of the monomer [35]. For polymer chains of comparable molecular weight but different monomer structure, intermolecular interaction energies were found to differ by up to 4 times. CNT-polymer interactions are the strongest for conjugated polymers with aromatic rings on the polymer backbone, since these rings are able to line up parallel to the nanotube surface and thus provide strong interfacial adhesion, this matrix modification is most interesting. In the presence of well-separated CNTs, the different polymer chains unravel and line up along the CNTs, covering the nanotube surface (envelopment). This is a general observation for all polymers studied; however, the effect is most pronounced for PmPV (Fig. 9.), which combines a certain flexibility in the main chain structure, flexible side chains and strong interaction with the nanotube surface.

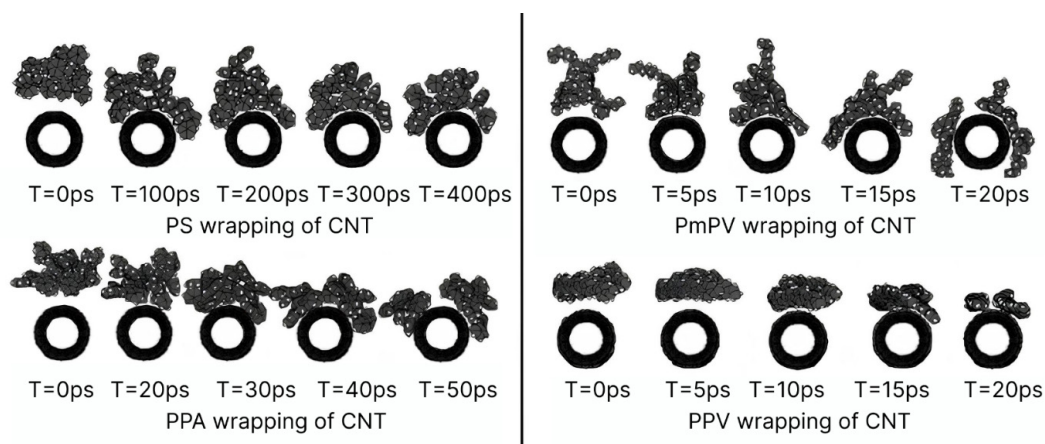


Fig. 9. Snapshots of MD simulations. Adapted from Ref. [35].

#### 4. CONCLUSIONS

This brief review covers experimental and molecular modeling work on mechanical loading optimization. The article describes methods for improving the bond between carbon nanotubes and a polymer, such as functionalization (covalent and non-covalent), reinforcement with embedded nanoparticles, and structural modification of the matrix. Although experimental work has shown interesting results, it is difficult to find work related to molecular dynamics on the topic of adding nanoparticles to a polymer with CNTs, which is partly justified by the complexity of the computational process. From the review, it is evident that covalent functionalization is one of the most common types of functionalization to improve the bonding between CNTs and polymer, preventing the sliding of nanotubes and optimizing/improving the mechanical properties of the composite.

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## Механические взаимодействия в полимерных материалах с углеродными нанотрубками: краткий обзор

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**Аннотация.** В этом кратком обзоре обобщены механические взаимодействия, происходящие в полимере с углеродными нанотрубками. Работа содержит подробное обсуждение методов, позволяющих улучшить механические характеристики полимерных композитов с углеродными нанотрубками для чего приводятся как экспериментальные, так и расчетные работы в этой области. В статье подробно рассмотрены такие методы улучшения связи углеродных нанотрубок с полимером, как функционализация (ковалентная и нековалентная), усиление внедренными наночастицами и структурная модификация матрицы. Обзор делает акцент на методе молекулярной динамики как одного из перспективных методов исследования механических взаимодействий в полимерных композитах с углеродными нанотрубками.

*Ключевые слова:* нанокompозиты; углеродные нанотрубки; полимеры; УНТ