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MOLECULAR DYNAMICS SIMULATION SHOWING THE INTERACTION BETWEEN MULTI WALLED CARBON NANOTUBE AND EPOXY RESIN / CURING AGENT

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ABSTRACT

Due to their exceptional outstanding characteristics, such as their extremely high young modulus, ultimate strength, and high electric and thermal conductivity, carbon nanotubes have attracted attention in the field of nanomaterials. As a result, carbon nanotubes are regarded as one of the best reinforcements for creating advanced nanocomposite due to their exceptional thermo-mechanical characteristics. Single-walled nanotubes and multi-walled carbon nanotubes have similar properties. But with multiwalled nanotubes, the outer walls can shield the interior carbon nanotubes from chemical reactions with outside substances (polymer, monomer, or any desirable substance). Multi-walled nanotubes have a higher tensile strength than single-walled nanotubes. To determine the molecular interactions between the MWNT/F-MWNT, Epon 862 (Diglycidyl Ether of Bisphenol F), and DETDA (Diethyltoluenediamine) curing agent molecules, molecular dynamics (MD) simulations were performed in this study using Material Studio 7.0. Epon 862 and DETDA were used to interact with MWNT, and the interaction energy was measured. The MWNT was further functionalized by adding hydroxy, amino, and carboxylic groups to its outer wall. The study provides interaction energy. The findings demonstrate that the resin's molecules interact with MWNT and F-MWNT in a desirable manner. The results also demonstrated that F-MWNT (Amine) and Epon 862 and DETDA curing agent molecules exhibit good wetting characteristics when F-MWNT is functionalized with Amine, which has a high favourable interaction with the resin molecule as well as with the curing agent molecule. In order to structurally connect the MWNT/F-MWNT and resin-curing agent structures and improve the load transfer between them, it may be possible to extend resin cross-link networks into the MWNT/F-MWNT cavities. This could lead to extremely strong composites for structural applications that are lighter, stronger, and tougher than any polymer-based material.

Keywords: Carbon nanotubes, nanocomposites, multi-walled carbon nanotubes, single-walled carbon nanotubes, tensile strength, molecular dynamics simulation, DETDA.

1. Introduction

Due to their structures, large surface area, and high aspect ratio for cutting-edge applications in composites, carbon nanotubes are regarded as the best material for reinforcement (Raman et al., 2010). Due to its common class of thermosetting curing agent's high tensile strength, high adhesion and dimensional stability, chemical and corrosion resistance, and other properties that make it suitable for use in the fields of aeronautics, astronautics, electronics, and other engineering applications, recent research has focused heavily on curing agent-based carbon nanotube composites. (Murari et. al, 2013 & Osaman, Shrivastava, 2001). However, CNT have poor

dispersion in polymer matrix due to agglomeration and also high surface area of CNT results in high viscosity of the composite of CNT and polymer (Berben et. al., 2000). Multi-walled nanotubes (MWNTs) are the ideal reinforcing material in the field of nanocomposite due to their distinctive atomic structure, high aspect ratio, and high tensile strength (Zhiyong et al., 2004). According to Arash et al. (2014), the interfacial interaction between CNT and polymer matrices greatly affects the mechanical properties of composites. Multi-walled carbon nanotube (MWNT) loading in curing agent of approximately 0.5 weight percent is thought to be sufficient for structural applications to produce high impact-resistant structures (Rodney & Donald, 1995). When 5 weight percent of MWNTs were ultrasonically dispersed in the EPON 828 curing solution, Schadler et al. and Thakre (1998, 2009) noticed a 20% increase in both the tensile and compressive moduli of an. According to Qian et al., elastic moduli increased by 42% and break stress by 25% when MWNT (1%) was disseminated in a polystyrene matrix (2000, 2001). Engineering appropriate dispersion and orientation of functionalized MWCNTs in curing agent remains a difficulty despite the success in functionalizing MWCNTs with desired chemical groups (Schlick, 2002). The covalent or noncovalent functionalization of MWCNTs, which enhances their interaction with solvents and/or polymers and improves their dispersibility, is a solution to this problem (Dujardin et al. & Raghvan et al., 1998, 2010). According to Arun et al. (2012), the organisation of hydrogen bonds in functional carboxyl groups has an impact on the mechanical characteristics of carbon nanotube fibres, and this effect is significant for both small and large diameter carbon nanotubes. Researchers Potschke et al. and Kinlock et al. looked on the improved dispersion of nanocomposites with functionalized CNTs (2002). Gou et al. (2004) concluded that functionalizing nanotubes, which can then be chemically attached to the chains of the cured epoxy resin molecule, may provide a robust interface on nanotubes. Further, Mohan et al. (2012) found a correlation between an increase in CNT structure defect and a decrease in CNT-epoxy nanocomposite. Fan et al. performed an MD simulation for triethylenetetramine (TETA)-curing cross-linked EPON 862 epoxy. He thoroughly described the MD simulation methods before figuring out the cross-linked network's Young's modulus and glass transition temperature (2007). As it is very challenging to conduct various types of experiments to research the interfacial properties of nanocomposites, atomistic simulation may be a valuable tool to investigate the interfacial reinforcement processes of nanocomposites (Zhu et. al. & Liao et. al., 2007, 2001). However, there hasn't been any documented direct proof of covalent interactions between modified CNT and epoxies. This is probably owing in part to the difficulty in isolating the reaction due to the comparatively low concentration of functional groups on the CNT surface when dispersed into the epoxy resin/curing agent mixture.

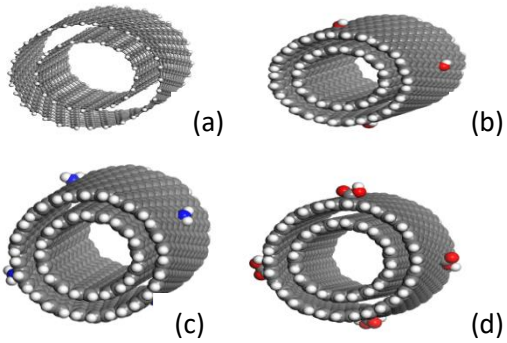
In this study, molecular dynamics (MD) simulations were run to determine how the molecules DETDA and MWNT/F-MWNT interacted. Based on the findings from the MD simulations, the wetting properties of the MWNT/F-MWNT and DETDA molecules were also investigated, which can help with the creation of CNT-based polymeric composites.The Material Studio 7.0 software programme, created by Accelrys Inc. (BIOVIA), was used to run MD simulations. The necessary force field calculations were carried out by the Material Studio 7.0 software's condensed phase optimisation molecular potentials for atomistic simulation studies (COMPASS) module. Condensed-phase properties of polymers and low molecular weight compounds were used to optimise this approach, which was parameterized using ab initio calculations of model compounds. Valence and non-bond components can be separated out of the overall potential energy determined by COMPASS. Cross coupling terms that are diagonal and off-diagonal are included in

the valence component. The bond stretching energy, angle energy, torsion energy, and out of plane deformation energy are further subgroups of the diagonal term. Bond-bond, angle-angle, angle-torsion, central bond-torsion, and terminal bond-torsion interactions are included in the off-diagonal cross coupling term. The columbic electrostatic interaction and the van der Waals energy of the Lennard-Jones function are both included in the non-bond potential energy term. Each MD simulation step typically had a 2 femto second (fs) interval. Using NVT ensembles (constant number of particles, constant volume, and constant temperature), all calculations were done at a starting temperature of 300 K.

2. Molecular model

2.1. Molecular model of MWNT/F-MWNT

Materials Studio was used to create the molecular models of MWNT and F-MWNT (Hydroxy, Amine, and Carboxyl). The finite length and diameter of the modelled MWNT were 24.60 and 13.56 respectively. The MWNT that was built had a structure of (10,10) and two concentric walls with a wall separation of 3.347 inches. By attaching functional groups such as hydroxyl, amine, and carboxyl to the MWNT's exterior wall, it was also functionalized. The interactions depicted in Fig. 1 were performed using the MWNT and F-MWNT molecular models. The carbon nanotube was modified by include hydrogen atoms at both ends to prevent the unsaturated boundary effect. C-C bonds were 1.42 in length and 1.10 in length for C-H bonds. Carbon atoms had a charge of -0.1268e and hydrogen atoms had a charge of +0.1268e. All four molecule configurations were subjected to energy minimization molecular mechanics in order to produce the lowest possible potential energy, which serves as the starting point for MD simulation. The geometry optimisation task of the forcite module was used to reduce energy.



g.1. Molecular model of (a)MWNT, (b)F-MWNT(Hydroxy), (c)F-MWNT(Amine), (d)F-MWNT(Carboxyl)

2.2. Molecular model of EPON 862

Epon 862 is a low molecular weight Bisphenol-F epoxy resin that has high mechanical qualities for use in composite applications and low viscosity. Bisphenol-F and epicholrhydrin are used in its production.The molecular model and chemical composition of Epon 862 resin are depicted in Fig. 2. In order to get the minimal potential energy, the resin molecule was additionally geometrically optimised using the forcite module. Under this minimum energy the molecule had approximate dimension of 8Å.

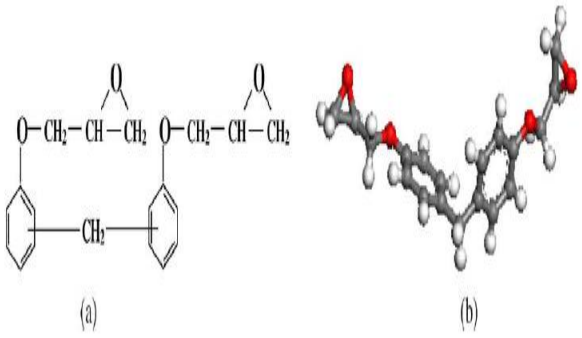


Fig.2. (a) Chemical structure and (b) Molecular model of Epon 862 epoxy resin molecule

2.3. Molecular model of DETDA curing agent

Diethyltoluenediamine, generally known as DETDA, is one of the main components of EPI-CURE curing agent W.The DETDA curative agent

molecule's molecular model and chemical composition are depicted in Fig. 3. In order to achieve the minimal potential energy, the curing agent molecule was geometrically optimised as well. The molecule's dimensions under this lowest energy were roughly 6.7Å ×6.5Å ×1.8Å.

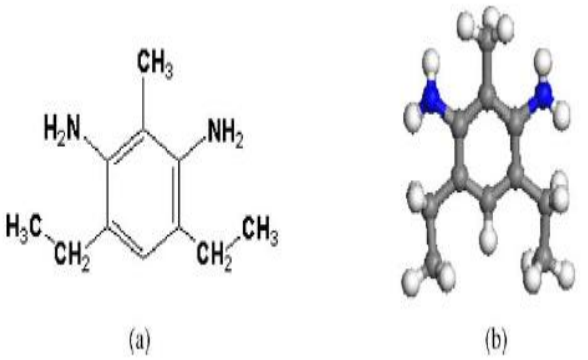


Fig.3. (a) Chemical structure and (b) Molecular model of DETDA curing agent molecule

3. Results and discussion

Interaction energy is calculated according to the following formula in Kcal/mol.:

$$E_{Interaction} = E_{Total} - (E_{MWNT/F\text{-}MWNT} + E_{Epon})$$

3.1. Interaction between MWNT and Epon 862 molecule/DETDA curing agent molecule.

The MD simulation model was created by first positioning the Epon 862 molecule at the side of the MWNT inside the cutoff distance of 10 of van der Waals interactions in order to mimic the interaction between the two molecules. The Epon 862 molecule had one end positioned close to the MWNT wall and the other end placed farther away. We can see in Fig. 4 that the atoms that were initially far from the MWNT wall gradually travel towards the wall based on the simulation results given in the snapshots. As the simulation came to a close, the resin molecule had a tendency to spirally wrap around the MWNT's surface until equilibrium was reached.

As demonstrated in Fig. 5, the interaction energy between the resin molecule and MWNT may be tracked. The Epon 862 epoxy resin molecule is moving towards the MWNT, as indicated by the negative interaction energy, as a result of an attractive force. Up to the system's equilibrium state, the interaction energy keeps going down. Based on MD simulation, the MWNT and Epon 862 resin molecule contact energy at the end of the simulation was 57 Kcal/mol.

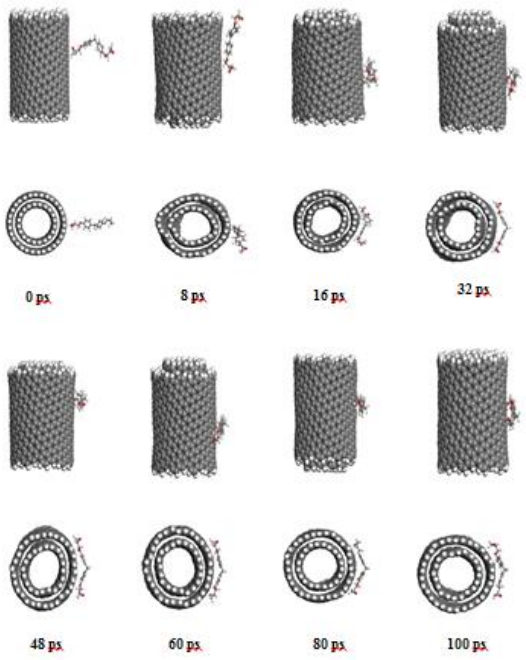


Fig.4. MD simulation snapshots of MWNT.

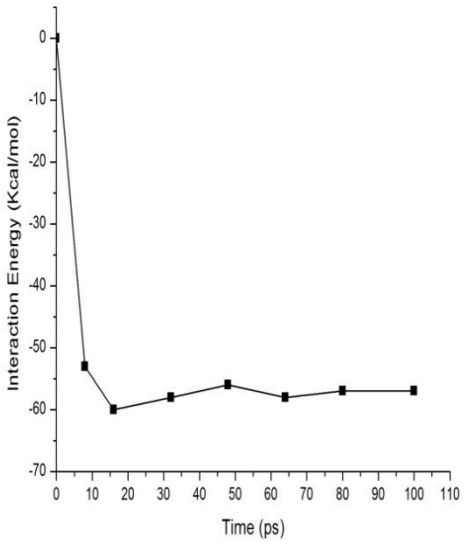


Fig.5.Interaction energy of the MWNT && Epon 862 epoxy resin molecule

Similarly interaction energy was calculated by running MD simulation between MWNT and DETDA curing agent molecule as shown in Fig.6.

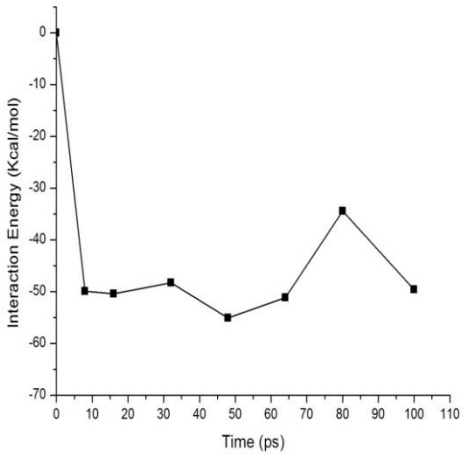


Fig.6. Interaction energy of the MWNT && DETDA curing agent molecule

3.2. Interaction between F-MWNT and Epon 862 molecule and DETDA curing agent molecule.

The same method was used to conduct the MD simulations of the interactions between Epon 862 resin and F-MWNT (Hydroxy, Amine & Carboxyl). Figure 7 displays the findings from the MD simulation. Fig. 8 shows the interaction energy between the Epon 862 epoxy resin molecule and the F-MWNT. According to the results of the MD simulation, MWNT functionalized with an amine group interacts with the environment more than MWNT functionalized with a hydroxyl or carboxyl group. Because Amine group and Epon 862 epoxy resin interact well, this is the case.

Similar MD simulations between MWNT/F-MWNT and the DETDA curing agent (EPICURE) were run, and the results showed that the MWNT functionalized with Amine group was having high contact with the DETDA curing agent. This interaction energy is illustrated in Figures 9 and 10.

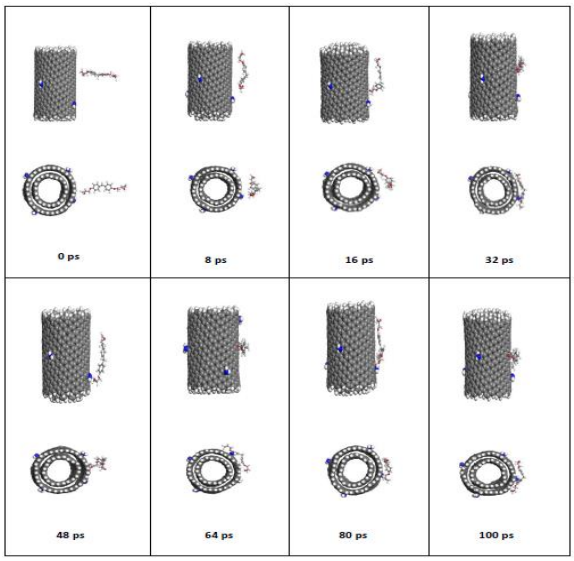


Fig.7. MD simulation snapshot of F-MWNT(Amine) & Epon 862 epoxy resin molecule interaction.

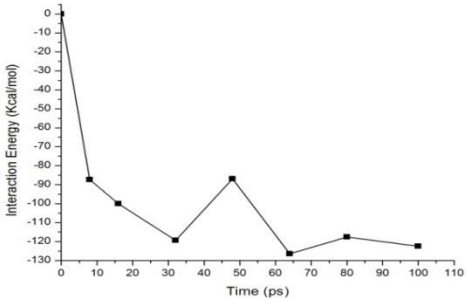


Fig.8. Interaction energy between F-MWNT(Amine) and Epon 862 resin molecule.

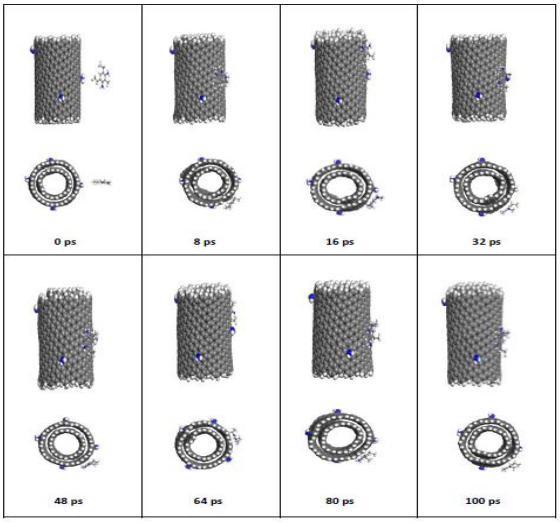


Fig.9. MD simulation snapshot of F-MWNT(Amine) &DETDA curing agent molecule interaction.

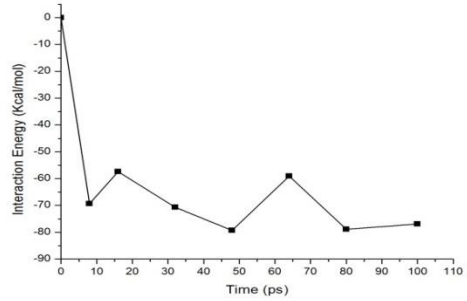


Fig.10. Interaction energy between F-MWNT(Amine) and DETDA curing agent molecule.

4. Conclusions

The chemical interaction between MWNT/F-MWNT and molecules of Epon 862 and DETDA curing agent was predicted using molecular dynamic simulations. According to the simulation results, MWNT and F-MWNT interact attractively and obviously with both Epon 862 and DETDA molecules. The outcomes also showed that MWNT exhibits extremely alluring properties with both Epon 862 and DETDA molecules when it is functionalized with Amine. It is reasonable to anticipate good wetting properties between MWNT/F-MWNT and Epon 862/DETDA molecules. In order to structurally connect the MWNT/F-MWNT and resin-curing agent structures and improve the load transfer between them, it may be possible to extend resin cross-link networks into the MWNT/F-MWNT cavities. This could lead to highly strong composites for structural applications that are lighter, stronger, and tougher.

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