Thermomechanical Properties of the Polymeric Nanocomposite Predicted by Molecular Dynamics

Majid Hadipeykani
Department of Mechanical Engineering, Khomeinishahr Branch,
Islamic Azad University, Khomeinishahr, Iran
E-mail: m.hadipeykani@gmail.com
mailto:Jmechanic@iaumajlesi.ac.ir

Farshid Aghadavoudi*
Department of Mechanical Engineering, Khomeinishahr Branch,
Islamic Azad University, Khomeinishahr, Iran
E-mail: davoodi@iaukhsh.ac.ir
*Corresponding author

Davood Toghraie
Department of Mechanical Engineering, Khomeinishahr Branch,
Islamic Azad University, Khomeinishahr, Iran
E-mail: toghraee@iaukhsh.ac.ir

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Abstract: A molecular dynamics simulation study is employed to investigate the elastic and basic thermal properties of thermoset polymer based nanocomposite sample reinforced by CNT. The COMPASS force filed was used to construct the simulation box. The simulation box contains the cured epoxy resin molecules obtained from cross linking process of DGEBA and DETA which were located around the CNT (10,10). NVT and NPT ensembles were performed to equilibrate the system and convergence of temperature, energy and density have been checked. The elastic constants of molecular sample of nanocomposite were determined based on stiffness matrix and compared with the molecular results of pure resin. The results show that the Young's modulus in the transverse direction of nanocomposite model is less than that in longitudinal direction indicating the transversely isotropic behaviour at atomic scale. Glass transition temperature (T_g) and coefficient of thermal expansion (CTE) were calculated through the linear fitting of density-temperature diagram for the CNT-reinforced nanocomposite model. Atomistic simulation results showed decrease in T_g and CTE comparing to the pure epoxy. Moreover, the simulation results were compared with the measured values and good agreements are observed.

keywords: CNT, Epoxy, Molecular Dynamics, Nanocomposite, Thermomechanical Property

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Biographical notes: Farshid Aghadavoudi is an assistant professor at the Department of Mechanical Engineering, Khomeinishahr Branch, Islamic Azad University, Iran. His current research interests include modelling of nanocomposites and molecular dynamics. **Majid Hadipeykani** is an MSc student of mechanical engineering at Khomeinishahr Branch, Islamic Azad University. **Davood Toghraie** is currently an associate professor at the Department of Mechanical Engineering, Khomeinishahr Branch, Islamic Azad University, Iran. His research interests focus on molecular dynamics simulation.

1 INTRODUCTION

1.1. Background

Polymer based nanocomposites are a class of novel materials that have great applicability in modern industries such as aerospace or biomedical engineering [1-6]. Predicting of the physical and mechanical properties of new materials is the important need of researchers because understanding the estimated values of these materials properties reduces cost of experimental test. However, numerical and analytical methods have been used for modelling and measuring the properties of nanocomposites by many researchers [7-10]. Molecular dynamics as a numerical method at atomistic scale have been successfully used to predict the mechanical and physical properties of complex organic and inorganic materials [11-12]. The fundamental properties of the polymeric materials such as Young's modulus, glass transition temperature (T_g) and coefficient of thermal expansion (CTE) have been calculated using the molecular dynamic simulations [13-16].

Epoxy as the thermoset polymeric matrix and carbon nanotubes (CNT) as reinforcement have been used in constructing the nanocomposites. Considering that the production of samples of these nanocomposites is time consuming and costly, material modelling should be used to obtain the optimum properties [11]. Due to the phenomenon of cross linking, atomistic modelling of the thermoset polymers and curing agent atoms have computational challenges [17]. Moreover, the interfacial bonding between CNT and surrounding polymeric matrix effects on the thermomechnical nanocomposite properties, which may be modelled accurately in molecular dynamics simulations [18]. It is noteworthy that despite the high mechanical properties of CNT, the experimental results did not show a significant increase in nanocomposite properties compared to pure polymers [11], [19]. Consequently, modification factors should be used to relate the experimental measurement to simulation results [11].

1.2. Pervious Works

Many researchers have used molecular dynamics simulations for modelling the behaviour of the materials. Kafash et al. studied the temperature's effect on the properties of cubic and cylindrical shapes atomistic model using molecular dynamics simulations [20]. Moreover, they used 2D molecular model to find the effects of force on AFM cantilever's tip. Aghadavoudi et al. investigated the CNT defects on longitudinal and transverse Young's moduli of nanocomposite models by molecular dynamics [21]. They concluded that the CNT defects significantly affect the elastic modulus in the transverse direction. Based on their simulation results correction factors must be used for predicting the mechanical properties by micromechanical theories at nano scale. The multiscale method is one of the ways in which it is possible to convert the molecular results into micromechanical results based on experimental values[11]. Moradi and co-worker used multiscale modelling with molecular dynamics (MD) simulations in nanoscale and Halpin-Tsai equations to calculate the elastic constants of the nanocomposite reinforced by defected CNTs [22]. They studied the stress distribution and deflection in sandwich plates with functionally graded nanocomposite using a first order shear deformation theory (FSDT) based mesh-free method. Farhadinia et al. investigated the characteristics of a polymer-based nanocomposite by molecular dynamics [12]. They have constructed a molecular model by embedding the CNT in a polycarbonate matrix and estimated the elastic constants employing the constant-strain method. They observed a significant increase of about 50% in elastic moduli with addition of 6.9wt% CNT to polymer.

Fasanella et al. performed a molecular dynamics study to calculate the thermomechnical properties of epoxy based nanocomposite reinforced by functionally and pristine CNT [13]. They used CVFF force field and obtained the coefficient of thermal expansion and stiffness of molecular model. According to their simulations, increases in stiffness and decreases in the CTE were observed when CNT was added to epoxy. Yang et al. studied the mechanical properties and thermal conductivity of carbon nanobud (CNB) reinforced DGEBA/MTHPA composite using atomistic modelling [23]. Based on their results, the T_g value of the DGEBA/MTHPA/FCNBs increases by 34.3% comparing to the pure matrix, whereas the improvement of the thermal conductivity was limited. Koloor et al. performed a non-equilibrium molecular dynamics simulation to study the effect of CNT length on the stiffness of the nanocomposites models [24]. The results showed that the reinforcing efficiency of the CNT decreases with decreasing its length. They derived an equation to predict the accurate elastic modulus of nanocomposite which was validated by some experimental tests.

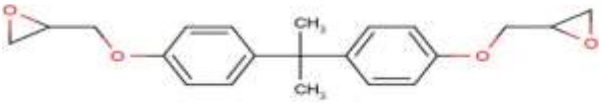
1.3. Objective of the Study

As mentioned above, limited studies have been performed on molecular modelling of CNT-reinforced epoxy based nanocomposites. Particularly, to the best of authors' knowledge, there has not been a molecular dynamics modelling to investigate the themomechnical properties of DGEBA/DETA based nanocomposites reinforced by armchair CNT. In this paper a molecular dynamics simulation is conducted to estimate the thermomechnical properties of a CNT-reinforced epoxy based nanocomposite model reinforced by CNT (10,10). Firstly, a molecular dynamics model for cross-linked epoxy was constructed and the repressive molecules of cured network were selected to create the nanocomposite model. The stiffness matrix and Young's and shear modulus as elastic properties and T_g and CTE as thermal specifications were calculated using the simulation results. The validity of the thermomechanical properties results was verified by comparing to experimental and simulation results for neat resin which are available in literatures.

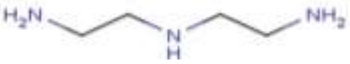
2 MATEIRAL AND METHOD

2.1. Materials

In this study, a nanocomposite molecular structure composed of cured DGEBA as matrix and CNT (10,10) as reinforcement was modelled using molecular dynamics. The molecular structures of DGEBA ($C_{21}H_{24}O_4$) as base resin and DETA curing agent ($C_4H_{13}N_3$) are illustrated in "Fig. 1" [25]. The epoxide group of DGEBA and reactive sites in DETA molecules may react in curing process. In curing process of DGEBA, as shown in the "Fig. 2", strong covalent bond was performed between epoxy and hardener atoms which is known as cross-linked network.



(a)



(b)

Fig. 1 Molecular structures: (a): DGEBA and (b): DETA [25].

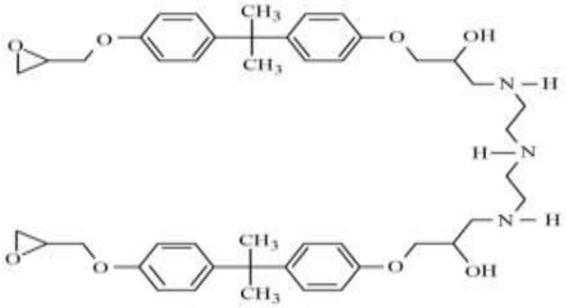


Fig. 2 Cross linked epoxy resin DGEBA/DETA.

In order to simulate cross-linked epoxy polymers using the MD method, a dynamic approach including minimization, equilibration, and bonding has been employed [21]. After verification of the atomistic polymer structure, a representative cross-linked molecule that has a certain degree of cross linking is selected to construct the simulation box of two-phase nanocomposite. As illustrated in Fig. 3, the CNT (10,10) molecule has been embed in the cross-linked epoxy networks along z direction. For atomistic modelling, a rectangular box of size 54 ×54×23 Å^3 have been considered.

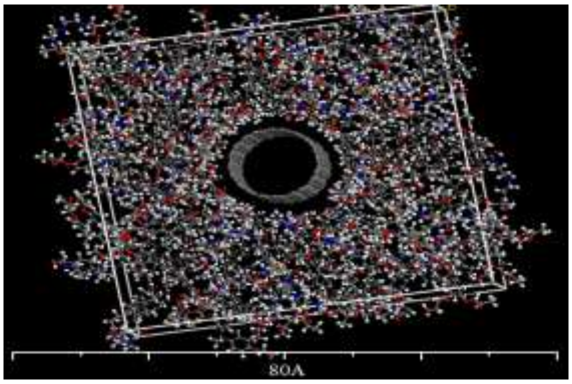


Fig. 3 Composite simulation box of CNT+ DGEBA/DETA.

2.2. Force-Field

The Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies (COMPASS) as an appropriate force-field for polymers [25-26] was employed in this study. In compass force-field, the energy potential function E_t includes the valence energy, cross-coupling energy and non-bonded energy as follows [8]:

$$E_t = E_{valence} + E_{cross} + E_{non-bond} \tag{1}$$

$$E_{valence} = E_{bond} + E_{angle} + E_{torsion} + E_{out-of-plane} \tag{2}$$

The terms of energy in equations (1) and (2) are:

$$E_{bond} = \sum_b [K_2(b-b_0)^2 + K_3(b-b_0)^3 + K_4(b-b_0)^4] \tag{3}$$

$$E_{angle} = \sum_\theta [H_2(\theta-\theta_0)^2 + H_3(\theta-\theta_0)^3 + H_4(\theta-\theta_0)^4] \tag{4}$$

$$E_{torsion} = \sum_\emptyset [V_1\{1-\cos(\emptyset-\emptyset_1^0)\} + V_2\{1-\cos(2\emptyset-\emptyset_2^0)\} + V_3\{1-\cos(3\emptyset-\emptyset_3^0)\}] \tag{5}$$

$$E_{out-of-plane} = \sum_\chi K_\chi \chi^2 \tag{6}$$

In above equations, V_i, H_i, K_i are dependent parameters of system which have been achieved from ab-into quantum mechanics calculations [26]. The term of b-b exhibits the length of the two neighbors' bond from the equilibrium state. $\theta, \emptyset$ and χ are angles of bond, dihrealtorsion, out of plane respectively. The E_{Cross} includes several terms that have been described in literatures [27-28]. The $E_{non\text{-}bond}$ includes the Coulomb and Van der Waals potentials. The latter is expressed by the following equations:

$$E_{non-bond} = E_{Van\ der\ Waals} + E_{Coulomb} \tag{7}$$

$$E_{Vander\ Waals} = \sum_{i>j} D_0 \left[2\left(\frac{r_{ij}^0}{r_{ij}}\right)^9 - 3\left(\frac{r_{ij}^0}{r_{ij}}\right)^6 \right] \tag{8}$$

$$E_{Coulomb} = \sum_{i>j} \frac{q_i q_j}{\varepsilon r_{ij}} \tag{9}$$

Where, D_0 and ε are Lenard-Jones and dielectric constants and q is the atomic electrical load. In this study, for the purpose of calculating Van der Waals and Coulomb potentials, the cut-off distance of 10Å was used.

2.3. Simulation Details of Nanocomposite

A simulation box has been built with CNT (10,10) surrounding by cured epoxy molecules. The mole ratio of epoxy resin and curing agent molecule was selected as 2:1based on experimental results [11], [25]. In this step, the density was set at 1 g/cm^3 and the temperature was fixed at 298 K. In the packing process, geometry optimization was used by a smart algorithm. The dynamic process and optimization subjected to the system can be divided into the following steps:

Step A: Geometry optimization and energy minimization were applied to molecular structures using a smart algorithm which is a cascade of the steepest descent, ABNR, and quasi-Newton methods to reach the nearest local minimum with convergence tolerance of 10^{-4} (kcal/mol).

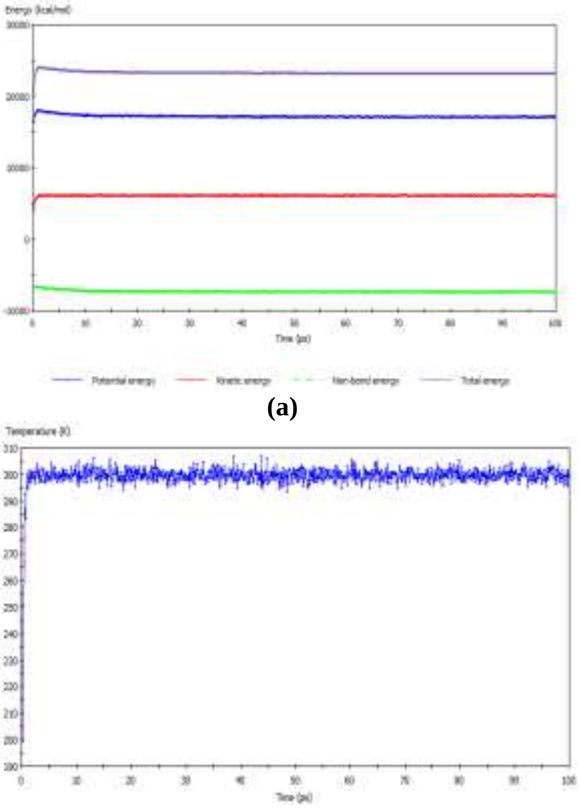
Step B: The system was equilibrated using NVT (isothermal-isochoric) dynamic simulation for 100 ps at a high temperature of 600 K (above curing temperature) using a time step of 1 fs to give adequate kinetic energy to molecules. The initial density was set at 1 g/cm^3 in this step.

Step C: NPT (isothermal-isobaric) ensemble was used to achieve the final density of simulation box for 100 ps with a time step of 1 fs at a pressure of 1 atm and a temperature of 298 K. In NVT and NPT ensembles, Berendsen thermostat and barostat were used for controlling the pressure and temperature during the equilibrium process. In order to eliminate the surface effects, periodic boundary conditions were employed. In both ensembles, 100 frames of dynamic atom configurations were saved as the trajectory files for computing the average properties of molecular structures.

3 RESULTS AND DISCUSSION

3.1. Energy and Density at Equilibrium

Statistical calculations on the molecular sample were performed to verify the equilibrium of atomistic structure after molecular dynamics simulations. The variation of energy terms and temperature during NPT calculations are illustrated in “Fig. 4”.



(a)

(b)

Fig. 4 Variation of: (a): energy terms and (b): temperature during NPT.

As can be shown in “Fig. 4”, the temperature was controlled at 300K and the energy fluctuations are very small less than 5% of the final value. Based on the results, it can be assumed that the system has reached a state of equilibrium.

Figure 5 Shows the variation of average density of molecular composite model during NPT. The final density equilibrated at 300 K is about 1.12 g/cm^{3}which is close to the values obtained in the previous MD simulations.

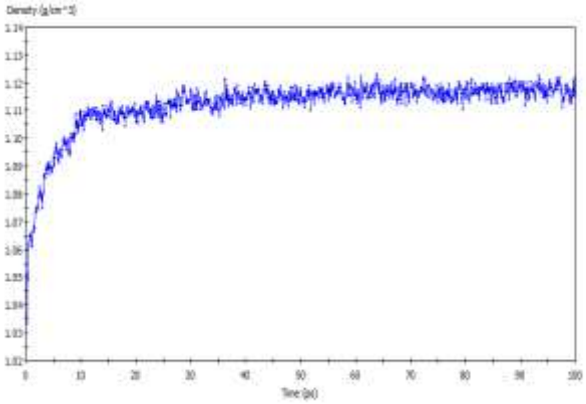


Fig. 5 Variation of density during NPT calculations.

3.2. Mechanical Properties

Constant-strain minimization method was employed on the simulation box to determine nanocomposite elastic constants. For this purpose, three-dimensional normal and shear strains with the same magnitudes were applied along the three principal axes of the unit cell. The maximum strain magnitude was set at ±0.003 to avoid nonlinearity of nanocomposite due to large strains. The stress components at the atomic level, for deformed configuration, were determined under these loadings. Based on Hooke's law for an elastic material, using Voigt notation, the stiffness matrix components, C_{ij}, can be calculated using:

$$\boldsymbol{\sigma_i = C_{ij}\varepsilon_j} \tag{10}$$

Where, σ_i are the six independent components of the stress tensor, and ε_j are the six strain components. For a specific strain vector, the stress components are calculated using molecular dynamics simulations and substituted in “Eq. (10)” to determine the stiffness matrix components, C_{ij}. Based on Voight notation, five independent elastic constants are required to calculate the elements of the stiffness matrix of the transversely isotropic nanocomposite. The stiffness matrix for the molecular sample is as follows:

$$C_{ij}\,(GPa) = \begin{bmatrix} 3.8 & 1.2 & 1.1 & -0.0 & 0.2 & 0.2 \\ 1.2 & 3.0 & 1.5 & 0.4 & 0.0 & 0.2 \\ 1.1 & 1.5 & 47.1 & 0.0 & 0.3 & 0.4 \\ -0.0 & 0.4 & 0.0 & -0.0 & 0.0 & 0.1 \\ 0.2 & 0.0 & 0.3 & 0.0 & 2.3 & 0.1 \\ 0.2 & 0.2 & 0.4 & 0.1 & 0.1 & 1.11 \end{bmatrix}$$

As can be seen in the above matrix, the results indicate that the nanocomposite sample is nearly transversely isotropic. Also, note that the CNT strengthening effect is observed in the z-direction since C_{33} is much larger than the other diagonal components of the stiffness matrix. Using these results, the other mechanical properties such as Poisson's ratio, Young's and shear moduli were determined for the nanocomposite sample in “Table 1”.

Table 1 Mechanical properties of the nanocomposite and the pure epoxy molecular models

Mechanical properties	Nanocomposite (Current study)	Pure epoxy [30]Ref.
Longitudinal Young's Modulus(GPa)	47.1	3.4
Transverse Young's Modulus(GPa)	4.1	3.4
Shear Modulus(GPa)	4.0	1.3
Poisson's Ratio	0.22	0.32

These values were compared to the mechanical properties of pure epoxy obtained from molecular dynamics. As can be observed, the Young's modulus of composite molecular model, along main axis, is about 10 times higher than pure resin. However, according to the experimental investigations, adding CNT to pure resin may increase about 10 percent in Young's modulus [11]. Over predictions of Young's modulus for molecular dynamics simulations of nanocomposite have been observed by other researchers because in molecular models, macroscopic phenomena such as waviness and agglomeration and distribution of CNT have not be considered [11], [29].

3.3. Glass Transition Temperature (T_g) & Volumetric Thermal Expansion (CTE)

The glass transition temperature (T_g) is the temperature that nanocomposite’s state changes from hard and glassy to the soft and rubbery. In order to compute the T_g by molecular dynamics simulation, the NPT ensemble is employed at various temperatures, and density values of the systems have been achieved at each temperature. Reducing the temperature increases the density. At the T_g temperature, there is a change in the gradient of the density line, which interpolates the density values.

Variations in the density with the temperature for nanocomposite is shown in “Fig. 6”. The mass density is decreased from 1.119 gr /cm^3 at 250K to 1.091 gr /cm^3 at 550K. Using the linear fitting for density values temperature, two lines with different slopes are plotted as illustrated in “Fig. 6”, The intersection of these two lines determines the T_g. For nanocomposite, the T_g was obtained about 365K. The values of T_g for nanocomposite and pure epoxy have been compared in

“Table 2”. As can be observed, adding CNT to epoxy matrix decreases the T_g.

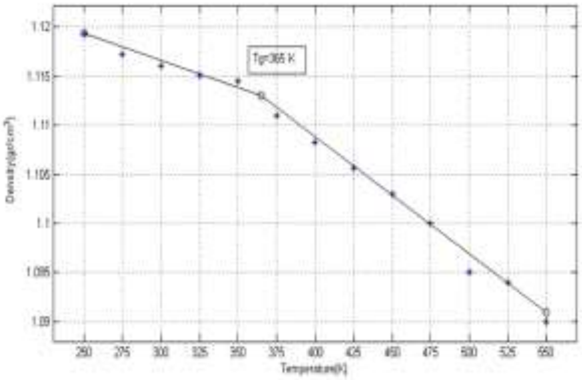


Fig. 6 Variation of the density as a function of temperature for nanocomposite sample.

Table 2 Glass transition temperature (T_g) and Coefficient of thermal expansion (β_1 and β_2) of nanocomposite and pure epoxy obtained from MD simulation

Thermal properties	Nanocomposite (Current study)	Pure epoxy [Reference No.]
T_g (K)	365	396 [25]
β_1 (below of T_g)(1/K)	49×10^{-6}	180×10^{-6}[31]
β_2 (above of T_g)(1/K)	108×10^{-6}	600×10^{-6}[31]

The coefficient of thermal expansion (CTE) as one of the most important thermal properties of materials is defined as follows [19]:

$$\beta = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \tag{10}$$

Where β is the coefficient of thermal expansion, V is the volume of the system, T is the temperature and P is pressure. In order to calculate the coefficient of thermal expansion, the volume of the system from MD simulation boxes in different temperatures from 250K to 550K was obtained. Figure 7 shows the volume changes of the cell structure as a function of the temperature which are given at glassy and rubbery state of the nanocomposite. As can be seen in the “Fig. 7”, with decreasing the temperature, the volume change has been decreased linearly. Moreover, the change in the slope of the curve is assigned to T_g. Using the linear regression, y=ax+b, at the temperatures above and below T_g, the volumetric coefficients of thermal expansion were determined by “Eq. (10)”.

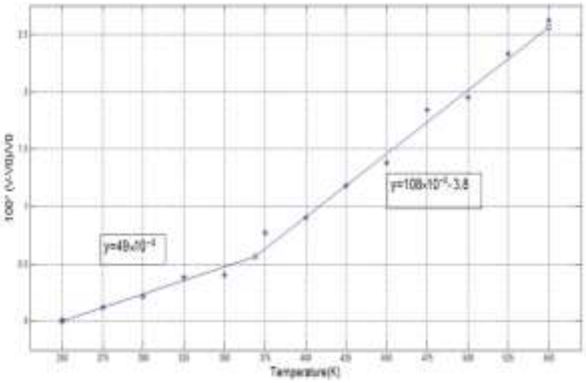


Fig. 7 Volume changes of simulation box of nanocomposite as a function of temperature and the two fitted straight lines.

The two slopes of the curves intercepts at the glass transition temperature and two values of the nanocomposite CTE for the glassy and rubbery state were obtained and listed in “Table 2”. Furthermore, “Table 2” shows that the CTE values for nanocomposite models at above and below of the T_g are less than those for pure epoxy.

4 CONCLUSIONS

Mechanical and thermal properties of epoxy based nanocomposite atomic sample were evaluated using molecular dynamics simulations. A cross-linked network of DGEBA and DETA molecules was constructed employing the COMPASS force field. The CNT (10,10) have embedded along axis of simulation box filled with cured epoxy molecules. After relaxation process, the equilibrium state was confirmed considering the density and temperature convergence during molecular dynamics simulation.

After equilibrium process, the mechanical properties of nanocomposite molecular sample were determined using constant strain method. The results show the transversely isotropic behaviour of the nanocomposite sample. The consistency of the simulation was validated through comparisons with pure resin simulation results. The longitudinal Young's modulus of molecular model was determined about 47GPa showing the large increase in stiffness compared to the neat resin. The glass transition temperature of nanocomposite was estimated as 365K which is lower than that for pure epoxy. Finally, the volumetric thermal expansion of polymeric based composite has been determined and good agreements are observed comparing to other simulation or experimental results in literatures.

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