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Research Article

Interfacial Characteristics of Graphene/Polymer Nanocomposites by Molecular Dynamics Simulation and Evaluating Effects of that on Mechanical Properties of Nanocomposites by FEM

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ABSTRACT

Nanocomposites are advanced materials that have excellent properties. For good usage of this material, it should be studied in detail. There is a phase between matrix and filler that is called interphase and also the properties of nanocomposites depend on the properties of that phase in addition to the matrix and filler. In this study, at first, the mechanical properties of the interphase of graphene/epoxy nanocomposite are extracted by molecular dynamic simulation and then by a Python code that is developed by the author and can be run by Abaqus, the best orientation distribution of fillers in RVE (representative volume element) according to weight percentage of fillers is predicted. The selection of graphene sheets as fillers has two important reasons the first is that graphene derivatives are the strongest materials compared to other materials in nature and the second reason is that the graphene sheet has a more active surface than other derivatives of that such as fullerene and nanotubes that causes more interphase zone formation that causes improvement of properties. The force field that is used in this study is DREIDING. For detection of the size of the interphase zone, the density distribution figure is used. The boundary conditions in RVE and the simulation box in all directions are periodic.

1. Introduction

Nowadays nanoscience is very applicable and a newfound technology. This technology consists of many branches like mechanics, chemistry, polymer, etc. To do significant work in this technology the researchers should have abilities in the mentioned knowledge. The results of these kinds of studies have usages in engineering branches such as electronics, aerospace, civil, etc. For success in this case of knowledge, the researchers should use the former scientists. Nanocomposites that consist of carbon structures and polymeric matrices, specially those kinds that are constructed from carbon nanotubes or graphene sheets, have attracted much attention to many functions of them. Despite traditional composites, nanocomposites without consideration of a phase that relates the filler to matric show a significant difference in their modeling of them [1]. After many tests on polymeric matrices with fillers like nanoparticles

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and nanotubes, the results showed that these fillers could be used for the improvement of mechanical properties of Nanocomposites that have many functions in wide aspects of engineering. Nowadays because reduction of weight of structures has been so important, these kinds of materials (nanocomposites) are so valuable for the edge of science studies. The modification of nanofillers in these studies will be so important and cause improvement in mechanical properties. Because of small dimensions, the usage of lab studies can not be very feasible and so the usage of computer simulation of MD (molecular dynamics) is bolded [2]. Among many kinds of fillers, graphene sheets have attracted attention because of their good mechanical, thermal, electrical, etc properties. Aradhana et al. [3] 2018 studied the effects of the addition of graphene oxide with zero to one percent loading on the adhesion strength of nanocomposite glued with an epoxy matrix. They show that reinforced glues with 0.5 % graphene oxide cause an increase of tension strength of about 30.7 % with respect to pure epoxy glue. Kernin [4] et al. 2019 studied the electrical and mechanical properties of nanocomposites with fillers of graphene oxide. They claimed that in reinforcement with a low amount of loading, the material that consists of graphene oxide as filler and epoxy as the matrix will have good electrical conduction and mechanical strength. Salom et al. [5] 2020 made two different kinds of nanocomposites: one of them consisted of fillers of functionalized graphene and pure graphene with epoxy as matric for both of them. They measured the Young modulus and deformation in rupture and mechanical strength and toughness of the nanocomposites. They showed that the Young modulus of the nanocomposites with 6 % weight of graphene as filler compared to the pure epoxy shows 40 % improvement. One of the reasons for epoxy usage is that they are corrosion which is not seen in fillers like graphene. It has been concluded that additives for matrices with a scale of nano, such as nanotubes, nanosheets, and nanoparticles, are good for enhancing many properties of nanocomposites with polymer base [6-10]. Jux et al. [11] introduced his hypothesis that reports the chemical crosslink between matrix and filler causes a decrease in crosslink density of matrices near the filler. In the case that we know the mechanical properties of matrix and fillers, some tests have been made that produced an analytical model such as the Hashin-Shtrikman model [12], or Mori-Tanaka model [13] that they can be combined and conclude the effective properties of interphase as e.g described in [14-17]. These analytical methods can not predict the interphase properties accurately and also they can not describe the gradient of these properties in the interphase of filler and matrix. The good modeling of interphase can be more accurately simulated by the FEM method and the FEM method can be used as a more accurate model than analytical methods as presented by Qiao and Brinson [18] and Bondioli [19]. Despite the recent developments in tests of mechanical properties of nanocomposites on a nanoscale, such as microscopy of atomic force [20], experimental methods can not model the direct modeling and measurement of properties of interphase [21]. There are many numerical studies of interphase mechanical properties. Shin et al. [22] studied the properties of interphase of nanocomposites of silicon carbide/polypropylene including effects of agglomeration. Some other studies showed similar approaches [23-25].

In our study, we develop a Python code that can be run by Abaqus software and predicts for each specific weight percentage which orientation distribution of fillers is the best according to mechanical behavior and properties. Instead of fullerene and nanotubes their inner surface is not active and can not form interphase, the graphene sheets are used.

2. Simulation Details

For extracting accurate results with low computational cost and with low effects of size in the simulation of RVE(representative volume element) and simulation box some assumptions are used in this study the most important assumption is that both RVE and simulation box are designed in which they are periodic in three orientations. Another assumption is that instead of adding interphase young modulus distribution we use the average young modulus of interphase.

2.1. Structure of Epoxy that is used in this Study

The structure of figure 1 consists of one cluster of DETA and four clusters of DGEBA that are connected to DETA. Number of each epoxy molecule is 216. As is depicted in figure 2 the link of N-H in cluster DETA and O-H in cluster DGEBA breaks and then a linkage of N-C is created and one cluster of DGEBA is connected to the DETA cluster and in the same manner the other three clusters of DGEBA connects to DETA. In the packing process, 40 clusters of crosslinked epoxy are assumed as simulation box that consists of 8640 atoms and then this box is replaced on both sides of the graphene plate the number of atoms of graphene is 1008 and the total number of simulation box atoms is 18288 [26].

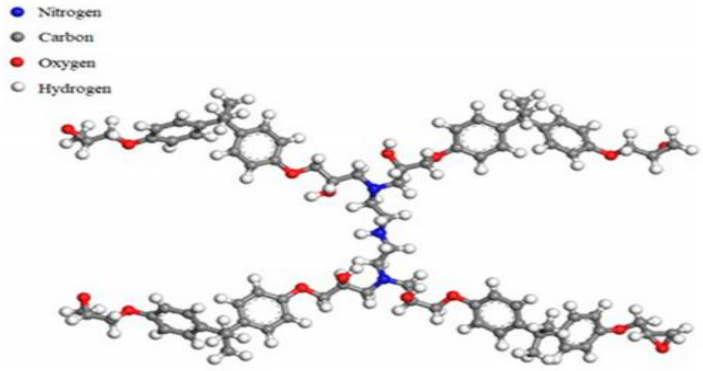

Fig. 1. Structure of epoxy that consists of nitrogen, carbon, oxygen, and hydrogen atoms[26]

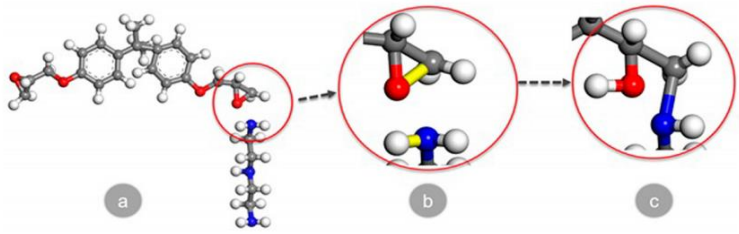

Fig. 2. Crosslinking process of a carbon atom at the end of one cluster of DGEBA with a nitrogen atom in the DETA cluster [26]

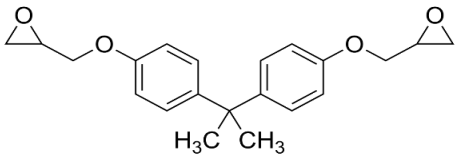

Fig. 3. chemical formulation of the DGEBA ($C_{21}H_{24}0_4$) [26]

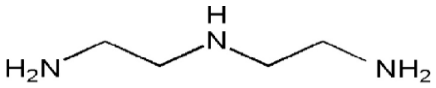

Fig. 4. chemical formulation of the DETA ($C_4H_{13}N_3$) [26]

2.2. Annealing and Relaxation

For uniform and homogeneous distribution of epoxy clusters, a simulation box from the annealing process between upper and lower temperatures in many cycles is used and this process ends by relaxation at room temperature the result is shown in Figure 5.

The lower temperature is about 100 kelvins and the upper temperature is about 600 kelvins. The time interval of each annealing process is about 50 picoseconds. The coordinate axes and simulation box in four sights are depicted in Figure 5 Reason for choosing the upper and lower temperatures is that the temperature should not be so low that the internal energy tends to zero and should not be so high that the structure of the simulation box deforms very high. This process consists of 14 stages. The cooling rate of this process is 10 K/ps.

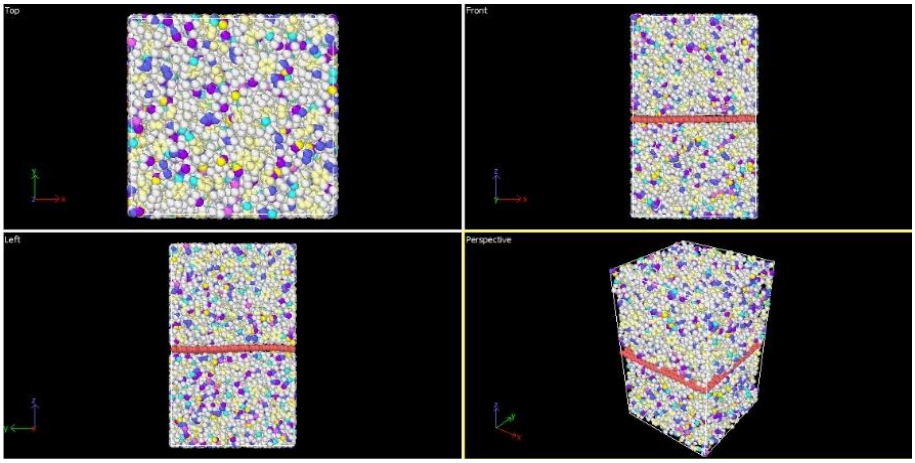

Fig. 5. Structure of simulation box after complete relaxation process

2.3. Simulation Process Explanation

The time duration In this simulation in the condition that in the NVT (ensemble with constant volume, temperature, and materials) ensemble that volume and temperature are constant and the time step is one femtosecond is 100 ps and for a condition that ensemble is NPT (ensemble with constant pressure, temperature, and materials) and the timestep of 1 femtosecond, is about 100 picoseconds. Pressure in NPT is set to zero atm. For simulation, DREIDING potential is used that is so suitable, easy to use, and practical. This potential of DREIDING is used by the advice of reference [27]. In these references, the reason for choosing this potential is described that is simple and practical.

2.4. Geometry of the Box of Pure Epoxy after Relaxing and Annealing

In the figure configuration of the pure epoxy box after the annealing and relaxing process is depicted. For uniform and homogeneous distribution of epoxy clusters in a box of pure epoxy from annealing, the relaxation process at room temperature is used. The upper and lower temperature of annealing is the same as before and the relaxation temperature is the room temperature (300 K).

2.5. Effect of Strain Rate on Results of Uniaxial Tensile Behavior

For more accuracy, the effect of strain rate is brought from reference 26 that this parameter has a negligible effect on the accuracy of results.

Table 1. Effect of strain rate on the result of uniaxial tensile test simulation [26]

Strain rate (S^{-1})	C_{11} (GPa)
10^9	93.099
10^8	92.48
10^7	92.32

2.6. Size and Boundary Conditions

In both the MD simulation and the FEM (finite element method) simulation we designed and programmed the simulation box and RVE that are periodic through the three orientations that helped us to extract good results with acceptable accuracy.

3. Results and Discussion

Graphene is not corrosion proof and also epoxy is not strong enough. It is concluded the simultaneous usage of both of them helps us to reach a strong material that is corrosion-proof.

There are three major novelties in our research: the first and the most important is that we programmed a code with Python language for each weight percentage and each filler orientation distribution predicts which orientation distribution for the specific weight percentage and loading direction is better. The orientation distribution is divided into two major types: 1- Regular and 2- Irregular. The regular one is also divided into two cases, the first case is the orientation distribution of the filler's surface that is perpendicular to the loading direction and the other type of Regular orientation distribution is which the orientation distribution of the surface of fillers is parallel to the loading direction. The irregular distribution is just one type.

The second novelty is that I used graphene plates as filler which is better than fullerene and nanotubes because its active surface is more than the fullerene and nanotube helps us to have more interphase zone that interphase zone helps to have a nanocomposite with stronger mechanical properties.

The third novelty is that we use a combination of epoxy which is corrosion proof and graphene which is a material with high strength properties that helps us to have a material that can be used in some industries such as marine and others that we need to a material that is corrosion proof and also strong.

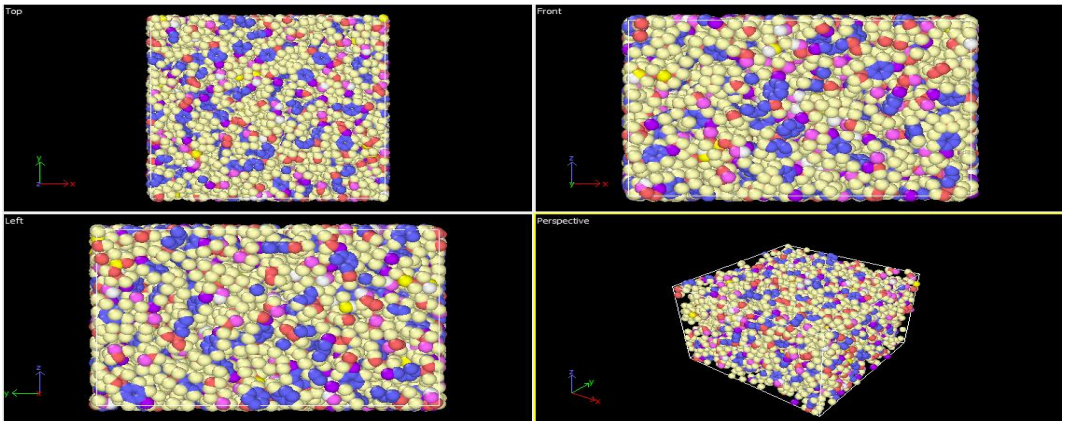

Fig. 6. Pure epoxy box after the annealing process

In this study for the calculation of density and Young's modulus the cell for simulation is divided into 0.05 bins in the thickness of it [1]. The applied boundary condition is periodic in all directions causing uniform distribution of atoms in the cell and is subjected to tension by starting the tension by increasing the magnitude of the displacement from zero to a specified magnitude and according to the stress-strain curve for each bin Young's modulus is obtained. This research is done for the prediction of RVE properties such as specific configuration that contains the best orientation distribution of fillers in this research is graphene plates for a specific weight percentage. This research helps to benefit the design of devices and stuff according to specific weight percentages and applications that need a high magnitude of a fraction of strength over weight. The study of RVE which contains numerous graphene pieces that are distributed in a matrix was made by FEM instead of MD because of decreasing computational costs. So just for extraction of interphase properties, the MD is used because in the MD simulation part, just interphase properties of a layer of graphene that is surrounded from bottom and top is extracted and this approach is the optimal work that can be done.

3.1. Figure of Density Distribution vs Time

In Figure 7 changes in density in the simulation box and pure epoxy vs time are depicted. Figure 7 shows that after elapsing 50 ps the magnitude of the density of pure epoxy and simulation box converges to a constant value that shows the system reaches stability and convergence.

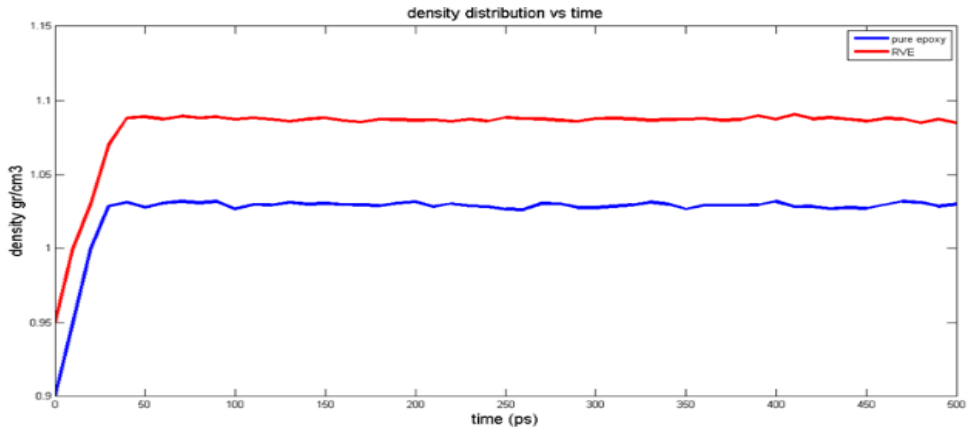

Fig. 7. The indicative figure of stability convergence of the material after a specific time

3.2. Figure of the Density Profile of Total Simulation Box vs Place of Nanocomposite along the z-Direction

The simulation box that is depicted in Figure 8 shows a density profile that has a lot of information about its configuration. For a depiction of segments with a size of 0.05 angstrom [1] in the z direction is considered and this figure is depicted perpendicular to the graphene sheet. Interphase thickness refers to the thickness in the place between the zone where the density value of graphene converges to zero and the place where the density value of epoxy converges to a constant value with so little fluctuation.

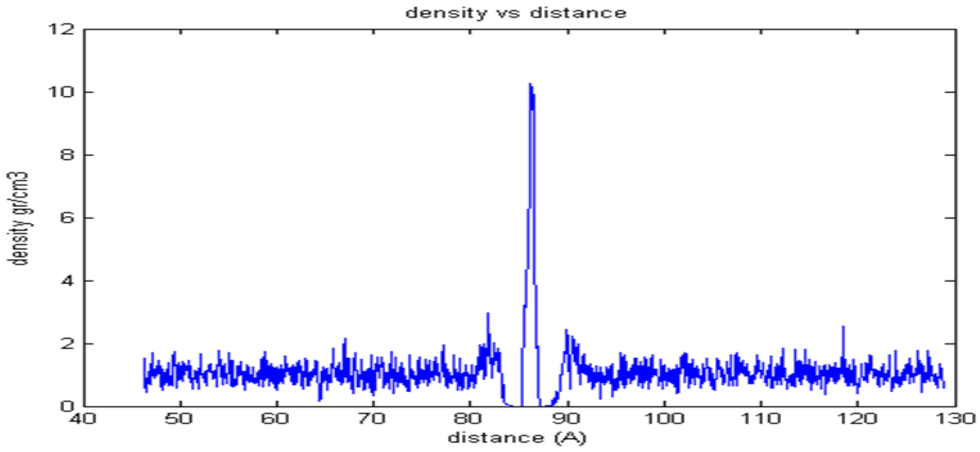

Fig. 8. Distribution of density in simulation box along z direction

Table 2. Information of simulation box and interphase zone

Bulk density	Peak density	Interphase thickness[2]	Wander vals thickness[1]
1.04 gr/cm^3	2.439 gr/cm^3	7.9 Å	2.9 Å

Table 3. Primitive data of simulation

cell length	82.33 Å^3
Volume of cell	205825 Å^3
Busy volume	181126 Å^3
Vacant volume	24699 Å^3
dimension along x	50 Å
dimension along y	50 Å
Total Young modulus	4.16 GPa
Young modulus of graphene sheet	800 GPa
Bulk Young modulus	1.2 GPa
Total number of atoms	18288
Number of graphene atoms	1008
Number of atoms of simulation of pure epoxy	8640

3.3. Figure of Stress vs Strain in Total Simulation Box

The figure of stress vs strain of the complete simulation box along the x direction is extracted from tension simulation in the x direction with changes in strain from zero to 2 percent and the slope of it shows Young's modulus of the simulation box that is about 4/16 GPa. A depiction of segments with a size of 0.05 angstrom [1] in the z-direction is considered and this figure is depicted perpendicular to the graphene sheet. Interphase thickness refers to the thickness in the place between the zone where the density value of graphene converges to zero and the place where the density value of epoxy converges to a constant value with so little fluctuation.

3.4. Figures of Distribution in Interphase and Total Interval of Simulation Box

The figure of distribution of Young modulus vs distances for interphase zone and total simulation box is brought in the following. Interphase configuration and properties of it is the day problem. Figure 11 shows that Young's modulus in the interphase zone is about 3/12 GPa. A depiction of segments with a size of 0.05 angstrom [1] in the z-direction is considered and this figure is depicted perpendicular to the graphene sheet. Interphase thickness refers to the thickness in the place between the zone where the density value of graphene converges to zero and the place where the density value of epoxy converges to a constant value with so little fluctuation. From the equality of the area of the interphase young modulus distribution along the interphase zone and the average young modulus area, we can achieve the average interphase young modulus for usage in FEM simulation that for accurate simulation we need it.

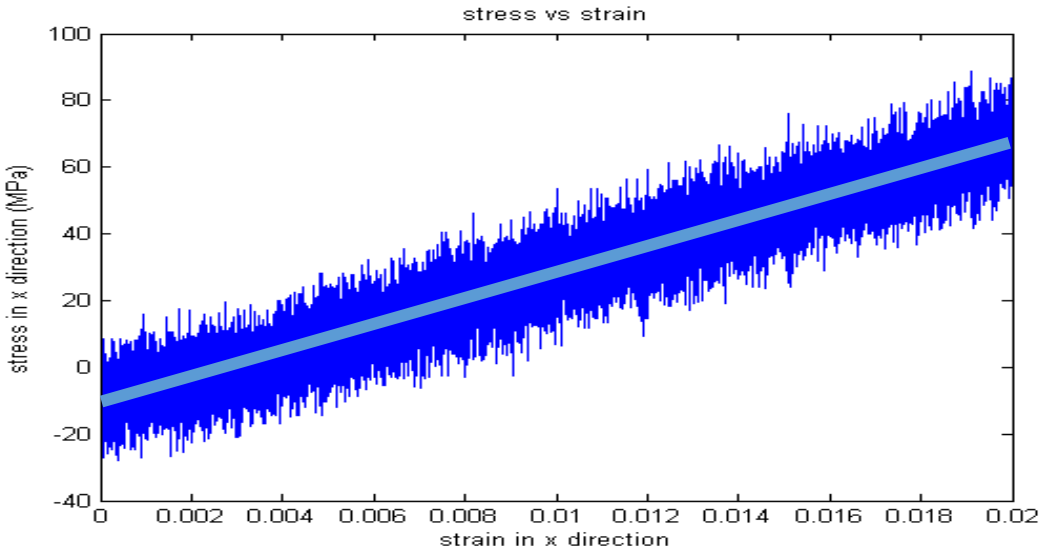

Fig. 9. Distribution of stress vs strain for total simulation box in traction along the x direction

[1] Thickness of vdw is a distance between graphene and epoxy in the distribution densty profile that in it the density is zero and the zone of it named vacant volume

[2] The thickness inwhich the place that density of graphene is zero to the place that density converges to a density magnitude that the fluctuation of density is zero

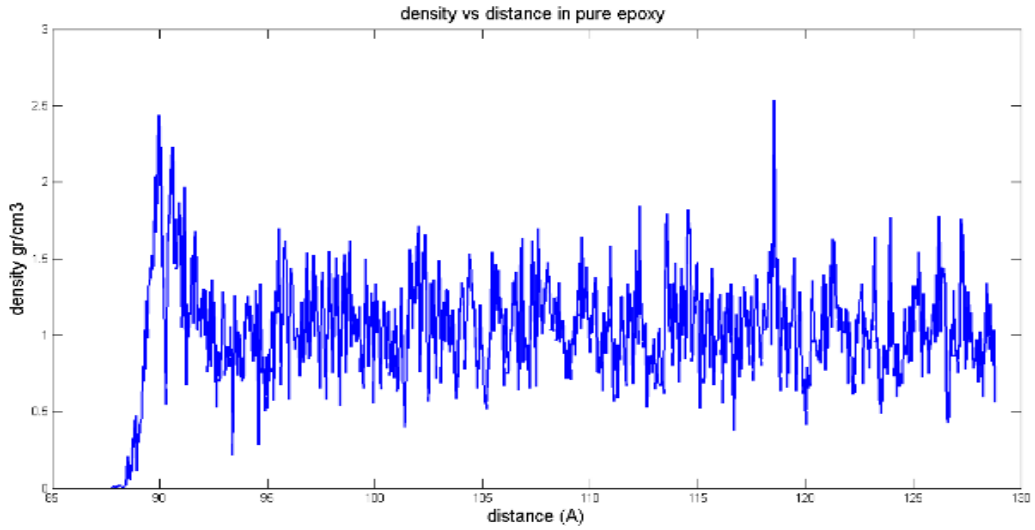

Fig. 10. Distribution of density along z direction of simulation box for epoxy (matrix) zone

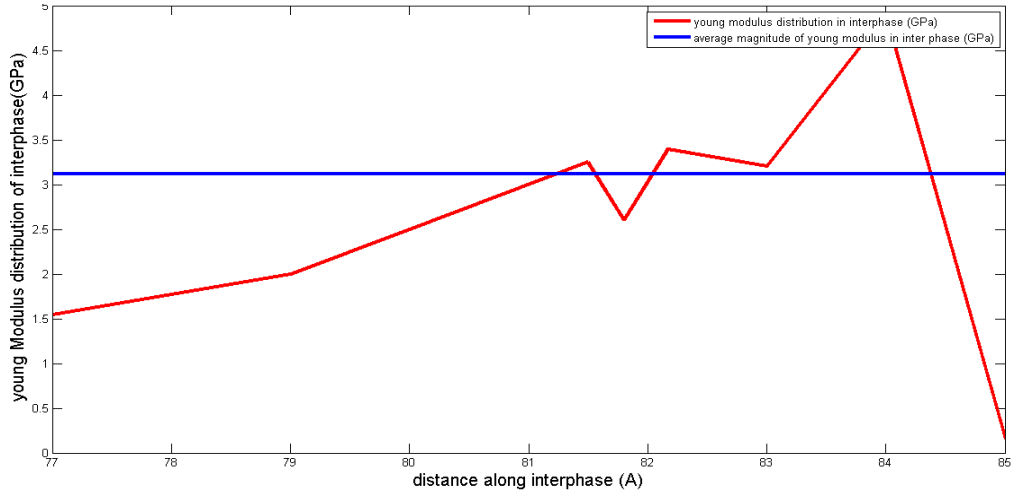

Fig. 11. Distribution of Young modulus along z direction for interphase zone

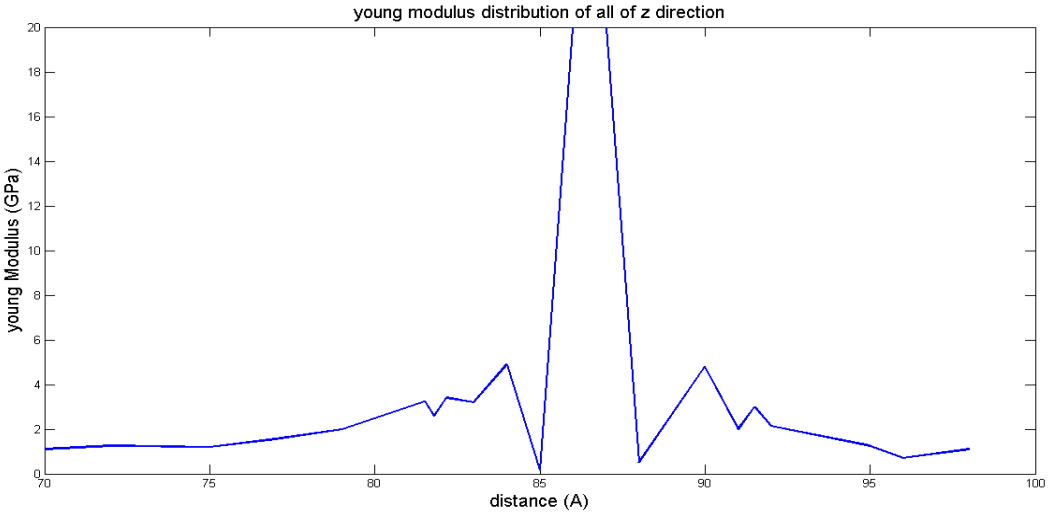

Fig. 12. Distribution of Young modulus along z direction for total simulation box

In Figure 12 the distribution of Young modulus in the total simulation box along the z-direction is shown that the highest value is for graphene sheet and tends to that of pure epoxy in both sides.

3.5. Magnitude of Shear Modulus and Poisson Ratio of Total Simulation Box on xy Plane

$$G_{xy} = \frac{E_{xx}}{2 \times (1 + \vartheta_{xy})} \text{ [26]} \quad (1)$$

G_{xy}=1.58GPa;

E_{xx}=4.16GPa;

ϑ_{xy}=0.317

3.6. Magnitude of Shear Modulus and Poisson Ratio for Interphase on xy Plane

The magnitude of shear modulus for interphase on the xy plane is 1/2 GPa and the Poisson ratio of that is 0/29.

3.7. Figure of Temperature Fluctuation vs Time for Pure Epoxy

In Figure 13 the fluctuation of temperature vs time is depicted. The stability of it illustrates the stage that came to convergence and stability of the system after treatment.

3.8. Extraction of Young Modulus for Total RVE That Consists of Specified Number of Nanoparticle with Erratic Orientation of Particles

The RVE is considered in which the dimension in all directions is equal and it has been considered that the dimension has a negligible effect on the results by some Python codes that enact the periodic boundary conditions just like the MD simulation. In the RVE three types of distribution of nanoparticles and for each type four models with 10, 20, 30, and 40 numbers of nanoparticles have been implemented. The simulation was implemented by considering the type of simulation of static general. The mesh definition was assumed in that the effects of the size of meshing do not affect the result considerably.

The erratic condition is the condition in which the orientation of particles is accidental. For choosing the type of modeling the static solver has been chosen. For the definition of properties, three types are defined that consist of pure epoxy, interphase, and filler. The filler that is used in this simulation is graphene nanosheets. The matrix in this simulation is pure epoxy and the interphase properties are extracted from the primary sections of this study.

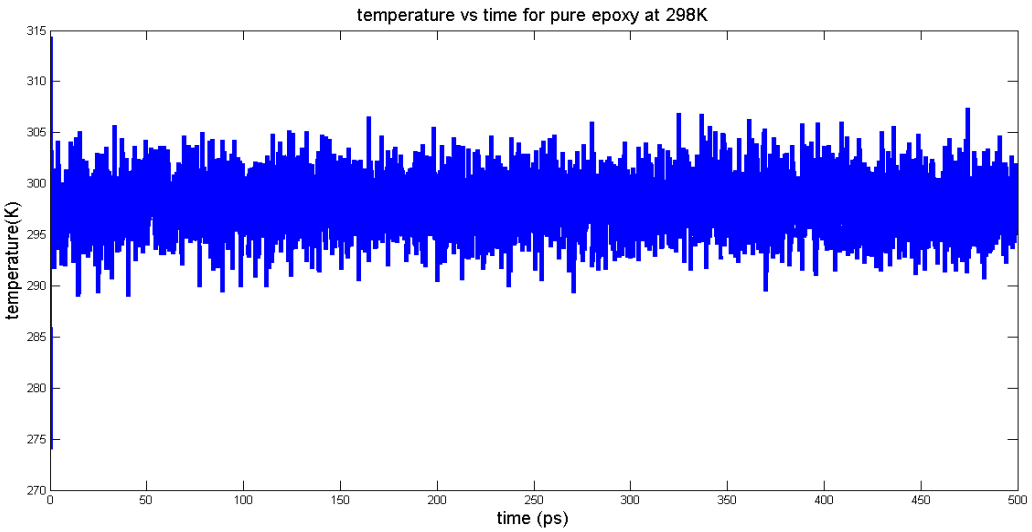

Fig. 13. Temperature vs time for pure epoxy in 298 K

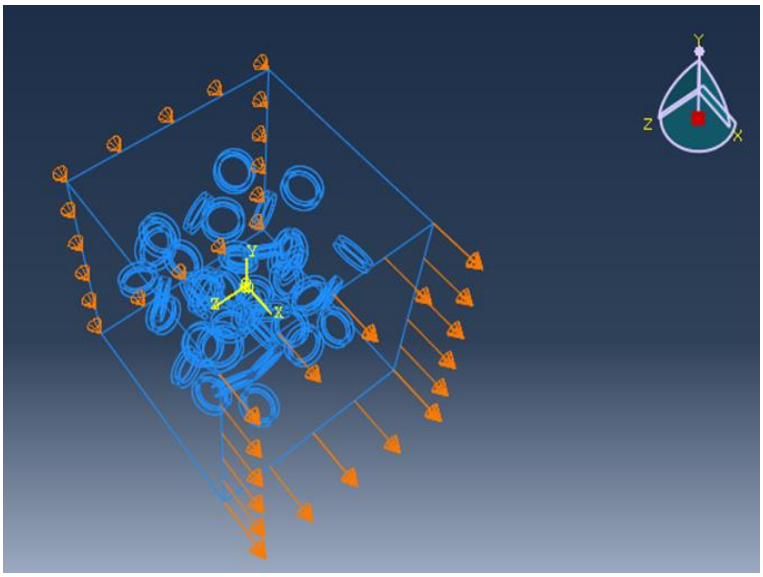

Fig. 14. Configuration of RVE in erratic distribution with loading condition of it

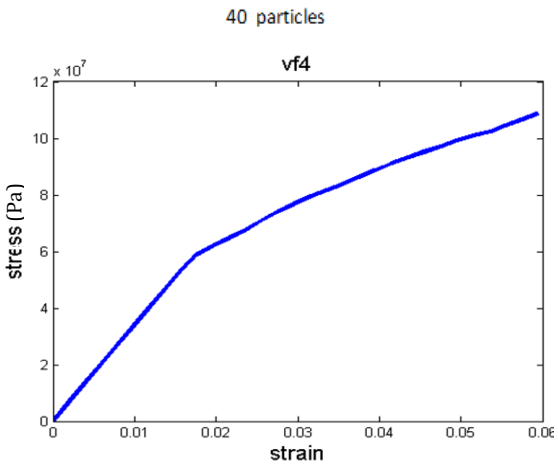

Fig. 15. Figure of stress vs strain for RVE with 40 nanoparticles

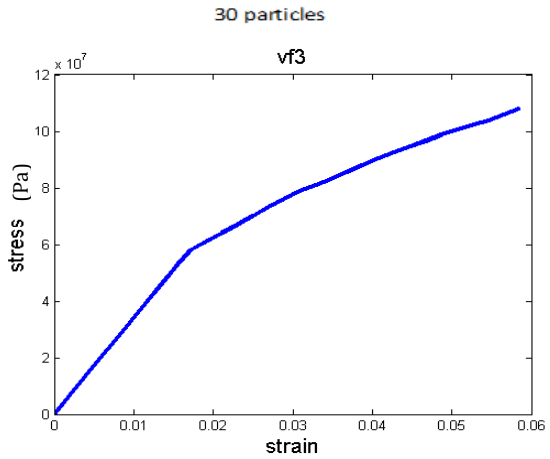

Fig. 16. Stress vs strain of RVE for 30 nanoparticles

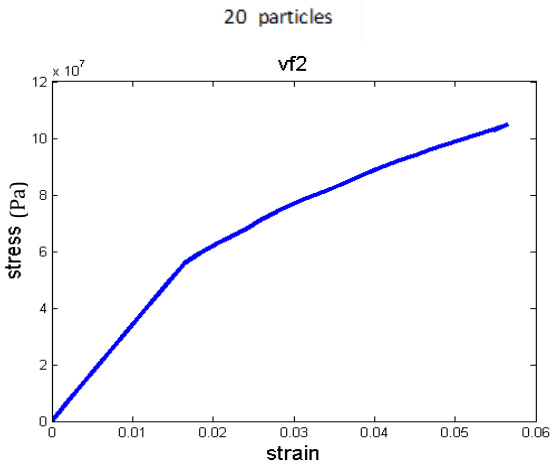

Fig. 17. Stress vs strain of RVE for 20 nanoparticles

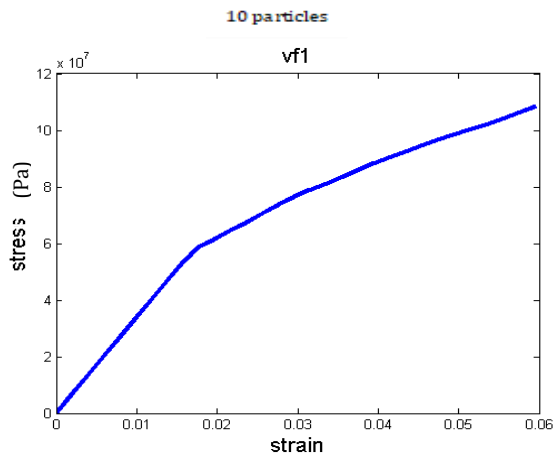

Fig. 18. Stress vs strain for RVE with 10 nanoparticles

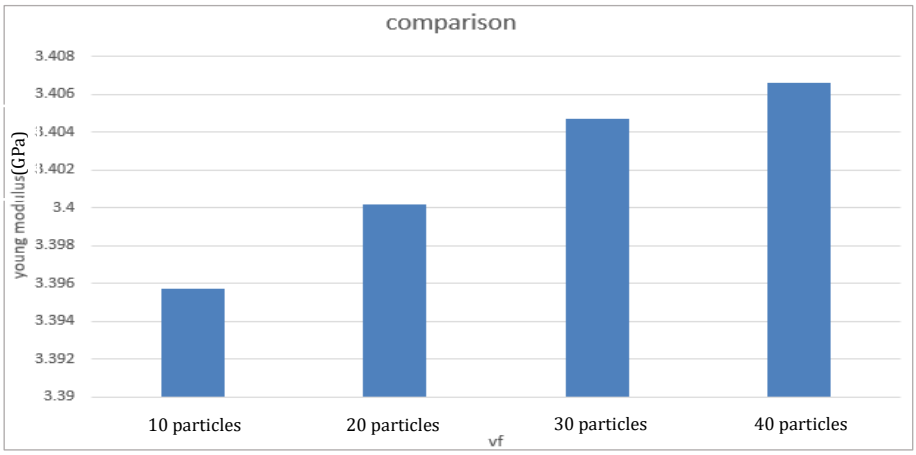

Fig. 19. Comparison of young modulus of RVE with different numbers of nanoparticles

3.9. Extraction of Young Modulus For RVE that Consists of Specified Number of Nanoparticles with Regular Orientation

The regular condition that is mentioned above is the condition in which the orientation of particles is parallel to each other.

For this case as well as the previous modeling the solver is static general and three materials have been simulated like before.

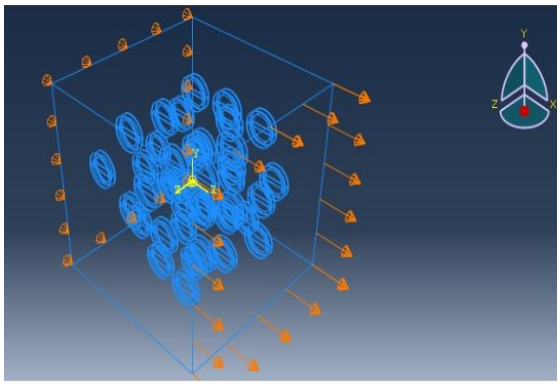

Fig. 20. Configuration of RVE for traction along the x direction

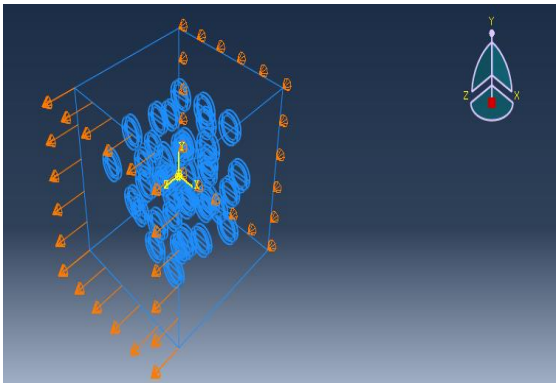

Fig. 21. Configuration of RVE for traction along the z-direction

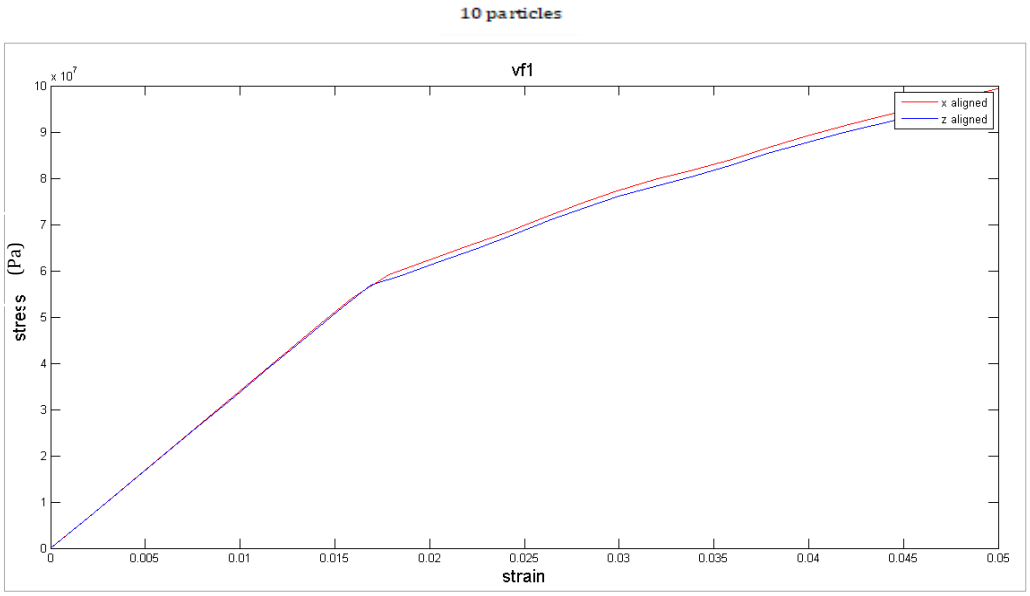

Fig. 22. Stress vs strain for RVE with 10 nanoparticles in two traction orientations along the x and z direction

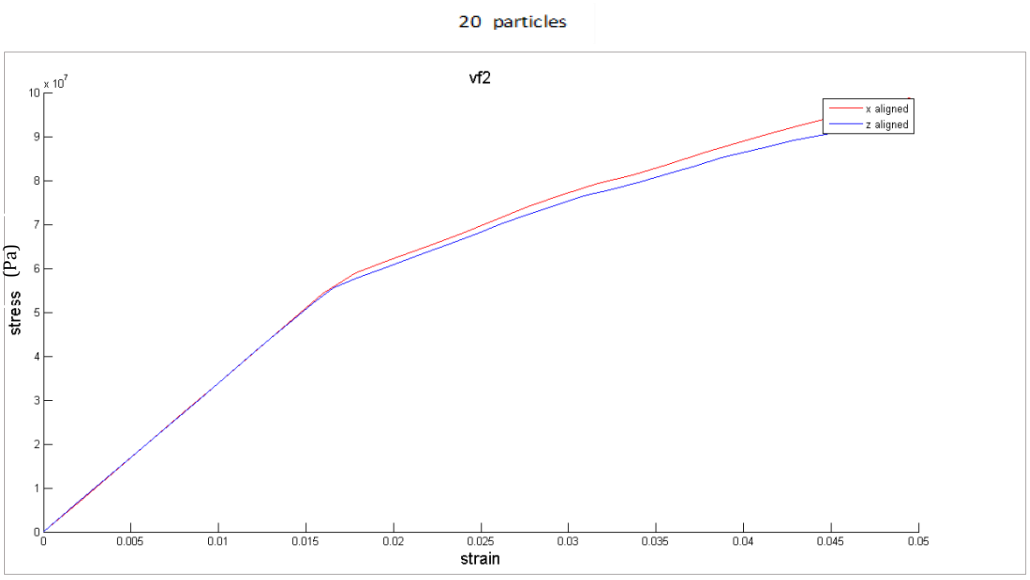

Fig. 23. Stress vs strain for RVE with 20 nanoparticles in two traction orientations along the x and z direction

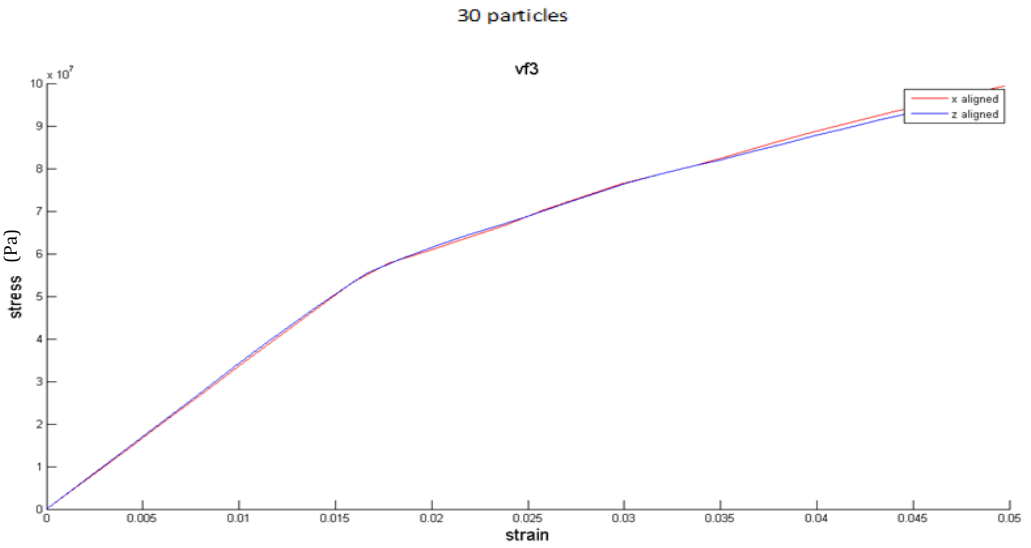

Fig. 24. Stress vs strain for RVE with 30 nanoparticles in two traction orientations along the x and z direction

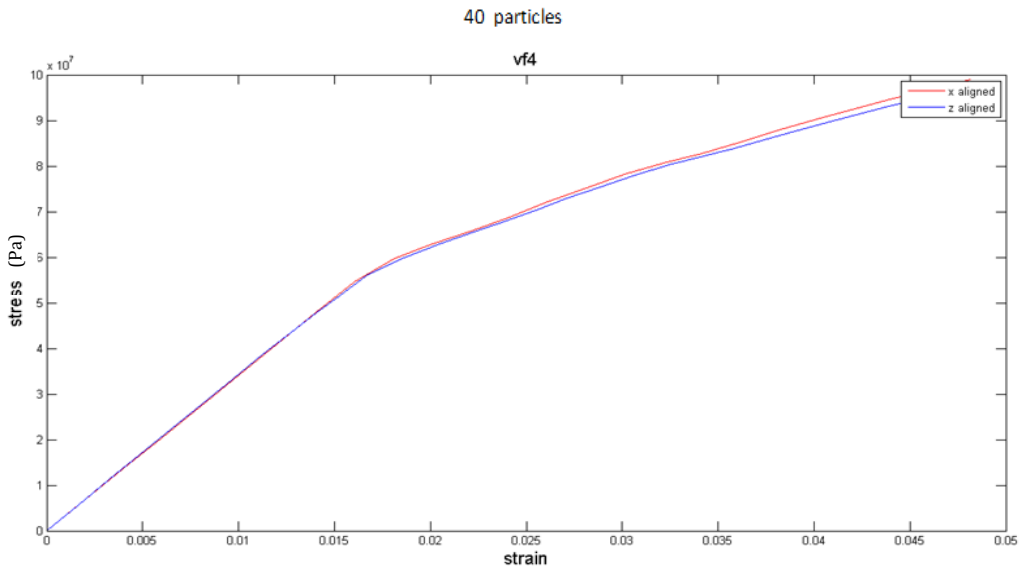

Fig. 25. Stress vs strain for RVE with 40 nanoparticles in two traction orientations along the x and z direction

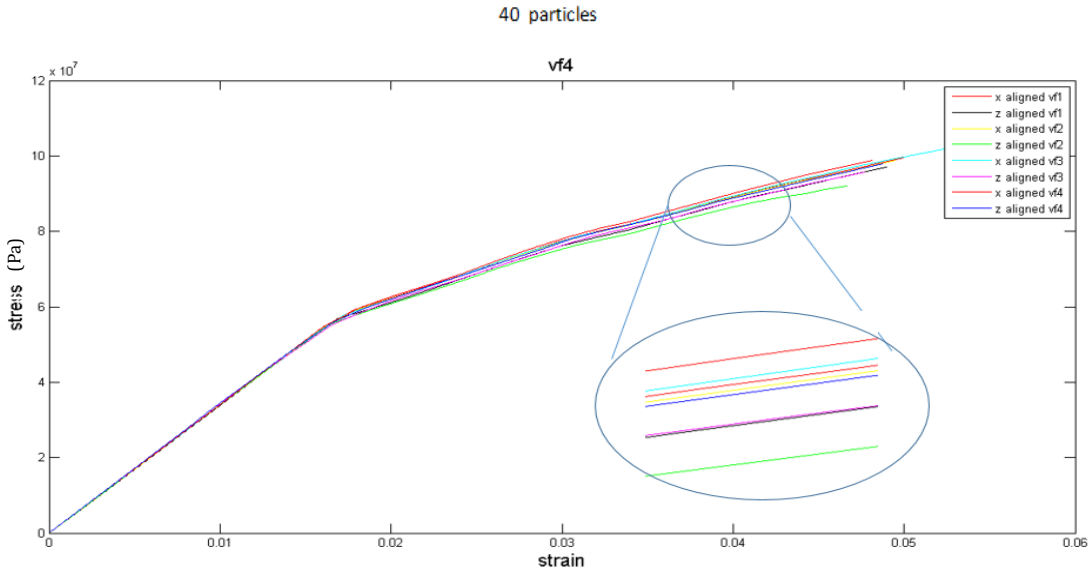

Fig. 26. Depicted figures for all conditions of above

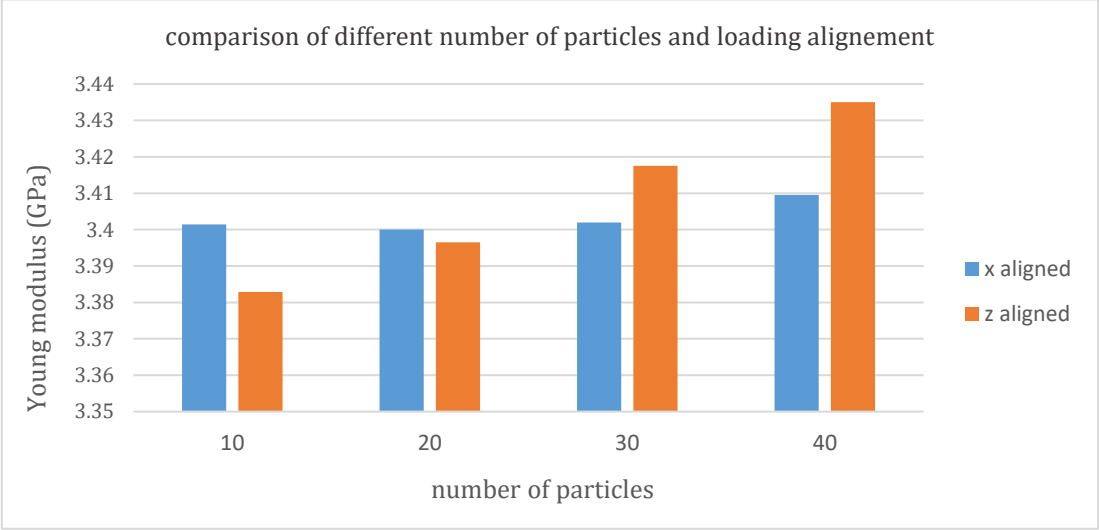

Fig. 27. Young modulus distribution of regular orientation of nanoparticles for different loading orientations

For ratios of the magnitude of interphase Young modulus over that of epoxy equal to 2.8, 2, 1.75, 1.5, and 0.75 consideration is made and the results are brought in the below

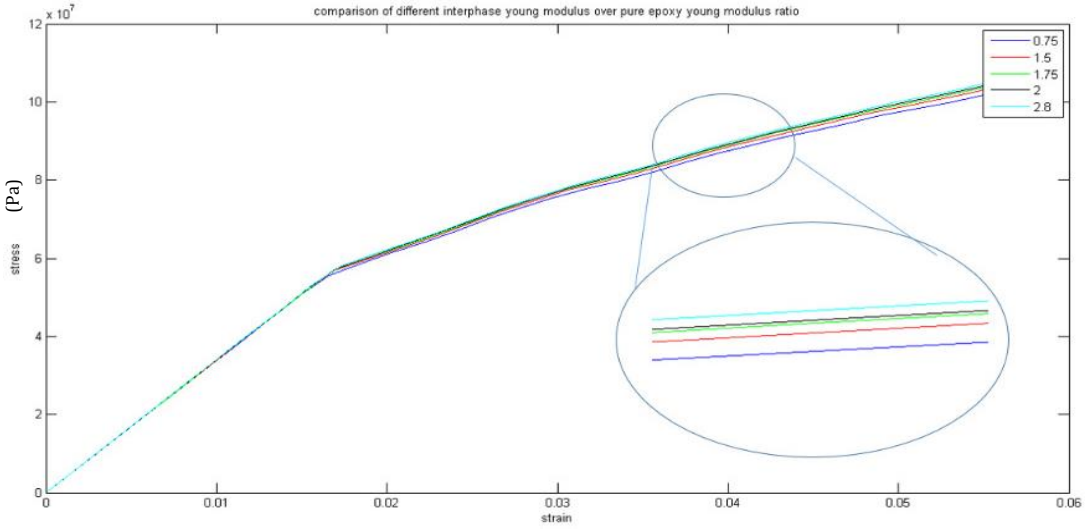

Fig. 28. Effects of different interphase over pure epoxy young modulus ratio magnitudes

In the above figure, the effects of specified ratios of Young modulus of interphase over that of pure epoxy are depicted for 40 nanoparticles in a defined dimension of RVE. This ratio for this study is about 2.8 and the corresponding figure of it is depicted in the highest place of the figure 28 with other ratio magnitudes that was mentioned above.

3.10. Validation of the Total RVE

For validation of the total RVE's mechanical properties we simulate RVE with specific volume factions and realized that in our study compared to experimental results, there are just 4 % errors.

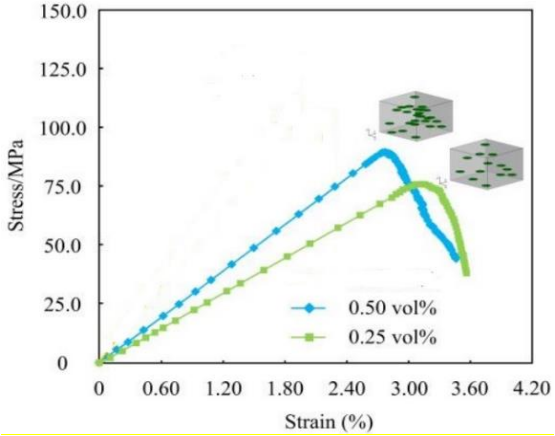

Fig. 29. Volume fraction effect on the mechanical behavior of graphene/epoxy nanocomposite (stress-strain curves) which our results with this reference just have 4 % errors [28]

4. Conclusions

In this study, the interphase and specification of it are considered and the properties of it are studied, because it helps to design more accurately. In this study, the FEM simulation for consideration of properties of RVEs with different conditions is studied. In the condition in which regular orientation of nanoparticles is chosen, in the loading in which the orientation of nanoparticles is parallel to loading orientation, with an increase in the number of nanoparticles, the Young modulus increases significantly. In a condition in which the direction of loading is perpendicular to the orientation of nanoparticles in regular orientation, with an increase in the number of nanoparticles the Young modulus does not increase significantly. In the erratic condition of nanoparticles in RVE, more particles cause a significant increase in the Young modulus of RVE. In the condition in which the graphene sheet is organized between two pure epoxy boxes with a 9 % weight ratio, a good magnitude of Young modulus is obtained. The best condition of loading is parallel to and in a regular condition of nanoparticles which is about 31 % higher than the condition in which the orientation of nanoparticles is regular and the orientation of loading is perpendicular to nanoparticles. As is concluded from the density profile of the simulation box, the density of interphase is 134 % higher than that of pure epoxy. The effective value of the Young modulus of interphase is 183 % higher than that of pure epoxy showing that the consideration of interphase in our study is obligatory for accurate design.

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Conflicts of Interest

The author declares that there is no conflict of interest regarding the publication of this article.

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