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Finite Element Modeling of A VGCF/Pp Nanocomposite Material To Measure The Strain Energy of A Representative Volume Element

Rameshwar Cambow[1], Ashok Kumar Bagha[2]

Lovely Professional University, Phagwara, India E-mail: rameshwar.20345@lpu.co.in
Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, India E-mail: baghaak@nitj.ac.in

Abstract

In this paper, strain energy of a representative volume element (RVE) is carried out analytically. The vapor developed carbon fibers are reinforced in a polypropylene matrix. In this paper, the two case studies are presented. In the one study, it is assumed that the fibers are throughout the RVE. And for the second study it is assumed that the fibers are enclosed inside the RVE. The loading direction is longitudinal and transverse direction. The main objective is to predict the strain energy of both RVEs at different loadings. The different RVE models are developed on NISA software for different fiber volume fractions (0.02 to 0.14) at constant fiber aspect ratio l/d = 19.

1. Introduction

Nanotechnologies and nanomaterials continue to be a preferable research topic for many researchers across the globe since the beginning of this century.It should be clearly understood at the beginning that nanoscience is much more than just miniaturization. It depicts anintegration of quantum physics, molecular biology, computer science, chemistry, and engineering. Advacements in nanoscience are prone to be marketed as improvement in holdof the atom-to-atom and molecule-to-molecule construction modification. A theorematicdescription of a nanomaterial relies on elemental theories. It must be preferred to go withapproach that each materialconsists of granules, in turnfurthermade up of atoms. Thegrains might be seen with the naked eye, as depends on its size, which varies from several microns to centimeters. The word ‘‘material’’ depicts a subject matter in a solid state, either in form of crystals or amorphous. As nanoparticles can form both nanomaterials and nanopowders, it must be noted that in mechanics, materials considered to be stable in shape, whereas powders considered to be in granular medium. Mostly, powders converted into materials by using different methods such as compression, sintering, irradiation etc. Composite structures withfeatureattributes at the nanoscale are known asnanocomposites.Ruoff and Lorents [1] used known elastic properties of graphite sheet to derive the mechanical properties i.e., tensile and bending stiffness constants for single walled carbon nanotubes (SWCNT’s) and multiwalled carbon nanotubes (MWCNT’s). As recommended, the thermal expansion of carbon nanotubes isideally isotropic, thus itcould be counterpointed with powerful anisotropic enlargement in regular fibers (big diameter fibers) and in graphite. On the other hand, the thermal conductivity might be extremely anisotropic and through the lenghty axis more than any others. The authors also presented a brief introduction about topological constraints to surface chemistry in refined multi-walled nanotubes and highlighted the relevance of powerfulportwithin nanotube and matrix to makestrong nanotube –reinforced composites. The authors calculated the young’s modulus of all the tubes by calculating the force on the end rings and by using the cross-sectional area of the tube. The results obtained from the simulation approach are used for deriving the formula which is used for different radii carbon nanotubes to predict the Young’s modulus in compression. The results obtained using this approachmatches with 1% of the simulated values for carbon tubes with radius ranging from 5 to 22A^{o}.Ajayan et al., [2] observed the forcedistribution to the nanotubes in composites is more in compression. The value of the compression modulus is much more than tensile modulus because during the load distribution in multiwalled nanotubes only the outer layer is seen to be in tension whereas other layers in compression.Odegard et al., [3] developed anapproachto formstructure-property relations of nano-structured materials. Basic approach here relates to replacement of the discrete molecular structures with equivalent continuum model in computational chemistry and solid mechanics which has been achieved by comparing the vibration potential energy of a nano-integrated material with the strain energy of presented figures. This continuum model is also utilised to determine the effective continuum geometry of graphene sheet. Further effective thickness is used for developing the representative volume element of equivalent continuum model.Odegard et al.,[4]developed a technique to present constitutionalmethodsto add polymer composite systems with single-walled carbon nanotubes. It is seen that the size scale of polymer matrix molecules and the carbon nanotubes are same, due to this reason that the interaction at the portstrongly depends on the local molecular structure and bonding between matrix/nano sizes reinforcing material. Moreover due to small size, the lattice structure is not continuous so the conventional micromechanical approach is not preferred for predicting the bulk behavior of nanocomposites. Thus authors suggested the application of equivalent continuum modeling methods to effective fiber. It is appropriate to note that the local polymer in vicinity of the nanotube and the port is named as an effective continuum fiber. The effective continuum fiber retained the continuity of structure so it is used for forecasting the bulk mechanical attributes of nanocomposites with various nanotube sizes and orientations. The dynamic mechanical thermal analyzer is used for measuring the storage modulus and damping of nanocomposites. The fiber injection direction is the preferred direction corresponding to which predicted and measured results are validated by the authors.Liu and Chen [5] used the conventional rule of mixture for long CNTs to find out the efficient elastic characterstics of nanocomposites whereas extended rule of mixture (ERM) for short fibers reinforced composites.Thus, it can be concluded from the different modeling methods as studied for the prediction of different properties of nanocomposites:(i) Most of work on molecular modeling studies in nanocomposite materials relates to prediction of elastic behavior of carbon nanotubes (CNTs). The effect of fiber-matrix interaction at the interface is accurately analyzed by the molecular modeling simulation methods with geometric parameters such as diameter, wall thickness and length.

2. MODELING OF NANOCOMPOSITES

In 1991, lijima discovered carbon nanotubes. Carbon nanotubes are filled up graphene sheets with a cylindrical shape with closed ends which can bementioned as long and slender fullerenes. The elastic modulus of carbon nanotubes proved to be more than 1 TPa and tensile strength surpassesas compared to the steel by almost an order of magnitude. Due to excellent characterstics of carbon nanotubes, it has been preferred as perfect reinforcements in composite system. For nanotube composite materials, Valavala and Odegard [6] have shown that a carbon nanotube weight fraction of 1% results in the same increase in composite elastic modulus as a composite with a 10% weight fraction of carbon fibers. This difference in elastic modulus is predicted even through the size scale of the two reinforcements differs by three orders of magnitude.

Nanoparticles with eminent aspects ratios resulted inexcellent reinforcing factor in polymers. Mostly in nanoparticle reinforced composites, the

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commonlyenquiredarrangementsdepend on silicates and clay particles. The enormous mechanical attributes of nanoparticlescould be noticed only in case ofpresence of excellentforcedistributionamong the ground substance and the reinforcement.

3. MODELING FOR DYNAMIC BEHAVIOR

Damping is the inbuilt characteristic of material that spreads out energy in case ofrepetitive load. Finite element modeling (FEM) could be utilised for mathematical calculations of bulk attributes depends on the geometry, characteristics, and volume division of element phases. FEM encompassescategorization of a material representative volume element (RVE) into elements where the elastic rootprovides stress and strain field. The granulairty of the categorizationgives the precision in result. Nanoscale RVEs of dissimilar geometricalsizescould be usedto simulatethe mechanical properties.

3.1 FINITE ELEMENT MODELING

It is conducted to analyse the reaction of a systemwithinspecifiedextremeconsiderations and time independent actingloads, when linear reactionconductconsidered withreliableprecision. The required reactionamounts are commonly, displacements, stresses, strains, reactions, and energy. Commonly, acting loads involvesspecified forces at nodes, variable pressure on the front of constituents along withgravitational force or centrifugal forces. The extremelimits are mentioned displacement integers at specified nodes or, it involves multi-point constraints, coupled displacements or fixed links. Mathematically, it can be expressed as

$$[K]\{u\} = \{p\} \qquad (3a)$$

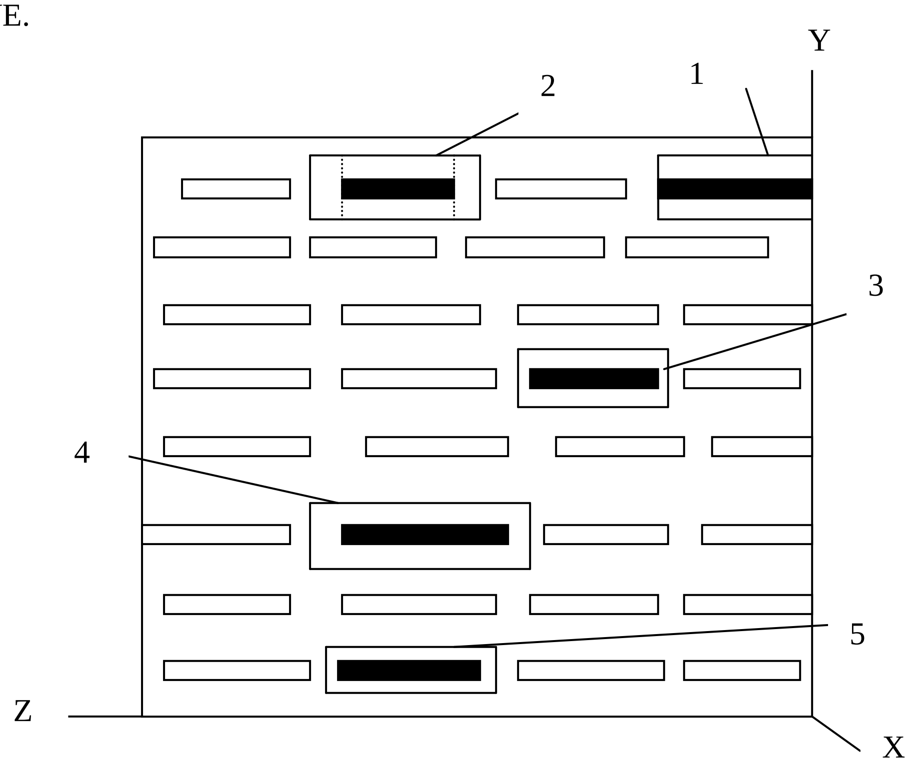
Where, [K] is the linear stiffness matrix for the defined structure, {u} is the undefined nodal displacement vector and {p} is the defined load vector.

Several square RVE models for VGCF in a matrix material are analysedwith the FEM so as to measure the characteristics of the VGCF-based nanocomposites as shown in Figure 1. This figure represents the illustrations of unit cell for staggered arrays of straight fibers. The vapor grown carbon fibers are short and assumed aligned and straight in the unit cells but the unit cells are not regular in the arrays. That’s why it is called staggered arrays. For predicting the properties of the nanocomposite in this study it is assumed that the material is transversely isotropic. Here, the Z-direction symbolizes the fiber direction and X and Y-directions are perpendicular to the Z-direction and X and Y have same properties. Also single fiber cell 3-D model utilised for FEM analysis. The following RVEs are used for modeling the dynamic behavior of VGCF/pp nanocomposites:

(i) VGCF through the RVE: In this case, the vapor grown carbon fiber through the length of square RVE is used for modeling the nanocomposite. The length of fiber is equal to the length of RVE.

(ii) VGCF inside the RVE, V_f is considered only for center part: In this type of modeling, VGCF is inside the square RVE and the length of fiber is small as compared to the length of RVE. Also in this case the RVE is divided into two parts one center and other outer ends as explained in Chapter 3. Now volume fraction of fiber in RVE is considered only for center part length (L_c). The theoretical extended rule of mixture (ERM) is used to predict the longitudinal storage modulus E'_{11} of the nanocomposite. For modeling on NISA (Numerically integrated elements for system analysis) software the geometry of RVE is created based on center part V_f . This type of modeling is called ERM/FEM.

(iii)VGCF inside the RVE, V_f is considered for whole RVE: In this type of modeling, VGCF is inside the square RVE, again the RVE is divided into two parts but this time the volume fraction of fiber V_f is considered for whole RVE during analysis on NISA software. The FEMapproachutilised to calculate the attributes of nanocomposite.
(iv) VGCF inside the RVE, End length is half the fiber length:In this case, the VGCF again inside the square RVE, as earlier explained the RVE is divided into two parts. Both parts are important while modeling on simulation software. In this study the different end lengths are considered for modeling and calculating various properties. The ends length used are 500, 600, 1000, 1900 nm and also a case is considered when the end length is half the fiber length.
(v) VGCF inside the square RVE, l/d of fiber is equal to L/2a of composite: In this case, the VGCF is inside the square RVE, and aspect ratio of fiber l/d is equal to the L/2a of the square RVE.



1. VGCF via the distance of square RVE
2. VGCF inside the square RVE, V_f only for center part
3. VGCF inside the square RVE, V_f for whole RVE
4. VGCF inside the square RVE, End lengths (L_{e1}=L_{e2}) is half the fiber length
5. VGCF inside the square RVE, aspect ratio of fiber (l/d) is equal to aspect ratio of RVE (L/2a).

Figure 1:Illustrations of unit cell for staggered arrays of straight fibers.

3.1.1 VGCF through the length of square RVE:

Here, the VGCF is through the RVE. The two types of cases are considered for modeling. In one case the longitudinal loading is applied on RVE, Longitudinal storage modulus E'_{11} , longitudinal loss modulus E''_{11} , longitudinal loss factor η_{11} is predicted by using FEM/Strain energy method (SEM) and in other one the transverse uniform loading is applied on RVE and transverse storage modulus E'_{22}, transverse loss modulus E''_{22} , transverse

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loss factor η_{22} is predicted and compare with rule of mixtures. For modeling on NISA software various volume fractions of fiber are considered between 0.02 to 0.14 at constant aspect ratio of fiber l/d =19.

(i) For longitudinal loading,Uz = 0.001: First, a representative volume element (RVE) for VGCF through the length of square RVE under longitudinal loading similar to one shown in Figure 4.2 is studied. The diameter (d) of the VGCF is 200 nm and length is 3800 nm (Finegan et al.,) [7]. Here in the models, L represents the total length of RVE, and 2a represents the width and thickness of the RVE, Δa is the change in width and thickness after applying Uz deformation i.e., 0.001 in Z direction. The material properties of the constituents are shown in Table 1.

A 3-D structurewithsingle VGCF utilised for analysis as depicted in Figure 3.A single fiber cell model is used for VGCF, where it is sufficient to get precise FEM outcomes. The polyhedron constituents utilisedin meshing. Net aggregate is 15522, in fiber the number of elements are 8640 and in matrix 6912. The extremelimitsof given loadis depicted in Table 2. For longitudinal loading the displacement is given in Z direction. The magnitude of displacement is 0.001 as shown in Figure 4.The model is free in X and Y directions where constraints are applied but other degrees of freedom i.e., Uz, Tx, Ty, and Tz are zero. The SEMutilised to forecastthe attributes of the VGCF/ppnanocomposite. Between 0.02 to 0.14 volume fractions,it is formulated on NISA software at constant aspect ratio i.e., 19. The strain energy of models at different volume fractions is shown in Table 3 and at V_f = 0.02 the strain energy pattern in RVE is also shown in Figure 5. The outcome of SEMis noted on the NISA resultregister. As clear from the Figure 5 and Table 3 that maximum strains energy stored in fiber as compared to matrix. For VGCF along the distance of RVE i.e., the length of fiber (l) and RVE (L) is same, as the V_f increases the domination of fiber increases.

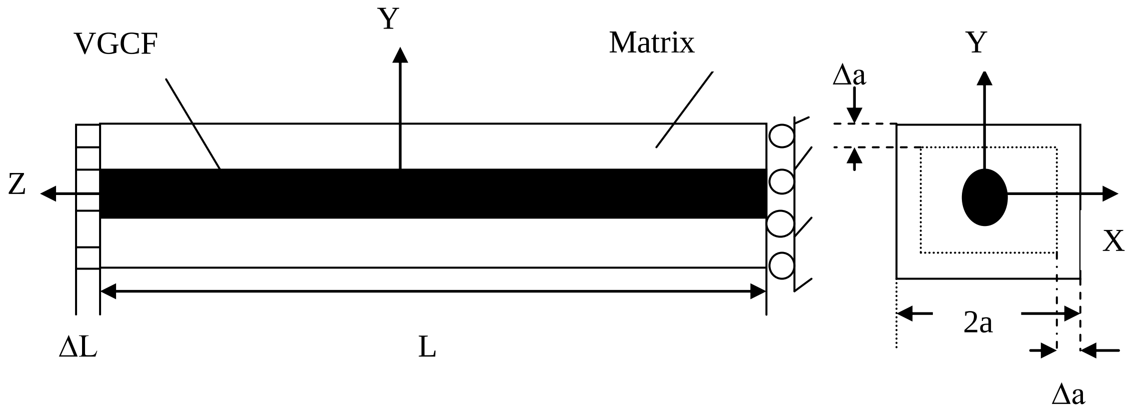

Figure 2: VGCF through the length of square RVE under axial deformation.

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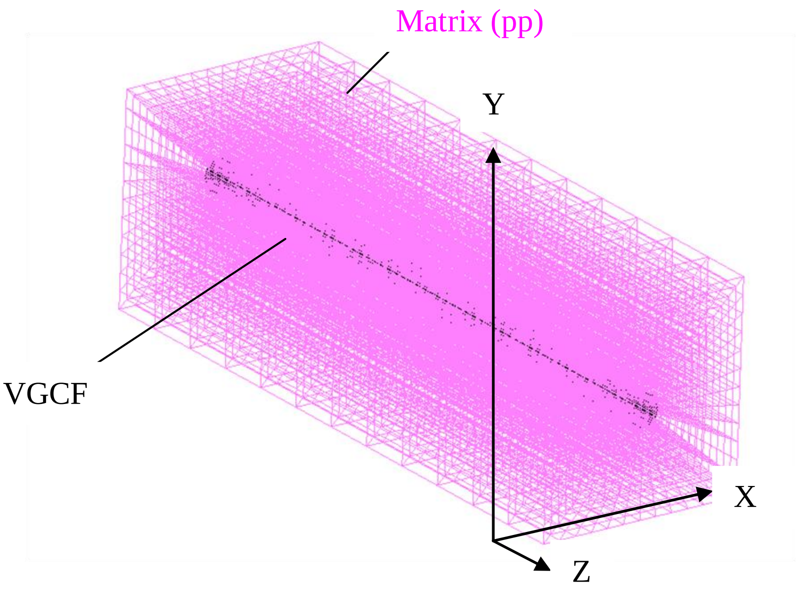

Figure 3: A full 3-D FE model for longitudinal loading.

Table 1: Dynamicalattributes of vapor grown carbon fibers and polypropylene [7]

S.No.	Dynamical attributes	VGCF	Polypropylene
1	Storage Moduli $E^{'}$ (GPa)	1000	1.23
2	Loss Modulus $E^{''}$ (GPa)	1.5	0.0738
3	Loss factor (η)	0.0015	0.06

Table 2 Boundary conditions for FE modeling for full 3-D model.

	Ux	Uy	Uz	Tx	Ty	Tz
Longitudinal Load						
Constraints			0	0	0	0
Force/Displacements			0.001	0	0	0
Transverse Load						
Constraints			0	0	0	0
Pressure XZ plane	0	-1	0	0	0	0

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(ii) Square RVE within a sidelong consistent force p: A RVE for VGCF through the length of square RVE under lateral loading similar to one shown in Figure 6 is studied. Here in the models, L is the total length of RVE; p is the negative pressure acting along transverse plane, for instance, the Y-direction. Δx and Δy are the deformation in width and thickness. Another 3-D structurewith single VGCF utilised for analysis. The polyhedron six sided constituents created the meshing. Net aggregate comes out to be 15522, in fiber the number of elements are8640 and in matrix 6912. The extremelimitsin the given case are depicted in Table 2. The RVE is restrcitedin direction perpendicular to XY plane

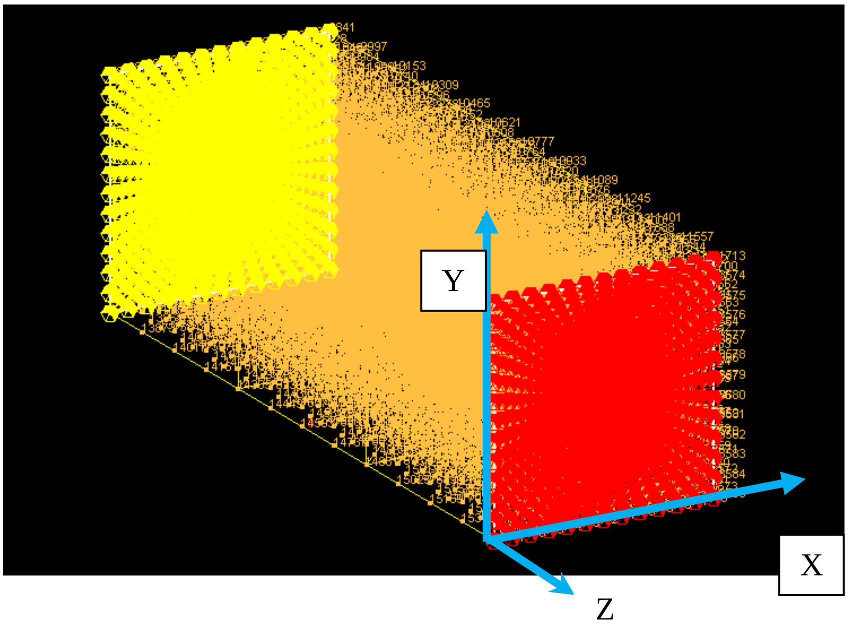

Figure 4: Boundary conditions for longitudinal loading.

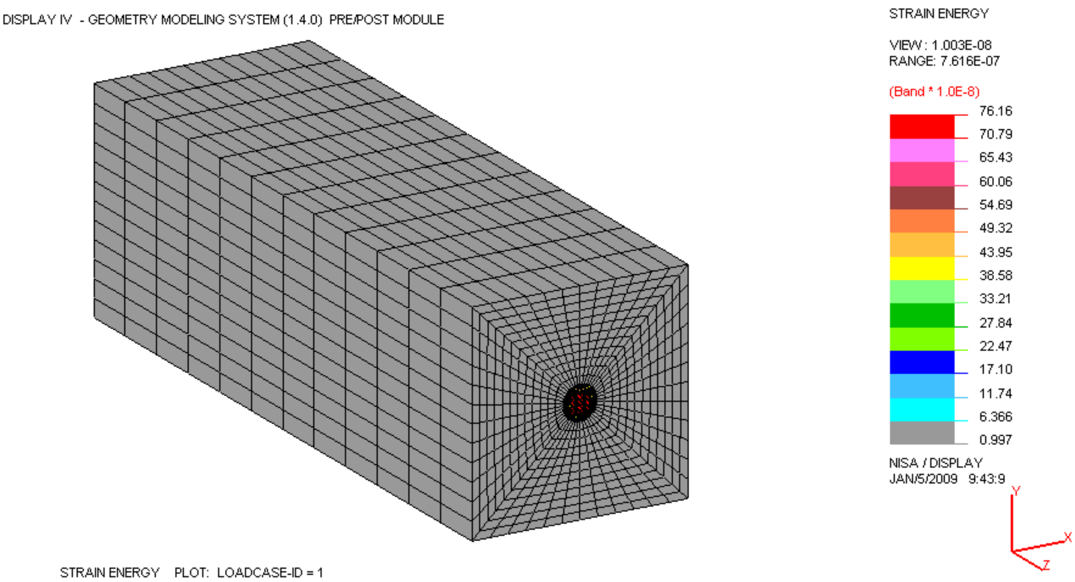

Figure 5 Strain energy distributions in RVE at $V_f = 0.02$, l/d =19.

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Table 3: Strain energy at different fiber volume fractions.

V_f	W	Wf	Wm	% difference (fiber)
0.02	4.38E-03	4.13E-03	2.47E-04	5.70
0.04	4.25E-03	4.13E-03	1.20E-04	2.82
0.06	4.21E-03	4.13E-03	7.75E-05	1.9
0.08	4.19E-03	4.13E-03	5.64E-05	1.4
0.10	4.17E-03	4.13E-03	4.37E-05	0.95
0.12	4.17E-03	4.13E-03	3.52E-05	0.95
0.14	4.16E-03	4.13E-03	2.92E-05	0.72

is maintained, in order to simulate the interaction of the RVE with surrounding material in the Z-direction. The pressure is acting in the XZ plane as shown in Figure 7. The deformation of RVE is shown in Figure 8. In this case the strain energy is maximum in matrix for fiber volume fractions (0.02 to 0.14) because in transverse direction the matrix properties are dominating. The strain energy pattern is shown in Figure 9.

3.1.2 VGCF inside the square RVE:

Here, the fiber kept inside the RVE and the length of fiber (l) is small as compared to length of RVE. As earlier explained the RVE bifurcated in following types: first typedescribing extreme limits with full lengthL_{te} (L_{te} = L_{e1}+L_{e2}) and Young's modulus E_m and another segment accounting for the center part with a length of L_c and Young's modulus E_c as shown in Figure 10. A full 3-D model used for analysis of the nanocomposite is shown in Figure 11. 3-D FEM model consists of total numbers of hexahedron elements 15522, number of elements in fiber 2560 and in matrix 12962. The material properties and boundary conditions are same are same as shown in Table 1 and 2.

(i) For longitudinal load: In this case, longitudinal displacement in Z direction is applied on RVE. The different strcuctures are developedusing NISA software for several fiber volume fractions (0.02 to 0.14) at constant fiber aspect ratio l/d = 19. FEM models are also analysed for fiber aspect vary from 5 to 1000 with constant volume fractionequal to 0.03. The effect of different end lengths (L_{e1}=L_{e2}) is considered as an important parameter.

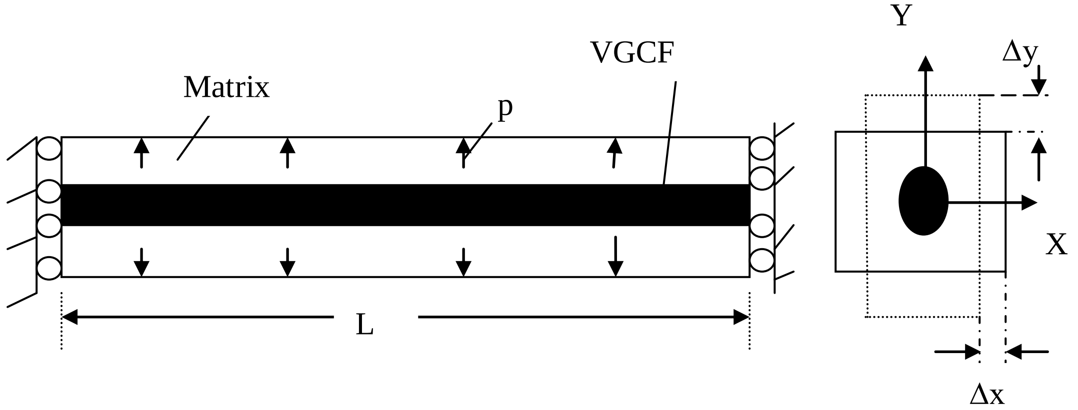

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Figure 6 VGCF through the length of square RVE withlateral consistentforce p.

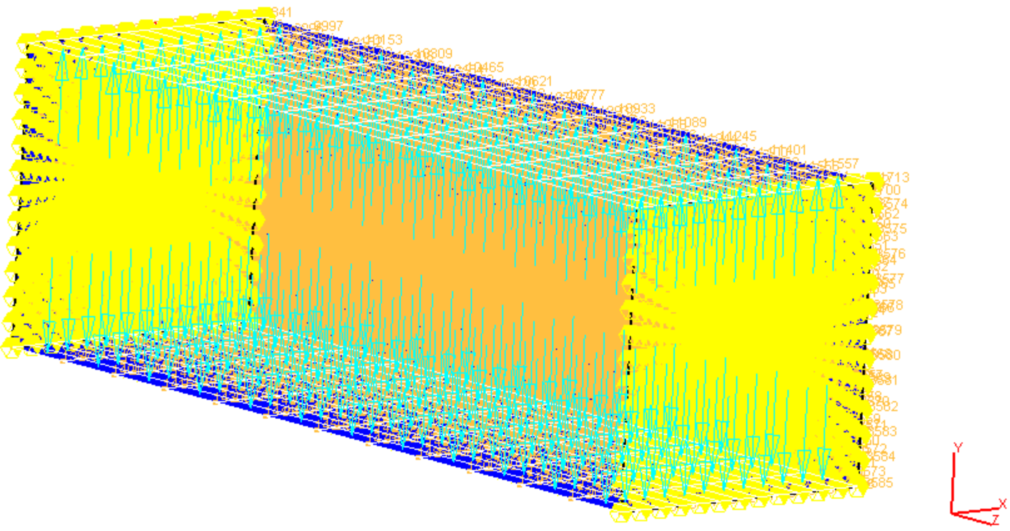

Figure 7 A 3-D FE model for transverse loading.

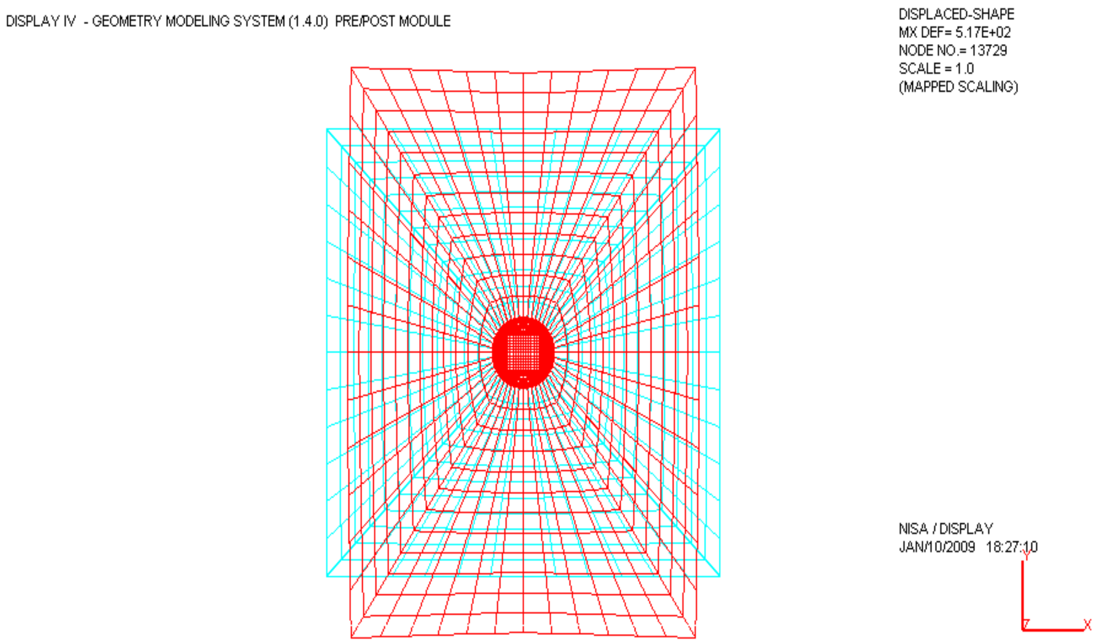

Figure 8 Deformation of RVE in lateral direction.

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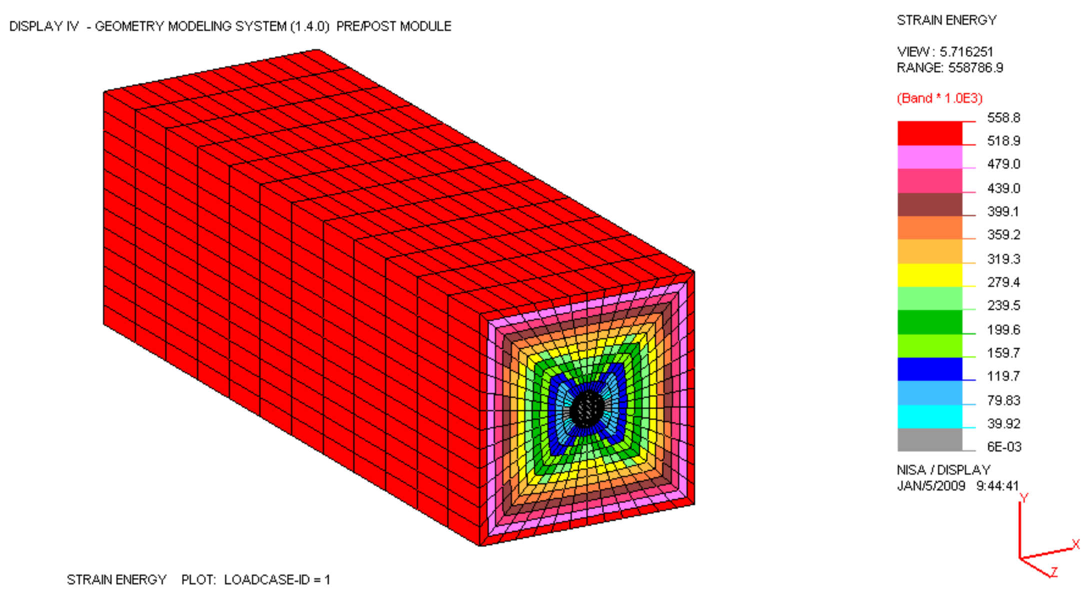

Figure 9 Strain energy (SE) pattern in transverse direction for 0.02 volume fraction.

(ii) When V_f is very from 0.02 to 0.14 and l/d = 19 and end lengths = 500 nm: In this case, VGCF is inside the RVE and volume fraction is considered for whole RVE. The end length are L_{e1} =500 nm and L_{e2}=500 nm and center length is always 3800 nm as shown in Figure 12. The properties of VGCF are predicted by using strain energy method. The strain energy pattern is shown in Figure 13 and Table 4 represents the SEin case of several fiber volume divisions.

Table 4: SEin case of several fibre volume divisions.

V_f	W	W_f	W_m	% difference (fiber)
0.02	1.81E-04	3.05E-06	1.78E-04	98.3
0.04	1.02E-04	1.54E-06	1.01E-04	98.4
0.06	7.23E-05	9.14E-07	7.14E-05	98.7
0.08	5.63E-05	6.04E-07	5.56E-05	98.9
0.10	4.61E-05	4.28E-07	4.57E-05	99
0.12	3.91E-05	3.19E-07	3.88E-05	99.1
0.14	3.39E-05	2.48E-07	3.37E-05	99.2

As clear from the Table 4 that the maximum strain energy in matrix as compared to fiber. This is also clear from here that for VGCF inside the RVE, the domination properties are matrix. Now geometry is also created when the volume fraction is considered for center part only i.e., V_f is only for center part length. The ERM/FEM is used for predicting the storage modulus in longitudinal direction, loss modulus and loss factor in fiber direction. The results of this modeling are approximately same for the case when the volume fraction of

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fiber is considered for whole RVE. For different end lengths such as 1000 nm and 1900nm the results are also predicted from FEM/SEM and ERM/FEM for different volume fractions (0.02 to 0.14) at constant l/d =19. The strain energy pattern is shown in Figure 14 and 15 for end length 1000 and 1900nm respectively. The volume fraction 0.02% to 0.14% is also considered for modeling the nanocomposite behavior. The strain energy pattern for 0.04% is shown in Figure16. From NISA output file the strain energy for fiber and matrix elements are taken for predicting the properties. The results show that the strain energy in matrix is more as compared to fiber, approximately 100% matrix properties are dominating.
(iii) When V_f is constant = 0.03 and aspect ratio is vary from 5 to 1000 and end lengths = 500 nm: In this case the volume fraction of fiber is constant i.e., 0.03 but aspect ratio of the fiber is varying from small l/d to large l/d. For this case also SEMutilized to forecastthe longitudinal storage moduli, loss moduliwith damping loss factor. The material and boundary conditions are same as used for VGCF within the RVE. Here, again the end length is taken as very important parameter for modeling on NISA software. The end lengths used are 600 nm and 1000 nm and simulation results are also predicted when end length is half the fiber length. For end length L_{e1} and L_{e2} =500 nm, the strain energy is shown in Table 5 for different aspect ratios. Strain energy pattern for l/d =5 and 100 is shown in Figure 17 and 18. It can be seen that as the aspect ratio increases the strain energy in matrix decreases because as length of fiber increases in constant volume fraction the fiber properties are more dominating.

Table 5: Strain energy for different volume fractions.

l/d	W	Wf	Wm	% difference(fiber)
5	1.73E-04	5.22E-07	1.72E-04	99.6
10	2.07E-04	2.32E-06	2.05E-04	98.8
20	2.30E-04	8.31E-06	2.22E-04	96.3
50	2.33E-04	2.75E-05	2.06E-04	88.1
100	2.12E-04	4.94E-05	1.63E-04	76.6
500	1.10E-04	7.05E-05	3.93E-05	35.9
1000	6.75E-05	5.37E-05	1.38E-05	20.44

(a) Square RVE with lateral consistentforce p: Here, the transverse load actingperpendicular to XZ plane. For end length $L_{e1,2}$=1900 nm, the transverse effect is predicted when volume fraction is varying from 0.02 to 0.14 and aspect ratio is constant (l/d=19). The boundary conditions are same as used for VGCF through the RVE and lateral loading is applied. In this case, also the matrix properties are dominating. Using FEM/Strain energy approach the transverse storage modulus E'_{22}, transverse loss factor η_{22} is calculated.

4.Theoretical Formulation

For forecasting the attributes of VGCF/pp nanoparticles:

(a) Storage modulus $E'_{11} = \frac{2 \times W}{V \times \varepsilon^2}$ (4a)

Where,
W = Total strain energy
V = Total volume of RVE
ε = strain

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(b) Loss factor in longitudinal direction $\eta_{11} = \left(\frac{\eta_f W_f + \eta_m W_m}{W}\right)$ (4b) Where,

η_f = loss factor of fiber
η_m = loss factor of matrix
W_f = strain energy in fiber
W_m = strain energy in matrix
W = total strain energy

(c) Loss modulus in longitudinal direction $E''_{11} = \eta_{11} \times E'_{11}$ (4c)

(d) Conventional rule of mixtures (ROM) = $E'_{11} = E_f V_f + E_m V_m$ (4d)

Where,
E_z = Young's modulus in longitudinal fiber direction
E_f = Young's modulus of fiber
E_m = Young's modulus of matrix
V_f , V_m = volume fraction of fiber and matrix

(e) Rule of mixtures in transverse direction,

$$E'_{22} = \frac{E_f \times E_m}{E_f \times V_m + E_m V_f} \quad (4e)$$

(f) The transverse storage modulus is calculating by using Effective Young's modulus and Poisson's ratio in transverse direction and Eq. (4a). The transverse loss factor η_{22} is calculated by using Eq. (4b).

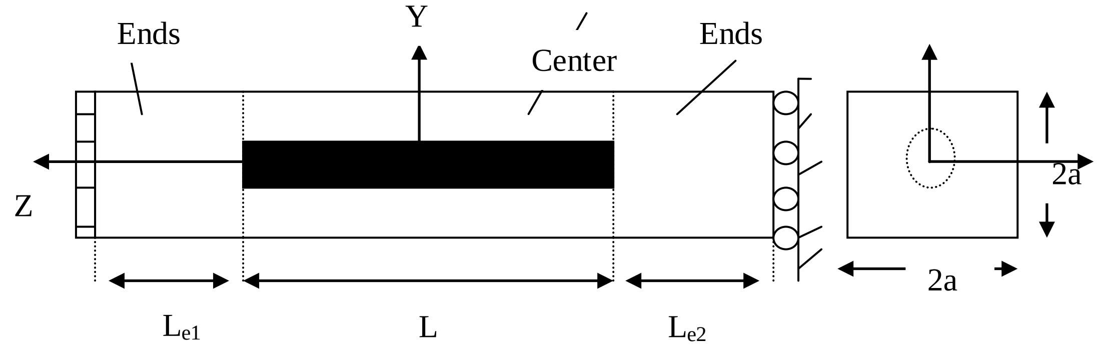

Figure 10: VGCF inside the RVE and axial stretch is applied.

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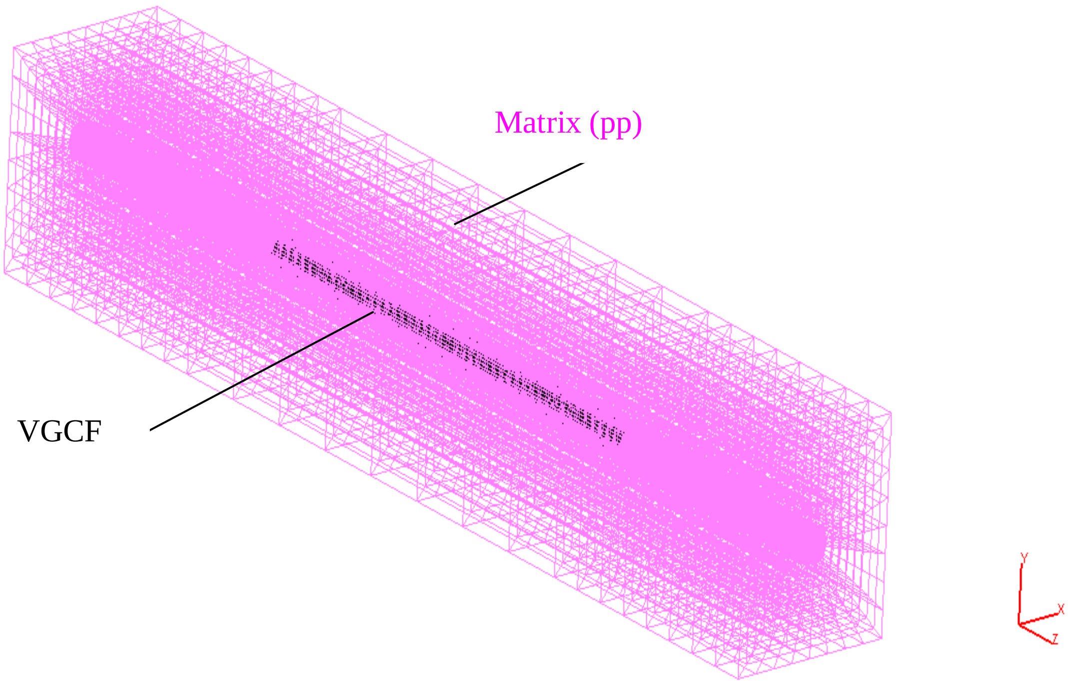

Figure 11: A full 3-D model for VGCF inside the RVE.

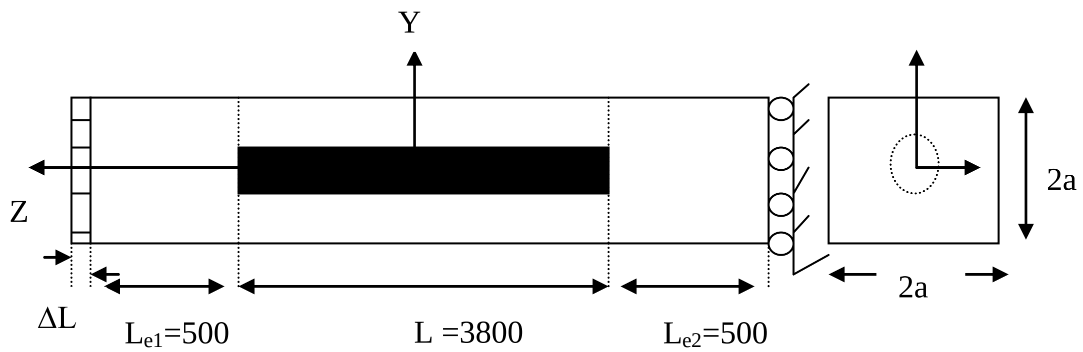

Figure 12: VGCF inside the RVE and end length (L_{e1}) =500.

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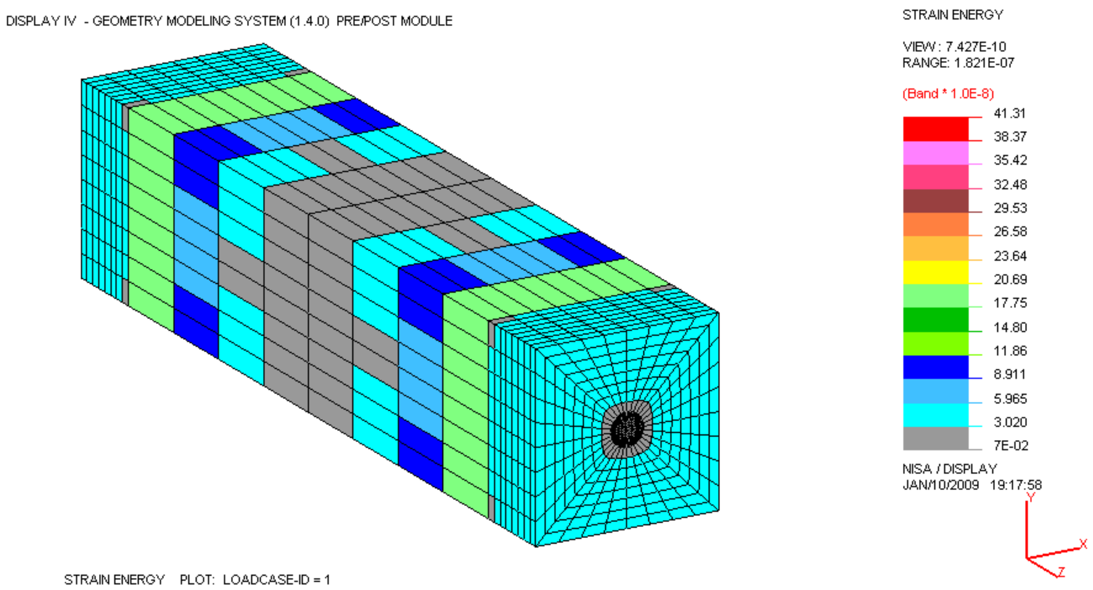

Figure 13: Strain energy when L_{e1} and L_{e2} =500, V_f = 0.02.

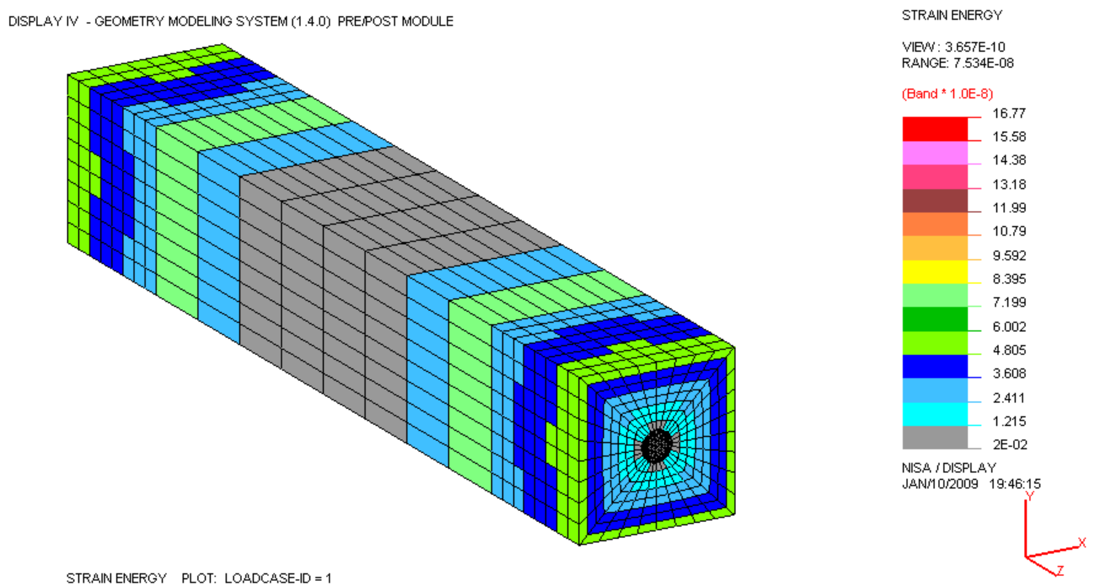

Figure 14: Strain energy when L_{e1} and L_{e2} =1000, V_f = 0.02, l/d =19.

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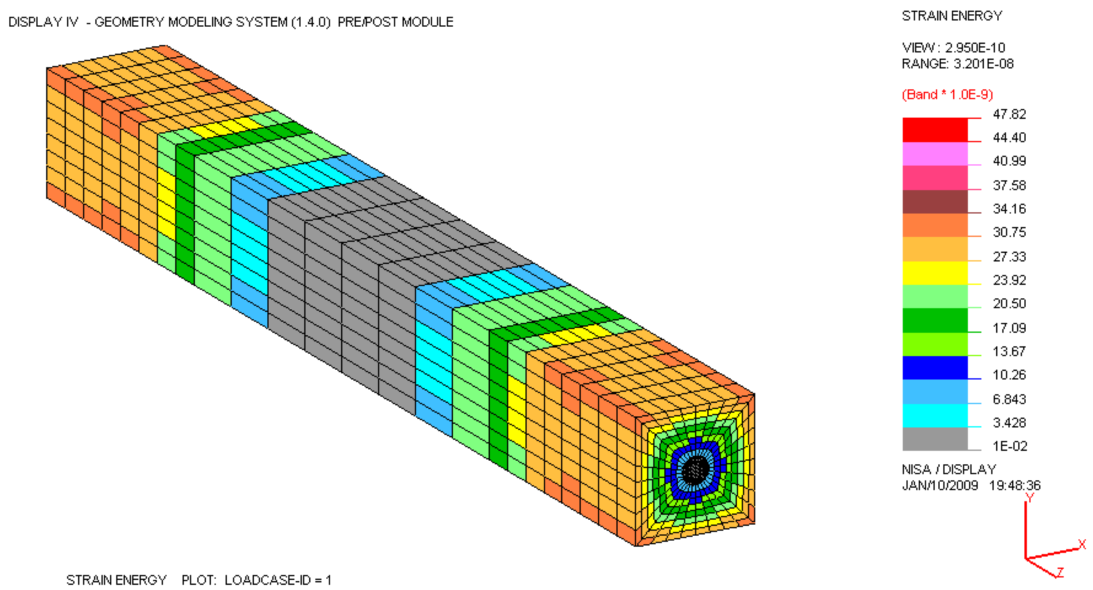

Figure 15: Strain energy when L_{e1} and L_{e2} =1900, V_f = 0.02, l/d =19.

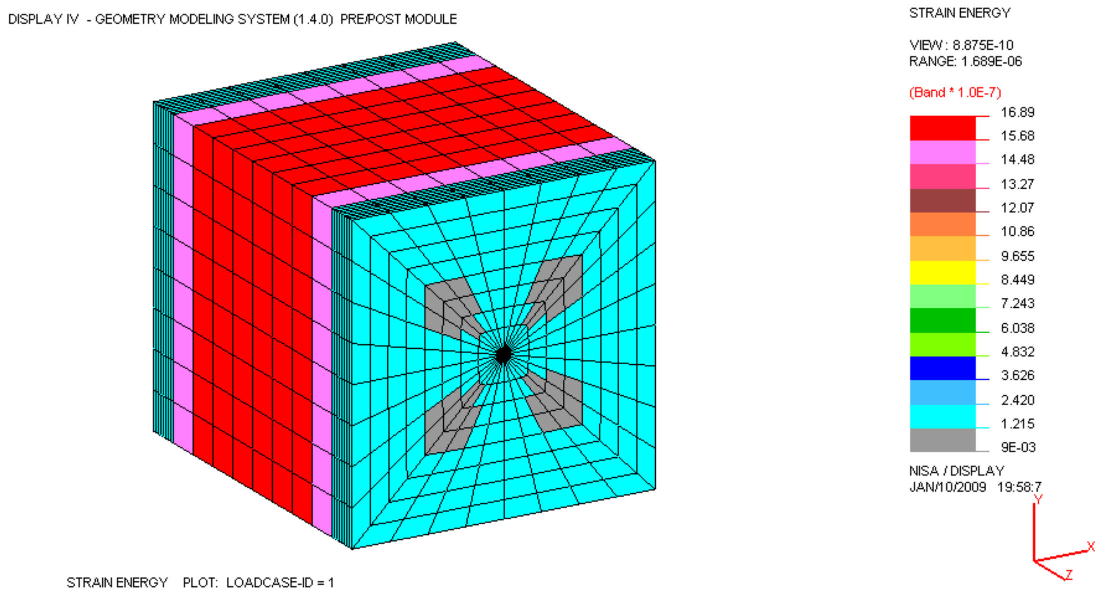

Figure 16: Strain energy when l/d=19 and V_f=0.04%.

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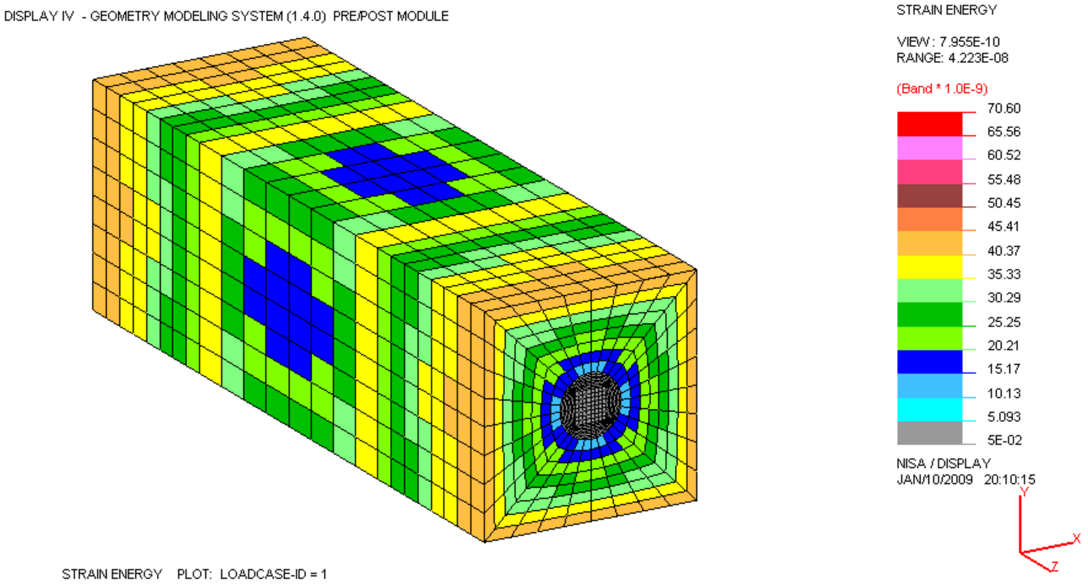

Figure 17: A 3-D model for longitudinal loading when V_f =0.03, l/d=5.

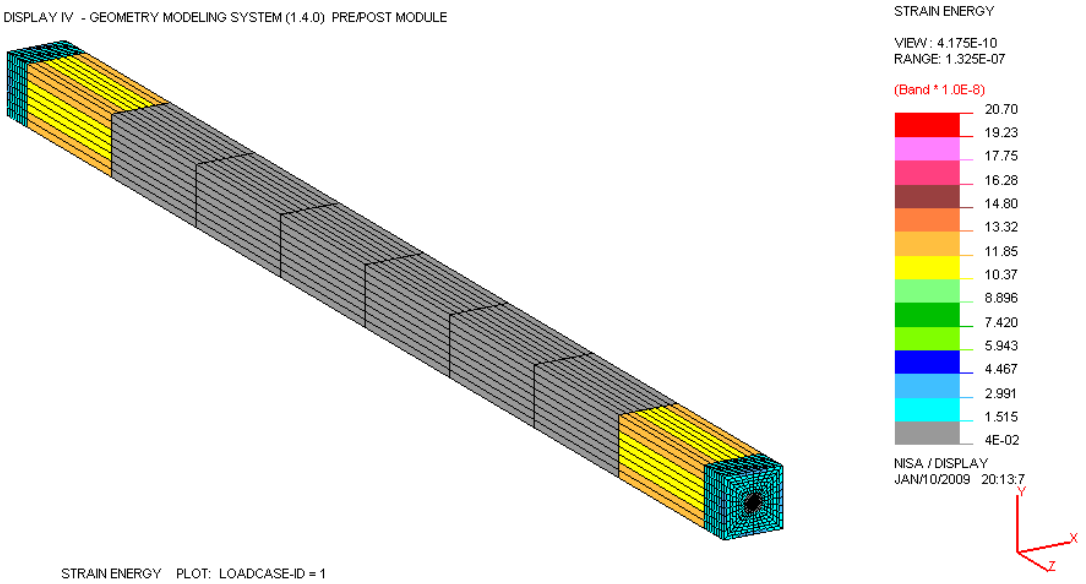

Figure 18: A 3-D model for longitudinal loading when V_f =0.03, l/d=100.

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5. Conclusions

VGCF weight fraction of 1% results in the same increase in composite elastic modulus as a composite with a 10% weight fraction of conventional carbon fibers. Continuum methods, molecular modeling and atomistic methods are used for predicting the various properties of nanocomposites. Some conclusions drawn on the basis of research conducted are presented here:

(i) FEM/Strain energy method can be used as an alternative tool for predicting the elastic and damping properties of VGCF/pp nanocomposites for longitudinal direction of fiber by considering geometric parameters.

(ii) Elastic modulus and loss factor predicted by FEM/Strain energy method correlate well with those obtained from experimental measurements.

(iii) As explained in the present study that the RVE for short fiber has two important segments: one center part and other are two ends on both face of center part. The end length is very important parameter for predicting the properties of nanocomposites by using simulation method.

(iv)Specimens of VGCF/pp nanocomposites can be fabricated successfully by using rectangular section die with extended nozzle on single screw extrusion machine.

(v)There is considerable improvement in longitudinal modulus of the VGCF/pp nanocomposite for addition of small amount of nanofiber.

(vi) The loss factor decreases 44% by adding 0.231% of fiber and 61% decrement at 0.464%.

Molecular modeling combined with continuum modelingcould be utilised for prediction the elastic and dynamic characteristics of nanocomposites. Finite element modeling of wavy fibers can also be done on simulation software.Sometimes the nano-reinforcement is hetergeneouslyspreaded out, forming groups with a higher density of SWNT. These groups are distributedall over the entire composite, creating restriction in locating isolated nanotubes. To anticipate the elastic and damping properties of these types of materials is a difficult task. During fabrication of the nanocomposites the nanomaterial agglomerates in the resin. To disperse the nanomaterials homogeneously in the polymer is a challenging work.

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