Evaluation of Mechanical Properties of Carbon Nanotubes Composite by Finite Element Method

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***Abstract*-Carbon nanotubes (CNTs) possess extremely high stiffness, strength and resilience and may provide ultimate reinforcing materials for the development of nanocomposites. Evaluating the effective material properties of such nanoscale materials is one of the important tasks. Simulations using molecular dynamics and continuum mechanics models can play significant roles in this development. Currently the continuum approach seems to be the only feasible approach for such large scale analysis.**

The finite element method-based continuum mechanics has been used to evaluate the mechanical properties of CNT based composites. The cylindrical as well as square representative volume element (RVEs) has been utilized in these simulations. Formulas to extract the effective material constants from solutions for the square RVEs under the axial stretch load is derived based on the elasticity theory. An extended rule of mixtures, based on the strength of materials theory for estimating the effective Young's modulus in the axial direction of the RVE, is applied for comparisons of FEM results. It has been observed that the addition of the CNTs in a matrix at volume fractions of only about 3.6%, the stiffness of the composite is increased by 33% for long CNT at $E^t/E^m = 10$, whereas there is no much improvement in stiffness has been noticed in case of short CNTS at $E^t/E^m = 10$. Effectiveness of composites is evaluated in terms of various dimensions like thickness, diameter and length of CNT. These results suggest that short CNTs in a matrix may not be as effective as long CNTs in reinforcing a composite.

The comparisons of mechanical properties between cylindrical and square RVE have also been made for single CNT bases composite. Since the mechanical properties obtained through cylindrical RVE overestimates the youngs's modulus thereby the square RVE is preferred for the simulations. The mechanical properties using cylindrical and square RVEs are also evaluated for multiple CNTs based composites and compared with each other.

Keywords—carbon nanotubes, finite element method, RVE, CNT.

I.INTRODUCTION

Carbon nanotubes (CNTs) discovered first by Iijima in 1991 [1] possess exceptionally high stiffness, strength and resilience as well as superior electrical and thermal properties which may become the ultimate reinforcing materials for the development of an entirely new class of composites. It has been demonstrated that with just 1% (by weight) of CNTs added in matrix, the stiffness of the resulting composite can increase between 36-42% and the tensile strength by 25%[2].The mechanical load carrying capacities of CNTs in nanocomposites have also been demonstrated in experiments [2] and preliminary simulations [5].All these studies show the great potentials of CNT based composites as well as the enormous challenges in the development of such nanocomposites.

Typically carbon nanotubes are long tiny cylinders of graphite structure with hemispherical cap at each end. The length of these nanotubes ranges from few tens of nanometers to several micrometers and the outer diameter usually extend from about 2.5mm to 30 mm .CNTs are in different sizes and forms when they are dispersed in a matrix to make nanocomposites. They can be single walled or multi-walled with length of few nanometers or few micrometers and can be straight, twisted and curled or in the forms of ropes. A single walled carbon nanotube (carbon SWNT) can be considered as a sheet of graphite that has been rolled into tube. Their distribution and orientation in the matrix can be uniform and unidirectional or random. The most important features of carbon nanotubes are their extremely stiff, strong and resilient and therefore may be ideal for reinforcing composite material.

A. Objective

The present work deals with the evaluation of the mechanical properties of carbon nanotube (CNT) composites by finite element analysis. The work has been presented in following sections by considering various aspects:

- Evaluation of mechanical properties of carbon nanotube composites using single CNT based model.
- To study the effect of CNT material properties on the overall mechanical properties of the CNT composites.
- Effect of CNT dimensions on the mechanical properties of carbon nanotube composites.
- Evaluation of mechanical properties of carbon nanotube composites using long and short CNT for square and cylindrical RVEs with hemispherical end cap and without hemispherical cap ends.
- Evaluation of mechanical properties of carbon nanotube composites with multiple CNTs.

II. EVALUATION OF EFFECTIVE MATERIAL PROPERTIES OF CARBON NANOTUBE BASED COMPOSITES USING CYLINDRICAL RVE

It is assumed that both the CNTs and matrix in RVE are continue of linearly elastic, isotropic and homogeneous materials with given Young's modulus and poisons ratio. It is also assumed that CNTs and matrix are perfectly bonded at the interfaces in the RVE to be studied. Other material models and interface conditions [7] can certainly be considered in more sophisticated investigations.

RVE containing single CNT or multiple CNT determine by the main criterion that it should be large enough to be representative of material and the small enough to model and analyzed efficiently using a solution method. Under the above assumptions there will be four effective material constants to be determined for the CNT based composite namely two young’s modulus and two poisons ratio.

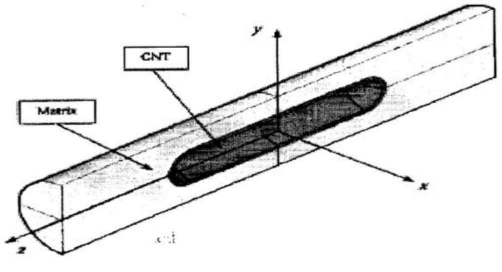

Fig.1: A cylindrical RVE shown in a cut- through view

To derive the formulas for extracting the material constants a homogenized elastically model corresponding to the RVE considered. The geometry of elasticity model is corresponding to hollow cylindrical RVE with length L, inner radius ri and outer radius R so that analytical solutions can be obtained.

This geometry can account for the cases when the CNT is relatively long and thus all the way through the length of RVE. In the case that the CNT is relatively short and does fully inside the RVE solid cylindrical RVE can be used for extracting the material constants since the elasticity solutions are difficult to find in this case. The elasticity model has single material with the four effective materials constant to be determined. The material of elasticity model is transversely isotropic and the general 3-D stress strain relation in the coordinates (x,y,z).

To determine the four unknown material constant four equations based on the elasticity theory will be needed. Three loading cases have been devised in the following subsections to provide four such equations. Note that for transversely isotropic materials the other materials are related to four constants. From three loading cases only one loading case with cylindrical RVE under and axial stretch have been devised to provide such a equations based on elasticity theory.

A. CNT through the length of the RVE

This is the case when the CNT is relatively long with the large aspect ratio and therefore a segment can be modeled using an RVE.

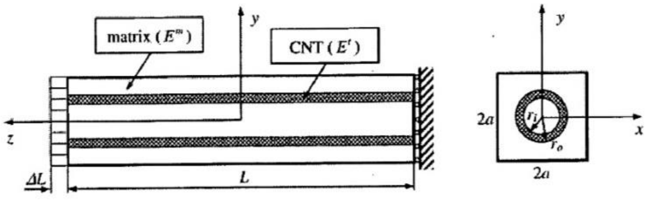

Fig 2: CNT through the length of the RVE

The volume fraction of the CNT (a tube, fig 2) is given as

$V_t = (r_o^2 - r_i^2) / (R^2 - r_i^2)$

Apply the strength of materials theory and assume the matrix and CNT deform independently of each other under the stretch ΔL (Fig. 2) .By considering the compatibility of strain and equilibrium of stresses, one obtains the following expression for the effective Young’s modulus in the axial direction .

$E_z = E^t V^t + E^m (1- V^t)$

Where E^m and E^t are the young's modulus of the matrix and CNT respectively .This is the same rule of mixtures as applied for predicting the effective young's modulus in the fiber direction for conventional fiber reinforced composites and is a close approximation of or identical (if matrix and fiber have the same poisons ratio to the elasticity solution [12].

B. Numerical Results

To evaluate the effective material constant of a CNT based nanocomposite the cylindrical RVE for single wall carbon nanotube in a matrix material is studied using the finite element method .The deformation and stresses are computed first for the loading case. The FEM results are then processed applied to extract the effective Young's modulus and poisonous ratio for CNT based composite. Two examples are studied one an RVE with long CNT and other and RVE of same size but a short CNT. In all the cases asymmetric FEM models are used since RVE have asymmetric geometry. Quadratic elements for asymmetric problems are employed which are a second order elements and offer a better accuracy in stress analysis. The value of dimensions and material constant are chosen within the wide range of those for CNT as reported in a references [13-17] and can be modified or fine-tuned readily for a specific case in future simulations. The finite element mesh is small elements comparable in size to those for the CNT are also needed in the matrix surrounding the CNT ensure the connectivity and to avoid the elements with large aspect ratios.

The finite element mesh is shown in fig 3. Small elements comparable in sizes to those for the CNT are also needed in the matrix surrounding the CNT to ensure the connectivity and to avoid elements with large aspect ratios.

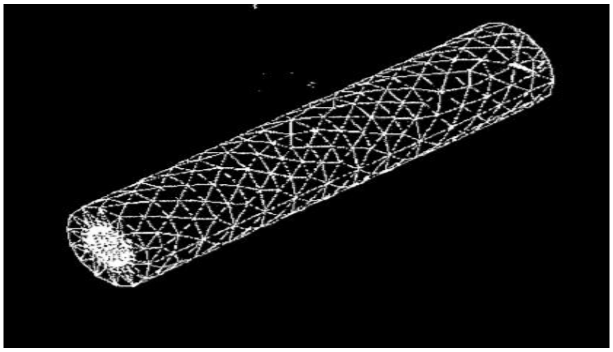

Fig 3: Finite element mesh for a CNT through the length of the cylindrical RVE

Table 1: Computed effective material constants for fig 2: CNT through the length of cylindrical RVE

E^t / E^m	FEM results		ERM results
	E_z / E_m	V_{zx}	E_z / E^m
5	1.2030	0.379	1.1948
10	1.4549	0.44	1.4384
50	3.3290	0.772	3.3866
200	10.7794	1.49	10.6925

The FEM results for the effective material constants of the CNT composite studied are listed table 1 .The strength of materials solutions for the effective Young's modulus E_z is also listed in table 3.1 for comparison. The strength of materials solutions is identical to those using the FEM for simple geometry and load condition.

The results reveal that the increase of the stiffness of the composite can be significant specially in the CNT exile direction. With the volume fraction of the CNT being at only about five percent the stiffness of the composite in the axial direction can increased by more than 9 times compared with that of matrix

A short CNT inside the RVE

Next an RVE for a short CNT in a matrix is studied. All the dimensions for the RVE are the same as in the previous example accept for the CNT total length which is reduced to 50 mm (with the two hemispherical end caps). The material constants used for the CNT and matrix are the same as in the first example.

Table 2: Computed effective material constants CNT inside the RVE

E^t / E^m	FEM results		ERM resultsE$_z$ / E^m
	E_z / E^m	V_{zx}	
5	0.9971	0.311	0.9701
10	1.0826	0.327	1.0628
50	1.5450	0.393	1.4550
200	1.8063	0.426	1.7879

Note: CNT modulus E^t = 1000GPa, CNT thickness= 0.4 mm, volume fraction=0.0211 at E^t / E^m = 10

The strength of materials solutions for the stiffness in the axial direction E_{zs} using the extended rule of mixtures are required closed to FEM solutions. Therefore, the extended rule of mixtures may serve as a quick tool to estimate the stiffness of a CNT based composite in the axial directions when the CNT are relatively short, while the conventional rule of mixtures can continue to serve in the cases when CNTs are relatively long.

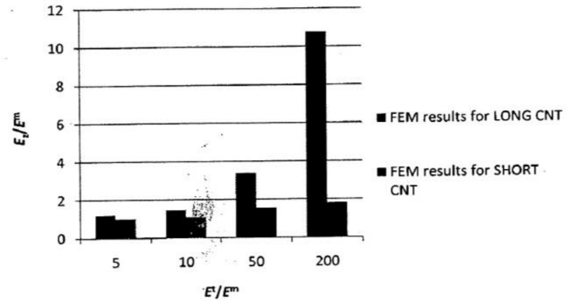

Fig 4: Comparison of FEM results for long and short CNTs using cylindrical RVE

The increases of the stiffness in axial direction are moderate for E^t / E^m = 10, 50 and 200 due to the small volume fraction of the CNT about (2%). At E^t / E^m =5, the stiffness is actually dropped due to reason that the increase of the stiffness in the CNT cannot compensate the loss of material due to reduced volume. All these results suggest that short CNT in matrix may not be as effective as long CNTs in a reinforcing the composites.

III.EVALUATION OF EFFECTIVE MATERIAL PROPERTIES OF CARBON NANOTUBE BASED COMPOSITES USING RVE

To derive the formulas for extracting the equivalent material constant a homogenized elasticity model for a square RVE is considered. The geometry of elasticity model is corresponding to solid square RVE with length and cross sectional area.

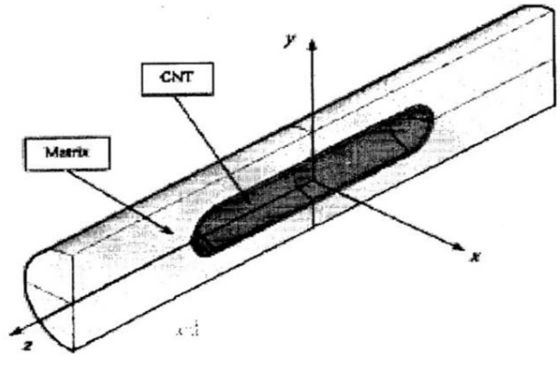

Fig 5: A square RVE containing a short CNT shown in cut through view

To determine the four unknown material constant for equation based on the elasticity theory will be needed .Two loading cases have been devised in the following subsections to provide a four such equations on the elasticity theory. From two loading cases only one loading case with a square RVE under axial stretch ΔL have been devised to provide such equations based on the elastic theory

Similar to cylindrical RVE cases simple rules of mixtures can be established based on the strength of materials theory. These rules of mixtures can be applied to verify the numerical results for the effective Young's modulus in the CNT axial direction. More general theories and extended results in the context of fiber reinforced composites its can be found in a reference [8].

A. NUMERICAL EXAMPLES

The FEM results are proceed to extract the effective young modulus and poisons ratio for the CNT based. Two numerical examples are studied one RVE with long CNT and other on RVE with short CNT. In all the cases quadratic solid elements are employed for the 3D models and quadratic 8 node elements are used for 2-D planes strain models both of which offer higher accuracy in FEM stress analysis.

Table 3: Computed effective material constants for CNT through the length of the square and cylindrical RVE

E^t / E^m	FEM results for square RVE		ERM results	FEM results for cylindrical RVE		ERM results
	E_z / E^m	V_{zx}	E_z / E^m	E_z / E^m	V_{zx}	E_z / E^m
5	1.1423	0.408	1.1446	1.2030	0.379	1.1948
10	1.3520	0.486	1.3255	1.4549	0.44	1.4384
50	2.696	0.645	2.7723	3.3290	0.472	3.3866
200	8.210	0.644	8.190	10.7794	0.49	10.6925

Note: Modulus ratio E^t / E^m = 10 , CNT thickness = 0.4 mm, volume fraction = 3.617 %

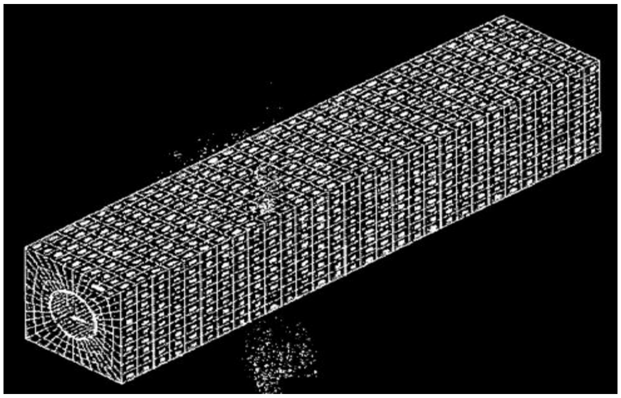

Fig 6 : A finite element mesh of a 3-D FEM model for the square RVE with a long CNT (CNT thickness = 0.4 mm)

The results reveal that increase of the stiffness of the composite can be significant in the CNT axial direction. With a volume fraction of the CNT being only about 3.6% the stiffness of the composite in the axial direction can increase by above 33% compared with that the matrix when $E^t / E^m = 10$

For comparison the effective material constants obtained using the cylindrical RVE which is of the same size (same length and same diameter of a cylindrical RVE = 2a of a square RVE) is listed in a table 3. It is a seen that the cylindrical RVE overestimate the young modulus. This is explained that the cylindrical RVE overestimate the volume fraction of CNT due to the negligence of the small amount of a matrix material (at the four corners of the square RVE) in the cylindrical RVE.

With addition of the CNT in a matrix at the volume fractions of 3.6% the stiffness of the composite increased by 33% as compared with that of the matrix in the case of a long CNT at $E^t / E^m = 10$ whereas in case of a short CNT in addition the stiffness in the axial direction is moderate due to the small volume fraction of the CNT about 1.6% .These result suggest that short CNT in a matrix may not be effective as long as CNT in the reinforced a composite.

The strength of a material solution for the stiffness in the axial direction using the extended rule of a mixture is quiet close to the FEM solution which is based on 3-D elasticity with a difference of only about 1%.

Therefore the extended rule of a mixture may serve as quick tool to estimate stiffness of the CNT based composite in the axial direction when the CNT is relatively short while the conventional rule of a mixtures can continue to serve in a case when CNTs are relatively long.

IV.FINITE ELEMENT ANALYSIS

The basic steps involved in finite element analysis given below:

1. Discretization of the domain
2. Application of field boundary conditions
3. Assembling the system equations
4. Solutions for the system equations
5. Review of results

1. Discretization of the domain:

Here the task would be divide the continent understanding into number of subdivisions called elements. Based upon the geometry the continuum or the system under study can be divided into number of elements.

- If the continuum is single point it can be discretized using point elements.
- If the continuum is 1-D it can be discretized using line elements
- If the continuum is 2-D it can be discretized using area elements
- If the continuum is 3D it can be discretized using volume elements

2.Once the discretization is done include the known field/boundary conditions which shall serve as a references and helps us in solving for the unknowns.

3. Once the reference or known conditions are imposed define a set of equations which are suitable to define the behavior of system. This involves formulation of respective characteristics equation matrices.

4. Once the equations are set up solve the same to know the unknowns and get insight into system behavior. That is basically the system of matrices which are nothing but a set of simultaneous equations are solved.

5. Upon the completion of a solution review the results

B. ANSYS FEATURES AND CAPABILITIES

ANSYS is a finite element modeling software package for analysing a wide variety of engineering problems. These problems include static/ dynamic analysis (both linear and non linear), heat transfer and fluid problems as well as acoustic and electromagnetic problems. The problems in employs the Matrix displacement method of analysis best on finite element idealization. In general a finite element solution may be broken into the following three stages (ANSYS manual 11.0) as given under.

Pre processing

In this is the first stage of analysis and it includes the following procedural steps

1. Defining the problem i.e structural , fluid or thermal
2. Selection of the element
3. Assigning the material properties, real constant (may be different for a different part of a structure)
4. Modeling of structure
5. Meshing to discretized the structure into elements

Solution

In this second stage of analysis solve the problems which is modeled in the pre-processor and it includes the following steps:

- Application of boundary conditions i.e displacement constraints
- Application of loading on the structure in terms of pressure, nodal loads ,inertia, surface load ,temperature etc
- Analysis type i.e static ,harmonic ,spectrum, transient etc
- Solve for a current load step.
- Solution provides the required results .This results are available in a graphical ,stress contour form and also in list format.

In general Post processor mode following important results can be observed

- Deflection
- Stresses and strains
- Nodal displacements
- Reaction solution
- Nodal displacements

ELEMENT USED IN ANALYSIS

For the analysis of carbon nanotube composite solid 186 element is used ANSYS for modeling.

SOLID 186 ELEMENT DESCRIPTION

SOLID 186 is higher order 3-D 20 node solid element that exhibit quadratic displacement behavior. The element is defined by 20 nodes having a three degree of freedom per node translation in the nodal x y and z directions. The element supports plasticity, hyper elasticity creep, stress stiffening, large deflection and large strain capabilities. It also has mixed formulation capability for simulating deformation of nearly incompressible elastoplastic materials and fully incompressible hyperelastic materials.

SOLID 186 is available into forms

- Structural solid (KEYOPT (3)=0 , the default)
- Layered solid (KEYOPT (3) = 1)

Solid 186 structural solid element descriptions

Solid 186 structural solid is well suited to modeling irregular meshes (such as those produced by various CAD / CAM systems). The element may have any spatial orientation.

SOLID 186 Structural Solid Geometry

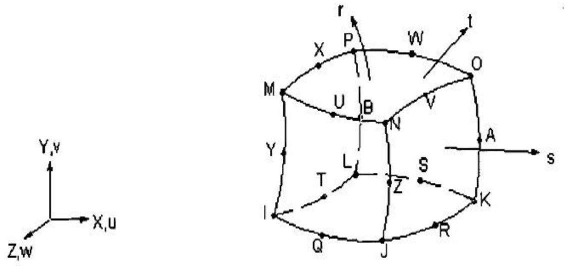

Fig 7: Solid 186 structural

Table 4 : Input data for SOLID 186 element

Element Name	SOLID 186 structural solid
Nodes	I, J, K,L,M,O,P,R,S,T,U,V,W,X,Y,Z,A,B
Degree of freedom	UX,UY,UZ
Material properties	EX,EY,EZ,ALPX,ALPY,ALPZ (or CTEX,CTEY,CTEZ or THSX,THSY,THSZ) PRXY,PRYZ,PRXZ(or NUXY,NUYZ,NUXZ) DENS,GXY,GYZ,GXZ,DAMP

5.6 MODELING OF CARBON NANOTUBES IN ANSYS 11.0

Table 5: Details of input and output data in ansys

1	Preferences	Structural
2	Element type	Solid 186 3 D 20 nodes solid element
3	Material properties	Define modulus of elasticity [E] for Matrix and CNT poisons ratio for Matrix and CNT (v)
4	Modeling of carbon nanotube	Create a key points in a plane .Create a lines and arks by joining the key points .Create areas by joining a lines and arcs. Generate a volume (and it corresponding key points lines areas) by offsetting from an area
5	Element size or number of divisions	Provide suitable element sizes (number of divisions) for the volume formation of purpose
6	Glue volumes	Generate new volumes by gluing input volumes
7	Meshing	Mesh the volume mapped 4 or 6 sided
8	Boundary conditions	Resisting the model at one end on the nodes by restraining all degree of freedom
9	Load application	Apply a uniform pressure on other end in the form of nodal loads .The pressure acting on the surface has been converted into nodal loads
10	Solution	Analyze the structure for a different load cases by performing current load steps

11	Post processing	Read the results in a general Post processor mode. Check the reaction solution deformation and stress values at different and required cross sections

V.RESULTS

C. Effect Of Material Properties On The Mechanical Properties Of The Cnt Composite

Case 1: CNT inside the cylindrical RVE with hemispherical end caps and without hemispherical end caps

In this case the material properties of cylindrical RVE evaluated using the hemispherical end caps and without using hemispherical and caps for CNT inside the RVE.

Table 6: Computed effective material constants for CNT inside the cylindrical RVE with and without hemispherical end cap

E^t / E^m	FEM results for cylindrical RVE with end caps		ERM results	FEM results for cylindrical RVE without end caps		ERM results
	E_z / E^m	V_{zx}	E_z / E^m	E_z / E^m	Vzx	E_z / E^m
5	0.9971	0.311	0.9701	0.9608	0.300	0.9701
10	1.0826	0.327	1.0628	1.0022	0.317	1.0628
50	1.5450	0.393	1.4550	1.2575	0.402	1.4550
200	1.8063	0.426	1.7879	1.5858	0.490	1.7879

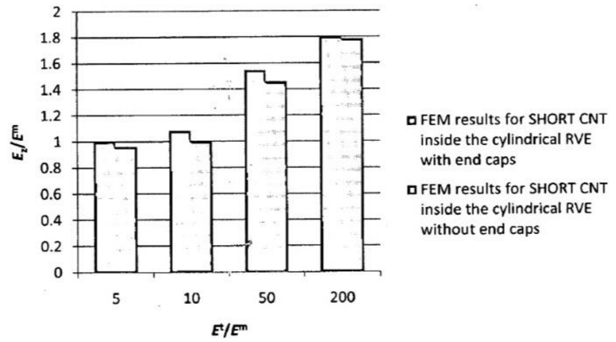

Fig 8: Comparison of FEM results for short CNTs inside the cylindrical RVE with and without using end caps

Case 2: CNT inside the square RVE with and without hemispherical end caps

Et / Em	FEM results for cylindrical RVE with end caps		ERM results	FEM results for square RVE without end caps		ERM results
	Ez / Em	Vzx	Ez / Em	Ez / Em	Vzx	Ez / Em
5	0.980	0.300	0.976	0.930	0.300	0.976
10	1.046	0.321	1.049	0.971	0.311	1.049
50	1.197	0.431	1.169	1.179	0.36	1.169
200	1.389	0.522	1.396	1.321	0.45	1.396

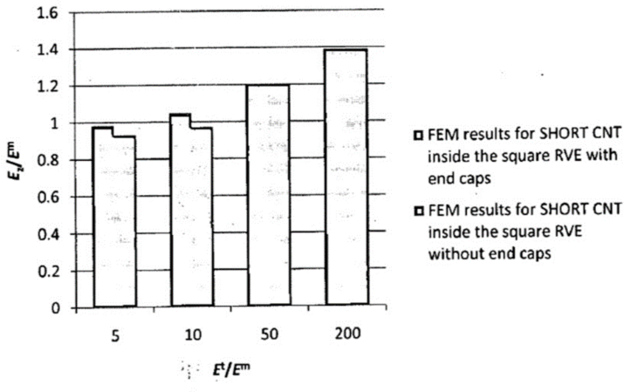

Fig.9: Comparison of FEM results for short CNTs inside the square RVE with and without using end caps hemispherical end caps are gives some difference in FEM results due to small change in effective length.

6.2 EFFECT OF CNT DIMENSIONS ON THE MECHANICALPROPERTIES OF CARBON NANOTUBE COMPOSITES

Changing thickness and diameter of carbon nanotube how the mechanical properties of carbon nanotube composites are going to change is shown through bar charts for both long and short cylindrical and square RVE.

The effect of CNT thickness

The dimensions are:

For matrix: Length L= 100 nm, outer radius R = 10 nm

For CNT: Length = 100 nm, outer radius r_o = 5 nm, inner radius r_i = 5nm

The young's moduli and poisons ratio used for the CNT and matrix are :

CNT: E^t = 1000 *n*N/m^2 (GPa), V^t = 0.3

Matrix : E^m = 5,20,100 and 200 *n*N/m^2 ,$V^{m = 0.3}$

Table 8: Computed effective material constants for the long CNT through length of the square and cylindrical RVE at E^t / E^m = 10

E^t / E^m	CNT thickness (t)	FEM results for square RVE		FEM results for cylindrical RVE	
		E_z / E^m	V_{zx}	E_z / E^m	V_{zx}
10	0.4	1.3520	0.486	1.4549	0.44
	0.6	1.4625	0.530	1.6994	0.489

	0.8	1.6177	0.566	1.8328	0.525
	1	1.7201	0.59	1.9742	0.555
	1.2	1.8237	0.665	2.0121	0.584

Material properties are also evaluated using multiple CNT for square and cylindrical RVE with short and long CNT and the material properties obtained by cylindrical RVE gives higher Young's modulus in axial direction due to negligence of small amount of matrix material (at the four corner of a square RVE) in the cylindrical RVE.

VI.CONCLUSION

Within the scope of the present study, the following conclusions are drawn.

- Comparison between square and cylindrical RVE for long CNT through the length are considered and observed that the cylindrical RVE overestimates the Young’s moduli. This can be explained as cylindrical RVE overestimates the volume fraction of the CNT due to the negligence of the small amount of matrix material (at the four corners of the square RVE) in the cylindrical RVE.
- At Et /Em = 5, the stiffness is actually dropped due to the reason that the increase of the stiffness in the CNT cannot compensate the loss of the material due to reduced volume in the case of short CNT. These results suggest that short CNTs in a matrix may not be as effective as long CNTs in reinforcing the composites.
- The effective material properties obtained by square and cylindrical RVE for CNT inside the RVE with and without hemispherical end caps gives some difference in FEM results due to small change in effective CNT length.
- The effect of change in diameter is more as compared to thickness for both square and cylindrical RVEs.
- Under axial stretch loading case for the square and cylindrical RVE the Young's modulus and poisons ratio are obtained in the axial direction in the present study. The other material properties young's modulus and positive ratio are evaluated in the transverse plane by considering lateral uniform load as a future work.
- From the three way of nanoscale representative volume elements for the analysis of CNT based composite only cylindrical and square RVE used in the present study. The other way is through hexagonal RVE also the properties of carbon nanotube composite can be evaluated.
- As the computing power and confidence in the simulations of the CNT based composite increase large scale 3-D models containing 100 or even more CNT can be employed to investigate the interaction among the CNT in a matrix and to evaluate the effective material properties.

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