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# Finite Element Analysis of Broken Single Walled Carbon Nanotube

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**ABSTRACT**: In CNT based composites one or more CNTs may break due to different reasons and it is possible that a CNT based composite is having broken CNTs in it. Therefore it is important to understand the influence of such broken CNT in the nanocomposites in terms of stress redistribution and possibilities of failure. Present study deals with studying the effect of a broken CNT in the composite in the form of normal and shear stress redistribution surrounding the broken CNT in a CNT-based composite. Near broken CNT small debonding between CNT and matrix has been considered as a crack. At the crack front stresses responsible for three modes of fracture have been studied and stress distributions ahead of crack front along the interface of CNT and matrix has been found. Components of strain energy release rates (SERR) responsible for three modes of fracture are also calculated using virtual crack closure integral technique (VCCT). It has also been found that the debonding between CNT and matrix is due to pure mode II component of stress and mode I and mode II stress components does not contribute to the debonding. Effect of volume fraction on stress distribution and on strain energy release rate has also been studied.

**KEYWORDS**: CNT based composites, strain energy release rate, Modes of fracture, stress distribution.

## I. INTRODUCTION

Composite material consists of two or more constituents/materials (or phases), designed to improve the overall mechanical properties. In general all composites have two or more constituents, in which the constituent that is continuous in the composite is called as the matrix. The basic idea of the composite is to optimize material properties of the composite, i.e., the properties of the matrix are to be improved by incorporating the reinforcement phase or reinforcement such as fiber, particles or flakes. In general, fibers are the principal load-carrying constituents while the surrounding matrix just helps to keep them in desired location and orientation and also act as a load transfer medium between them. Examples of composite materials are Concrete, Glass fiber reinforced plastic, Carbon nanotubes in polymer etc.

Since the discovery of carbon nanotubes by Ijimain 1991 [1], they have excited scientists and engineers in the research field. They are extremely small in size, having strengths 20 times that of high strength steel alloys and half as dense as aluminium. The diameter of CNT is in the nanometer range and their length can be in the micrometer range. Carbon nanotubes not only exhibit exceptionally high stiffness, strength and resilience but also possess superior electrical, thermal and mechanical properties. These nanotubes are also chemically inert and are able to sustain a high strain without breakage. These properties of CNTs are believed to be ideal for using them as reinforcements in high performance structural composites. Therefore, among many potential applications of nanotechnology, nano composites have been one of the latest research areas in the recent years and hence a large number of works has already been reported in the direction of modelling and characterization of CNT based composites.

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## II. RELATED WORK

Carbon nanotubes are fullerene-related structured discovered by a Japanese electron microscopistIijima S. [1]. Liu & Chen [2] determined the elastic and mechanical properties of CNTs using 3-D nanoscale representative volume element using FEM. Earlier works [3, 4] determined the elastic and mechanical properties of CNTs and reported that the Young's modulus and Poisson's ratio of CNTs were in the order of 1 TPa and 0.28 respectively. Thostenson et al. [5] and Lau and Hui [6] presented a comprehensive review on manufacturing processes, mechanical and electrical properties and applications of CNT-based composites. Odegard et al. [7] proposed a method for developing structure–property relationships of nano-structural materials. Montazeri et al. [8] investigated the mechanical properties of multi-walled CNT (MWCNT)/Epoxy composites and concluded that acid-treated MWCNT was more efficient as reinforcement in Epoxy matrix than untreated MWCNT.

Lau and Hui [9] reported that the use of MWCNTs as intrinsic reinforcements for composite structures might not allow the maximum strength to be achieved due to non-uniform axial deformation inside the MWNTs and hence the use of single-walled carbon nanotubes (SWCNTs) might be more beneficial for advanced composites structures. Effective mechanical properties of CNT-based composites are evaluated using a 3-D nanoscale RVE based on the 3-D elasticity theory and solved by the finite element method (FEM) by Chen and Liu [10]. Lusti and Gusev [11] performed FE analysis for calculation of Young's modulus and coefficients of thermal expansion (CTE) of CNT/Epoxy composites for different fiber orientation of CNTs in matrix, and concluded that CNTs could be more efficient as compared to conventional glass or carbon fibers.

## III. FINITE ELEMENT MODELLING OF CNT BASED COMPOSITES

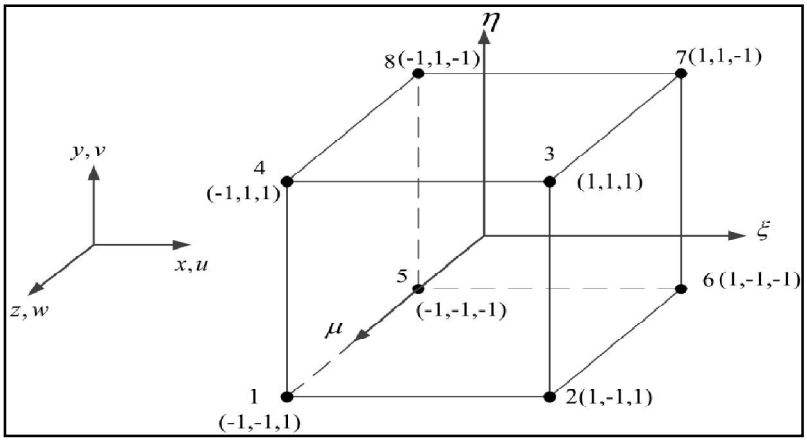


Fig.2. Eight noded SOLID45 element

Figure 3.1 shows the 8-noded SOLID45 element in natural coordinate system. Natural coordinate systems are dimensionless and have a maximum absolute magnitude of one. Being an isoperimetric element, the geometric variables are expressed in a similar way as field variable.

x, y, z = Geometric variables,
u, v, w = Field Variables
N1 (i =1, 2, 3….8) = shape functions
xi, yi, zi = Nodal co-ordinates
ui, vi, wi = Nodal displacements

$$x = N_1 x_1 + N_2 x_2 + N_3 x_3 + N_4 x_4 + N_5 x_5 + N_6 x_6 + N_7 x_7 + N_8 x_8$$

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$$y = N_1 y_1 + N_2 y_2 + N_3 y_3 + N_4 y_4 + N_5 y_5 + N_6 y_6 + N_7 y_7 + N_8 y_8$$

$$z = N_1 z_1 + N_2 z_2 + N_3 z_3 + N_4 z_4 + N_5 z_5 + N_6 z_6 + N_7 z_7 + N_8 z_8$$

Similarly, the field variables are also represented as

$$u = N_1 u_1 + N_2 u_2 + N_3 u_3 + N_4 u_4 + N_5 u_5 + N_6 u_6 + N_7 u_7 + N_8 u_8$$
$$v = N_1 v_1 + N_2 v_2 + N_3 v_3 + N_4 v_4 + N_5 v_5 + N_6 v_6 + N_7 v_7 + N_8 v_8$$
$$w = N_1 w_1 + N_2 w_2 + N_3 w_3 + N_4 w_4 + N_5 w_5 + N_6 w_6 + N_7 w_7 + N_8 w_8$$

Above equations can be written as

$$x = \sum_{i=1}^{8} N_i x_i y = \sum_{i=1}^{8} N_i y_i z = \sum_{i=1}^{8} N_i z_i$$

$$u = \sum_{i=1}^{8} N_i u_i v = \sum_{i=1}^{8} N_i u_i w = \sum_{i=1}^{8} N_i w_i$$

## IV. MODES OF FRACTURE AND STRAIN ENERGY RELEASE RATE

Debonding between fiber and matrix is probably the most critical and studied, failure mode of composite material. To characterize the onset and growth of debonding in composite materials the use of fracture mechanics has become common practice over the past two decades.

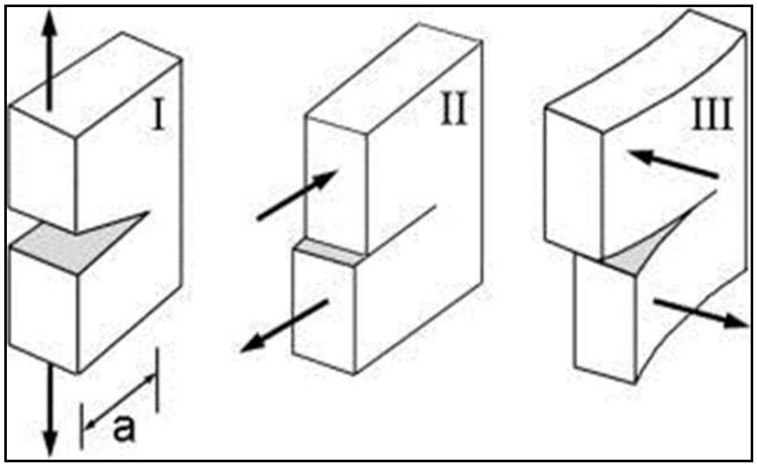


Fig.3. Modes of fracture

There are three modes of fracture viz. the mode I due to interfacial tension or opening, mode II due to interfacial sliding shear, and the mode III due to interfacial tearing as shown in Figure 3. Fracture mechanics principles can be used to study the behaviour of composite structures in presence of interfacial damage and to determine the conditions for the interfacial crack growth initiation.

Strain energy release rate ‘G’ is defined as the amount of strain energy released per unit extension of crack.

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$$G = - dU / dA$$

Where, $dU$ = change in strain energy $dA$= change in crack area
There are three components of strain energy release rate for three types of modes of fracture.

The total strain energy release rate (GT) is calculated from individual mode components as

$$G_T = G_I + G_{II} + G_{III}$$

Where $GI$ is the mode I component corresponding to interfacial tension
$GII$ is the mode II component corresponding to interfacial sliding shear
$GIII$ is the mode III component corresponding to interfacial tearing

Among the variables of fracture mechanics, the strain energy release rate components have been used most frequently in determining the initiation and growth of debonding in composite materials.

## V. RESULTS AND DISCUSSION

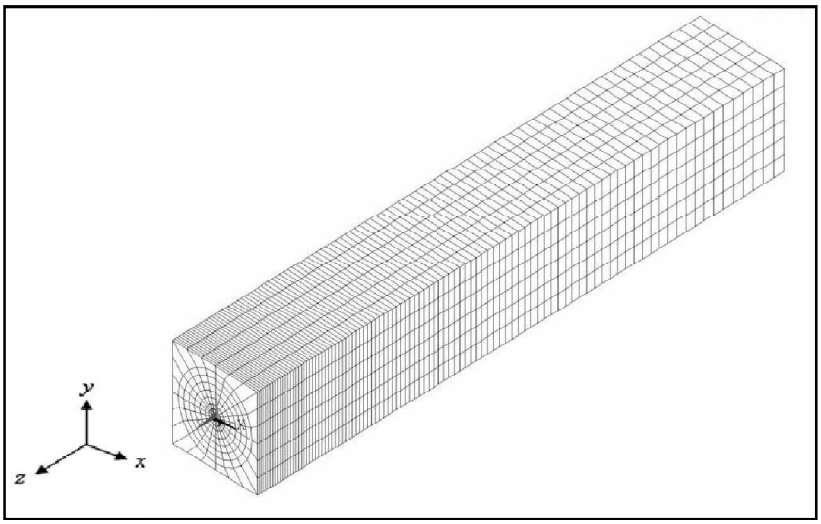


Fig.4 RVE of a CNT reinforced composite

As shown in Figure 4 a square RVE of a CNT reinforced composite is modelled in ANSYS where the *x–y* plane is the transverse plane and the *z*-axis is the axial direction. Two types of matrix materials viz. epoxy and copper are chosen to study the effect of matrix material on the stress distribution. Boundary conditions for half model and full model as explained in section are applied to study the axial normal stress distribution along CNT and interfacial shear stress distribution along interface of CNT/Epoxy and CNT/Copper composites to assess the severity of the fiber break, the results of which are discussed in section. After it is assumed that near the CNT break there is a debonding between CNT and matrix and the length of the debonding in axial direction is considered as $a$=1 nm. The debonding at the interface is considered over the entire circumference ahead of broken end of CNT for a length of 1 nm. This debonded area is the interfacial crack for the 3D square RVE. The virtual crack extension size is taken as $\Delta a$= 0.2 nm. Near the debonding or crack very fine mesh is used. The nodes which are placed at the interface of CNT and matrix have the same coordinates and are coupled through multi-point constraint equations. Interfacial stresses responsible for three modes of fracture is determined to further determine the components of strain energy release rate using VCCT the results of which are discussed in section.

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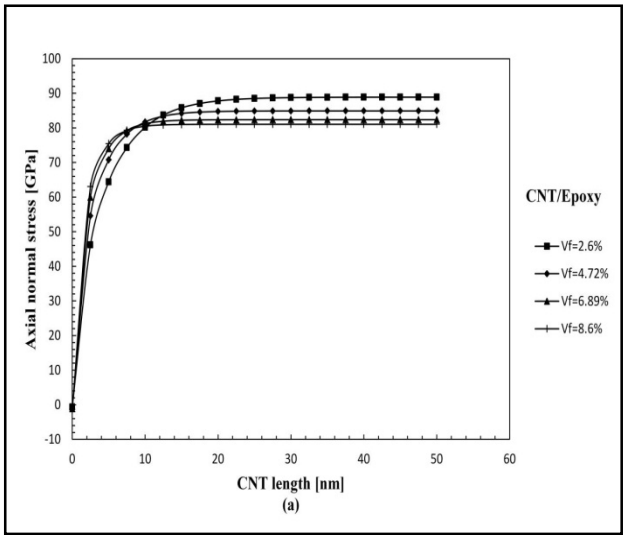
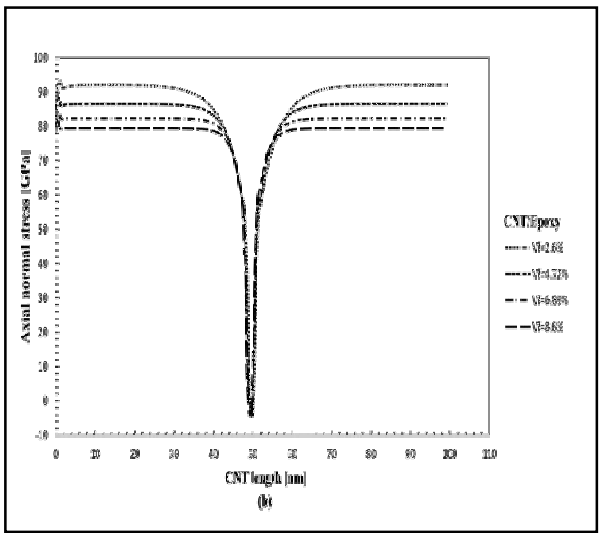
Generally the volume fraction of CNT in CNT-based composites is limited to 10% due to high cost of CNT and hence in the present analysis the volume fraction is varied from 2.6% to 8.6% and results are compared for CNT/Epoxy and CNT/Copper composites.

1) **Half model Variation of axial normal stress distribution for Epoxy composites**

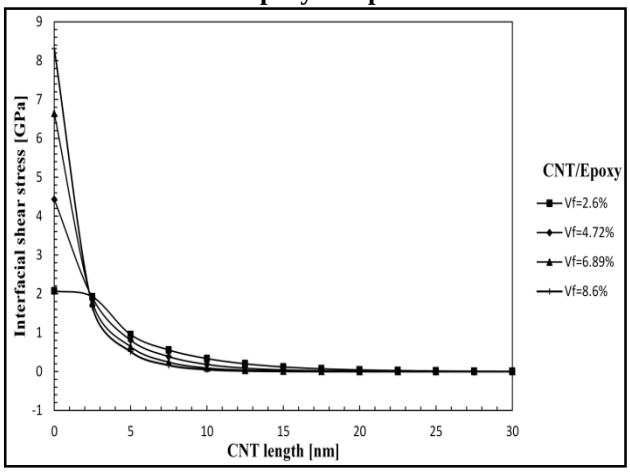



**Full model Variation of axial normal stress distribution for Epoxy composites**

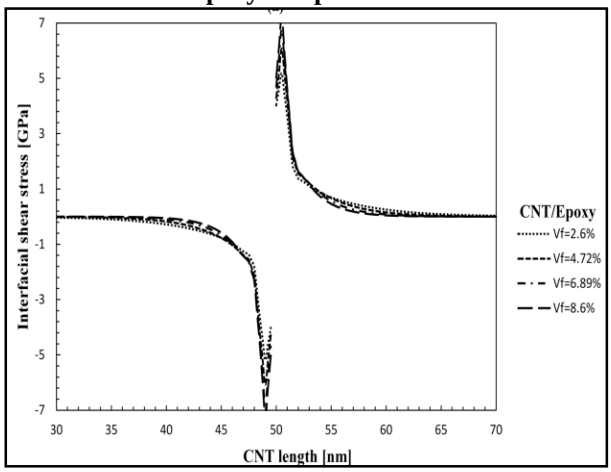



- Ineffective length is 15 nm……for Vf = 2.6 % 13 nm…….for Vf = 4.72%
  12.5 nm…..for Vf = 6.89% 11 nm……..for Vf = 8.6%
- Broken CNT is ineffective up to 30% of the length
- It contributes very less to the load bearing of the composite.
- Here, Vf = volume fraction

2) **Half model Variation of interfacial shear stress distribution for Epoxy composites**




**Full model Variation of interfacial shear stress distribution for Epoxy composites**




interfacial shear stress are 2.10 Gpa……..Vf = 2.6% 4.43 Gpa……Vf = 4.72%
6.64 Gpa……Vf = 6.89% 8.3 Gpa……..Vf = 8.6%

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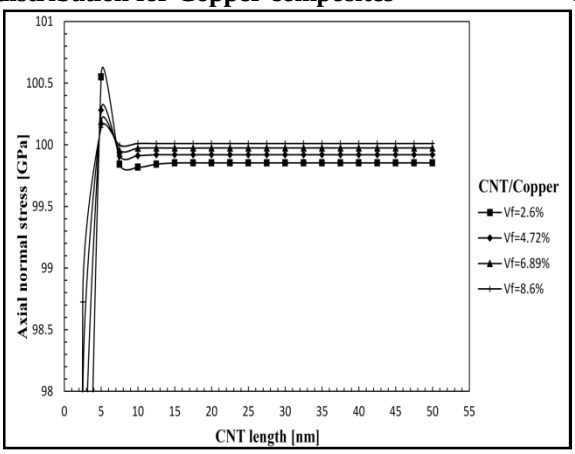
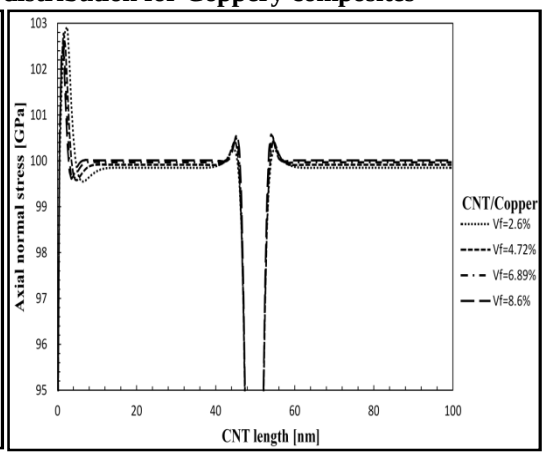
3) **Half model Variation of axial normal stress distribution for Copper composites**

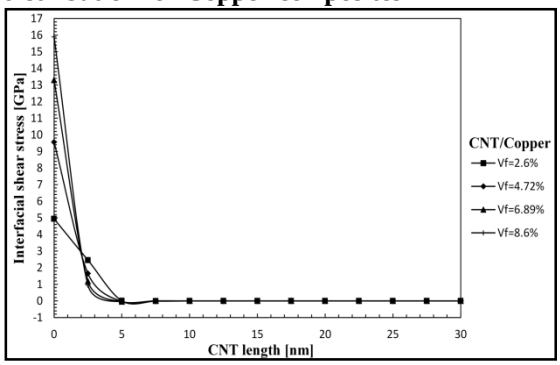



**Full model Variation of axial normal stress distribution for Coppery composites**

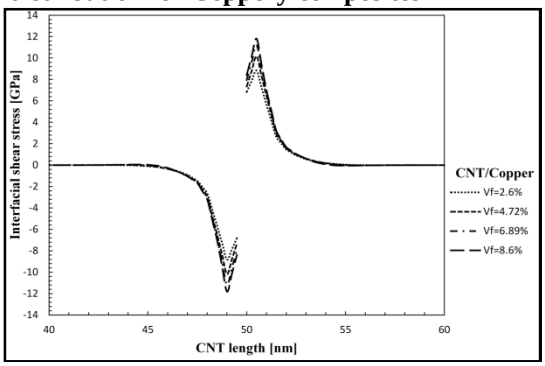



- Broken CNT regained nominal stress value after a length of 4 nm
- Therefore the ineffective length is 8%
- Li (Copper) < 4*Li (Epoxy)

4) **Half model Variation of interfacial shear stress distribution for Copper composites**




**Full model Variation of interfacial shear stress distribution for Coppery composites**




- shear stresses are : 4.94 Gpa…..Vf = 2.6% 9.56 Gpa…..Vf = 4.72%
  13.29 Gpa ….Vf = 6.89% 15.89 GPa ….Vf = 8.6%
- All these values are higher than Epoxy composites
- $t_{rz\ Copper} > t_{rz\ Epoxy}$ ……chance of debonding in Copper is higher

## VI. CONCLUSION

The following conclusions are drawn from the present study.

I. The ineffective length of the broken CNT in CNT/Epoxy composites is 30% whereas for CNT/Copper composites it is 8% at a volume fraction of 2.6% hence load bearing capacity of CNT/copper composites is more than the CNT/Epoxy composites. For CNT/Epoxy and CNT/Copper composites the ineffective length decreases with increase in volume fraction.

II. For both the CNT-based composites the magnitude of interfacial shear stress increases with increase in volume fraction of CNT. These values of interfacial shear stress for CNT/Copper composite are higher

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than that of the CNT/Epoxy composites for the same volume fraction. Therefore the chance of debonding at interface in CNT/Copper composites is higher than that in the CNT/Epoxy composites.

III. The ineffective length : Epoxy 30%: load bearing capacity is less
: Copper 8%: load bearing capacity is more

IV. Vf α (1/ Li) ……for both

V. Vf α $t_{rz}$ ……..…for both

VI. $t_{rz\ Copper} > t_{rz\ Epoxy}$ …… .Chance of debonding in Copper is higher

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