Mathematical Modelling of CNT to Derive its Different Parameter to Be used in Finite Element Analysis.

P K Mehta
Dept. of Mechanical Engineering,
City Engineering College, Bangalore, Karnataka, India

Abstract: **Carbon Nano Tubes have significant mechanical and electrical properties which have been subjected to many theoretical and experimental studies. Experimental studies are quite cumbersome and expensive, hence researchers are moving towards theoretical study of CNT. In this connection, modeling and analysis of CNT has given a tremendous help because of its result approximate to exact result. For modeling of CNT in FEM software, we need different dimensional parameter. In this paper, effort has been made to extract different dimensional parameter for CNT which can be used to model the CNT in FEM Software.**

Keywords- ***CNT,*** **Chirality, FEM.**

1. INTRODUCTION

Nanotechnology refer to the understanding and control of matter at the atomic levels, at the length scale of approximately 1 to 100 nanometers, where unique phenomena enable novel applications. Nanotechnologies are the design, characterization, production and application of structure, devices and systems by controlling shape and size at nanometer scale.

One of the fundamental components in nanotechnology is Carbon Nanotubes made of Carbon atoms arranged in a hexagonal lattice, whose diameter ranges from one to tens of nanometer and that are from hundreds up to thousands nanometers in lengths.

CNTs have incredible physical properties, both mechanical and electrical, and they are the basis of most of the new nano technological innovations. FEM and Molecular mechanics share a common ground of energy minimization, with respect to the nodes and to the discrete atoms, respectively.

2. MATHEMATICAL MODEL OF CNT

A SWCNT can be thought of as a sheet of graphite (a hexagonal lattice of carbon) rolled into an endless cylinder. It can be constructed by wrapping up a single sheet of graphite such that two equivalent sites of the hexagonal lattice coincide. The wrapping vector, C, which defines the relative location of the two sites, is specified by a pair of integer (n,m) that relate C to the two unit vectors, a_1 and a_2 and is given by the following equation.

$$Ch = na_1 + ma_2 \quad (1)$$

Where a1 and a2 are unit vector,

$$a_1 = \langle \frac{3}{2}a_{cc}, \frac{\sqrt{3}}{2}a_{cc} \rangle$$

$$a_2 = \langle \frac{3}{2}a_{cc}, -\frac{\sqrt{3}}{2}a_{cc} \rangle$$

Where acc =distance between nearest neighbour carbon atom.

Let a be the unit length of grapheme honeycomb lattice, then

$$a \equiv |\mathbf{a_1}| = |\mathbf{a_2}| = \sqrt{3}a_{C\,C} \quad (2)$$

A tube is called “armchair” if n equals m and “zigzag” in the case m=0. All other tubes are of the “chiral” type and have a finite wrapping angle θ with $0^\circ < \theta < 30^\circ$

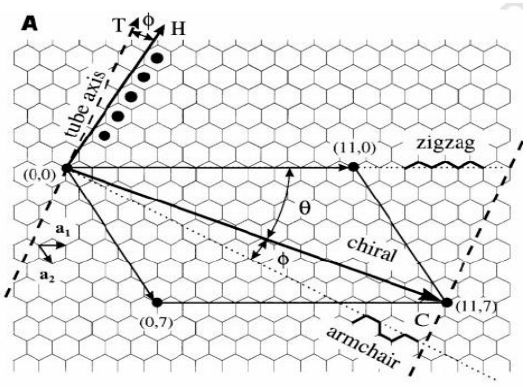

Fig 1

If we equate the length of chirality vector to the circumference of the tube, we will get the diameter of the tube.

$$C_h = 2\pi r = \pi d_t$$

$$d_t = C_h / \pi. \quad (3)$$

The magnitude of the chirality vector can also be determined in terms of the two lattice parameters, n and m, and the nearest-neighbor carbon distance:

$$\begin{aligned}\|C_h\|^2 &= C_h \cdot C_h = (na_1 + ma_2)\cdot(na_1 + ma_2)\\ &= n^2 a_1 \cdot a_1 + m^2 a_2 \cdot a_2 + 2nm a_1 \cdot a_2\\ &= n^2\left(\sqrt{3}a_{cc}\right)^2 + m^2\left(\sqrt{3}a_{cc}\right)^2 + 2nm\left(\frac{3}{2}a_{cc}^2\right)\\ &= \left(\sqrt{3}a_{cc}\right)^2\left(n^2 + nm + m^2\right)\end{aligned}$$

(4)

For an arm chair CNT (n,n) , *Ch* = 3*nacc*;

For a zigzag CNT *Ch* = √3n*acc*

Thus the diameter of the tube associated with an arbitrary chirality vector can be defined as

$$d_t = C_h /\pi.$$

$$d_t = \frac{\sqrt{\left(\sqrt{3}a_{cc}\right)^2\left(n^2 + nm + m^2\right)}}{\pi} = \frac{\sqrt{3}a_{cc}\sqrt{n^2 + nm + m^2}}{\pi}$$

The chiral angle ,Θ, determines the degree of helicity to the lattice, with a zig-zag (n; 0) lattice defined as Θ=0.This value can also be determined in terms of the lattice parameters.

Tangent of the chiral angle Θ

$$\tan\theta = \frac{\frac{3\sqrt{3}}{2} m\, a_{cc}^2}{\frac{3}{2}a_{cc}^2(2n + m)} = \frac{\sqrt{3}m}{(2n + m)}$$

$$\Rightarrow \theta = \arctan\frac{\sqrt{3}m}{(2n + m)} \quad (5)$$

For Arm chair CNT, m=n; $\Theta = \arctan(1/\sqrt{3}) = 30^\circ$,

For ZigZag CNT, m=0; $\Theta = \arctan(0) = 0^\circ$,

For Chiral CNT; $0 < \Theta < 30^\circ$.

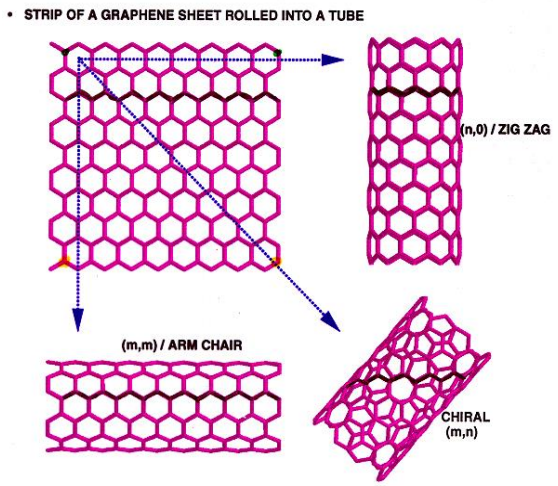

Fig 2

The **translational vector T** perpendicular to the chiral vector **Ch** is expressed as

$$\mathbf{T} = [(2m + n)\mathbf{a_1} - (2n + m)\mathbf{a_2}]/\, d_R$$

Otherwise

$$\mathbf{T} = [t_1\mathbf{a_1} + t_2\mathbf{a_2}]/d_R \ . \quad (6)$$

Where

$t_1 = (2m + n)/\, d_R$,
$t_2 = -(2n + m)/\, d_R$,
$d_R = d$, if $n - m$ is not a multiple of $3d$,
$d_R = 3d$, if $n - m$ is a multiple of $3d$

Where, d is is the highest common divisor of *n* and *m*.

The translational vector is

$$\mathbf{T} = [(2m + n)\mathbf{a_1} - (2n + m)\mathbf{a_2}]/\, d_R \ .$$

(6)

The length of translational vector is the **NT unit cell length *L*** along the nanotube axis direction:

$$L = |\mathbf{T}| = \sqrt{3}a(n^2 + nm + m^2)^{1/2}/\, d_R = \sqrt{3}C_h/\, d_R \ .$$

(7)

For arm chair CNT

$$m = n,\ d = n,\ d_R = 3d = 3n, \text{ and}$$
$$L = \sqrt{3}C_h/(3n) = 3n\sqrt{3}a_{CC}/(3n) = \sqrt{3}a_{CC}$$

For ZigZag CNT

$$m = 0,\ d = n,\ d_R = d = n, \text{ and}$$
$$L = \sqrt{3}C_h / n = 3na_{CC} / n = 3a_{CC}$$

Number of hexagons *N* in a nanotube unit cell is

$$N = 2(n^2 + nm + m^2)/d_R \ .$$

(8)

For arm chair CNT ,

m=n

$$N = 6n^2 / 3n = 2n$$

For ZigZag CNT, m=0

$$N = 2n^2 / n = 2n.$$

3. FINITE ELEMENT METHOD

CNTs carbon atoms are bonded together with covalent bonds forming an hexagonal lattice. These bonds have a characteristic bond length a C–C and bond angle in the 3D space. The displacement of individual atoms under an external force is constrained by the bonds. Therefore, the total deformation of the nanotube is the result of the interactions between the bonds. By considering the bonds as connecting load-carrying elements, and the atoms as joints of the connecting elements, CNTs may be simulated as space-frame structures.

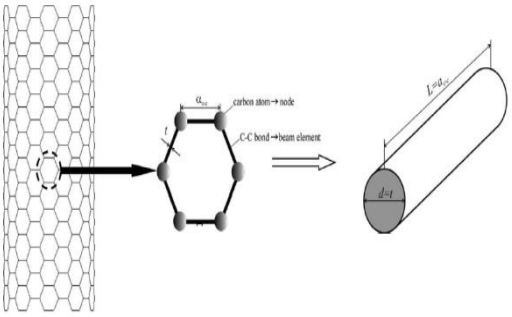

Fig 3

By treating CNTs as space-frame structures, their mechanical behavior can be analyzed using classical structural mechanics methods.

3.1 Finite element modeling with Representative Volume Element (RVE)

In RVE approach, a single nanotube with surrounding matrix material is modeled, with properly applied boundary and interface conditions to account for the effects of the surrounding materials it is possible to study the nanocomposite based on the single Representative volume element. This RVE model can be employed to study the interactions of the nanotube with the matrix. It is possible to model and evaluate the effective material properties of the nanocomposite.

According to the shape of the cross section, three types of representative volume elements are possible : cylindrical, square, and hexagonal RVEs shown in

Fig. 4 . Specifically, the cylindrical RVE is used to model carbon nanotubes with different diameters. The square RVE is applied when carbon nanotubes are arranged evenly in a square pattern, while the hexagonal RVE is adopted when carbon nanotubes are in a hexagonal pattern. Compared to the square RVE, the cylindrical RVE tends to overestimate the effective Young's module of carbon nanotube/polymer composites. This can be explained by the fact that a cylindrical RVE overestimates the volume fraction of carbon nanotube due to the negligence of the small amount of polymer matrix.

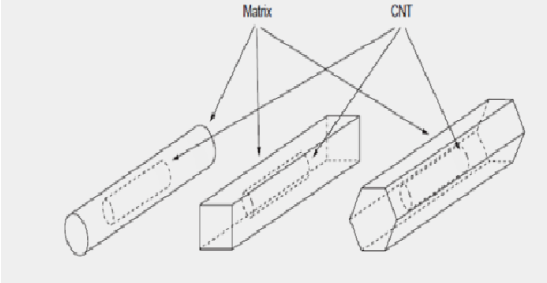

Fig.4 Three types of Representative Volume Elements (RVEs) (a) Cylindrical RVE (b) Square (c) Hexagonal

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