Chapter - 8
Chapter 8

SIMULATION STUDIES ON MODELING AND ANALYSIS OF MULTIWALLED CARBON NANOTUBES

8.1 OBJECTIVE

In this chapter, an F.E approach has been made to analyze and study the bending deformations and buckling behavior of multi walled carbon nanotubes (MWCNTs). The results calculated for the MWCNTs agree with the results of other similar numerical simulation studies available in literature and then establishing the validity of the present Finite Element approach. The analyses have been performed using ANSYS 11.0. The Nanotubes are modeled using shell93 (see section 3.14.4) elements from the ANSYS 11.0 library [187]. For analyses, the structures of MWCNTs are assumed as cantilever, loaded at the free end. Definite relationship is developed between the diameter and the critical buckling curvature of the CNTs. The deviations of bending load with bending curvature meant for the CNTs with dissimilar geometric constraints like different diameters of the CNT and lengths are analyzed in detail. Results of the analysis confirm the present F.E technique could be a helpful instrument for studying the mechanical behaviors of MWNTs as distinct units, and their usefulness in the field of nanocomposite materials. Finally, it seen that the present FEA approach is faster in computation. It can be used as a substitute competent method to study bending and buckling of the CNTs accurately.
8.2 MODELING OF MULTIWALLED CARBON NANOTUBES

By taking eight nodded shell93 element into consideration from ANYSIS11.0 library [187], the 13, 14 and 15 walled CNTs are modeled. Elastic shell theory can be derived for structures with 1D’s (thickness of the wall) extremely lesser than the other 2D’s, gives a natural approval for CNT that can be an idea of single graphene sheet of hexagonal lattice structure that may be enfolded into a continuous and perfect cylinder with no damage.

A thriving continuum model of the MWNTs may be constructed by suitable handling of the following 4 important aspects of CNTs. (a) Shell behavior of each and every nanotube wall is able to model by using shell theory with a proper set of elastic constants and a proper equivalent mechanical thickness of shell93 element. (b) The tube like character of the CNT structure desires an exit of pattern from a stress-free hexagonal-structure to an enclosed construction, containing an earlier internal stress due to its initial curvature. (c) A CNT wall act together through neighboring walls, with further portions of itself, and with via strong van der Waals interactions. (d) The shear resistance between successive walls is negligible and very minute.

8.2.1 Description for Geometrical Modeling of the MWCNTs

As geometric dimensions of the CNTs are very small, even a small error is not tolerated. To build the CNT model accurately eight nodded
Shell93 elements are used. The geometry and material properties of the carbon nanotube which are taken for analysis are as follows:

1. Inner diameter of the first tube : 0.34nm.
2. Thickness of the each tube’s wall : 0.314nm.
3. Gap between two successive tubes : 0.314nm.
4. Length of the tube : 100nm.
5. Young’s modulus : 4.84TPa.
6. Poisson’s ratio : 0.2.
7. Density : 0.14g/cm³.
8. Load : 10nN.
9. No. of tubes (i.e. MWCNTs) : 13, 14 & 15 walls.

The inner diameter of the first tube is taken as 0.34nm, the tube’s wall thickness and the gap between two successive tubes is 0.314nm, which is equal to distance between two successive carbon atoms. In this work carbon nanotube is analyzed and assumed it as a cantilever beam. The beam is modeled using shell elements (SHELL93). The shell element is having 6 degrees of freedom at each node i.e., 3 translational (d o f) and 3 rotational (d o f) in x, y, z-axes. In model problem, the MWCNT is fixed (all translations and rotations are zero) at one end. The load is applied at the free end as shown in Fig.8.2. Cross sections of Shell models of MWCNTs and geometry showing thickness of Carbon Nanotubes are shown in Fig.8.1.
The Fig. 8.2 shows the fine mesh of 15walled MWCNT with boundary and loading conditions. The thickness of each tube wall has been given in the real constants as 0.314nm. From the literature [93-103] the Young’s modulus (E) is taken as 4.48TPa and an assumed Poisson’s ratio (ν) is 0.2. Many authors considered this value as 0.18 and 0.19 in the literature. Finally, after solution is obtained, the results of first set have taken from each type of MWCNTs and analyzed in detail.
8.3 RESULTS AND DISCUSSIONS:

8.3.1 Bending Behavior of MWCNTs

In the previous chapter, the simulation studies on SWCNTs would provide important groundwork for MWCNTs in this chapter. However, there is no direct comparison between the two (because of the difficulty of setback of much no Molecular Dynamics (MD) simulation and other results accessible in the literature). The effects of nanoscale on the bending and buckling behaviors of MWCNTs have not been studied previously. In the present chapter, the bending and buckling of MWCNTs is broadly simulated by the FEA approach using ANSYS11.0. The analysis includes the influence of nanoscale effect and layer number on the critical bending and buckling load of MWCNTs.

As a first step, 13, 14 and 15 walled CNTs are modeled using shell93 element and meshed with fine mesh as applicable for structural shell element in the ANSYS11.0. Fig.8.2 shows the loading and boundary conditions, and deformed (total deformation) shapes of 13, 14 and 15 walled CNTs, simulated using the above software.

The maximum deformations (DMX) along X-direction of the tubes known from the simulation are 0.200E-9nm, 0.178E-9nm and 0.146E-9nm for 13, 14 and 15 walled CNTs respectively. Similarly, the maximum
deformations (DMX) along Y-axis are 0.201E-9nm, 0.174E-9nm and 0.146E-9nm for 13, 14 and 15 walled CNTs.

Fig: 8.2 Total Bending deformations for 13, 14 and 15 walled CNTs and boundary conditions and loads.

Fig: 8.3 show the comparison at bending deformations of 13, 14 and 15 walled CNTs for the same length and applied load. The graph is plotted between bending deformation vs. length of CNTs. Only 14 walled
CNT has slightly difference from other two CNTs plotted on the graph. All three CNTs are giving linear curves.

Fig: 8.3 comparison of bending deformations of 13, 14 and 15 walled CNTs for same lengths of CNTs (present FEA simulation results).

8.3.2 Buckling Behavior of MWCNTs.

It is experimentally observed that for the three MWCNTs i.e., 13, 14 and 15 walled CNTs, the diversity of flexural moment gives non-linearity for smaller bending angle, which is different from that the SWCNTs, presented earlier. The non-linearity of MWCNTs is due by the interlayer van der Waals forces. By additional increase in the angle of bending, flexural moment alters with the linearity of angle of bending. When the flexural moment reaches the angle of critical bending, it stops
its development. With still additional increase in angle of bending, the flexural moment goes down suddenly, and MWCNTs come up to post-buckling condition. It reveals that the post buckling equilibrium path of MWCNTs due to bending load is not stable. It may be observed that with the increase in MWCNTs inner-tube, the critical flexural moment increases clearly while the angle of critical bending and critical curvature of bending-buckling reduces. Fig.8.4 shows the change in curvature of critical buckling with the diameter of MWCNTs. For curve fitting, it is also noted that, for 13, 14 and 15walled MWCNTs with same length, the critical buckling curvature goes down as Inverse Square of the tube’s diameter. From the graph (Fig.8.5) it is observed that the buckling effect on 13, 14 and 15 walled CNTs are almost linear for the same length and load applied, irrespective of their outer diameters. It agrees well with the Transmission Electron Microscopic image of buckled MWCNT in CNT – polymer composites [187].
Fig. 8.4 Buckling effects on 13, 14 and 15 walled CNTs along U-sum.

Fig. 8.6 shows the change of critical buckling curvature with the diameter of CNTs. It is observed that, for all different MWCNTs, with equal length, the buckling curvature changes with Inverse Square of the tube diameter. The relationship between critical buckling curvature and nanotube diameter can be written as

$$K_{Cr-bending}^{FEA} = \frac{0.0478}{d^2} \quad (8.1)$$
Fig: 8.5 Variation of axial buckling with load on 13, 14 and 15 walled CNTs.

Fig: 8.6 Variation Critical buckling with diameter of 14walled CNT.
The correlation between critical buckling curvature and nanotube diameter for SWCNT, DWCNT and MWCNTs are compared and shown in Fig.8.7. Further, it is revealed that the critical buckling curvatures for SWCNT, DWCNT and MWCNT are approximately identical for the diameters $d > 4$ nm. The critical buckling curvatures for SWCNT is more than that of DWCNT and MWCNTs for diameters $d<4$nm.

The sound effects of different layers on the buckling property of MWCNTs are studied by applying the present customized F.E.A method. The geometrical configurations for 13, 14 and 15 walled CNTs with Length = 100nm at the preliminary buckling position shows the 3D
integral buckling deformation of MWCNTs. The shape of the proportioned plane in Fig.8.4 shows that the inter-layer spacing of MWCNTs have no observable effect during the bending position under the action of von der Waals (vdW) forces.

8.4 SUMMARY

A methodology for building continuum shell theory F.E. models of CNTs has been developed in the present work. General F.E.A. simulations are adopted to study the bending and buckling behaviors of MWCNTs. Correlations are developed between the geometry parameters and the critical buckling curvature of CNTs, like diameter of the tube and length of tube. Through the atomistic techniques, the present approach can significantly decrease the cost of computation of simulating the deformation of SWCNTs and MWCNTs, particularly for large Carbon Nanotubes and structures with a number of CNTs.