Continuum Modelling of Nanoindentation into Vertically Aligned Carbon Nanotubeforests by Finite Element Method

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Abstract— Nanoindentation is an appropriate technique to study the behavior of the materials at the nanoscale. Carbon nanotubes are allotropies of carbon with outstanding mechanical properties. Young's modulus is one such property dealing with its elastic behavior. Vertically Aligned Carbon Nanotubes (VANCT'S) are a cluster of carbon nanotubes that are grown during the synthesis of carbon nanotubes. Nanoindentation can be used to characterize the mechanical properties of VACNT'S. Alternately, numerical techniques such as Finite Element Modeling (FEM) can be used to simulate such a process to know the physics and mechanics of VANCT's. In the present work, continuum modeling has been used to simulate nanoindentation into vertically aligned carbon nanotubes. The load-displacement curves are obtained as the output of numerical simulation.

Keywords: Finite Element Method, Load-Displacement Curves, Nanoindentation, Vertically Aligned Carbon Nanotube Forests, Stress-Strain Distribution

I. Introduction

The nanoindentation process deals with a diamond tip pressed into the sample surface and subsequently, having reached a given maximum depth for the maximum load applied. The tip is brought back and removed. During the process, the loading and the displacement of the indenter are recorded. The recorded result of such an experiment is, therefore, not only a hardness value but also the complete history of the deformations occurring during the test. A load-displacement curve consists of a loading and an unloading curve. The loading curve shows the resistance of the sample against the penetration of the tip and reflects both the elastic and the plastic properties. The unloading curve is mainly determined by the elastic recovery of the indent. From such load-displacement curve, hardness nd Young's modulus of the specimen can be determined using an appropriate analysis model. Thus, the requirements for a successful application of the Nanoindentation technique are an apparatus capable of performing indentation experiments and simultaneously recording the applied load and the corresponding displacement of the indenter. The other requirement is a method for the analysis of the measured load-displacement curves.

The mechanical properties of Carbon Nano Tubes (CNT) play a major role in a variety of applications. The basic mechanical property of CNTs is its Young's modulus. Experimental techniques have been designed and molecular and continuum modeling and simulations have been done to extract the various mechanical properties like axial modulus, bending modulus of elasticity, etc. VACNTs have become a current topic of research because of applications starting from field emission devices to Microelectronics systems used for the formation of super-hydrophobic surfaces. Nowadays, the nanoindentation has become a reliable tool for the determination of mechanical properties of CNTs and the constituents VACNT forests, Hiroshi Kinoshita, et al. (2004) [1].

II. Literature Survey

Carbon nanotubes are small scale tubes carbon molecules with the diameter in few nanometers and length can be in micro or millimeters possessing superior mechanical properties, Iijima, (1991) [2].

The fundamental mechanical property of CNTs is its Young's modulus when it is modeled as a continuum hollow cylinder. Many experimental techniques have been used to measure Young's modulus of CNTs and stiffness at room temperature, Krishnan, et al. (1998) [3] and the electric, mechanical, and field emission properties, Wang, et al. (2000) [4], of CNTs. Elastic properties of CNTs have been estimated using an empirical force constant model, Lu, (1997) [5]. A model linking structural mechanics and MM of CNTs has been developed, Lie, and Chou, (2003) [6]. In general, nanoindentation has been used to characterize the mechanical properties of thin films and bulk materials. Numerical methods like FEM has been used to simulate the process and obtain the load-displacement characteristics. Bulk materials and thin films of Titanium and copper subjected to nanoindentation have been simulated by FEM technique [7]. FEM has been applied to simulate and obtain the elastic behavior of biological cells [8]. Nanoindentation into Vertically Aligned Carbon Nano Tubes (VACNTs) have been conducted to investigate the Micro tribological properties with film thickness 6 µm, and measure the critical shell-buckling load by axial compressing, Waters, et al. (2005) [9]. Based on the literature survey and available data, analytical equations have been obtained for the deformation of VANCNT's for bending, compression, and buckling loads [10]. The images of three different samples of VACNTs tilted at 25° on which nanoindentation experiments have been conducted are shown in Figure-1,2 and 3 respectively on three samples Qia, et al. (2003) [11]. Apart from nanoindentation, simple axial compression tests also have been conducted on VACNT's. Finite element analysis has been carried on uniaxial compression of cylindrical bundles of vertically aligned carbon nanotubes to study the deformation due to buckling [12].

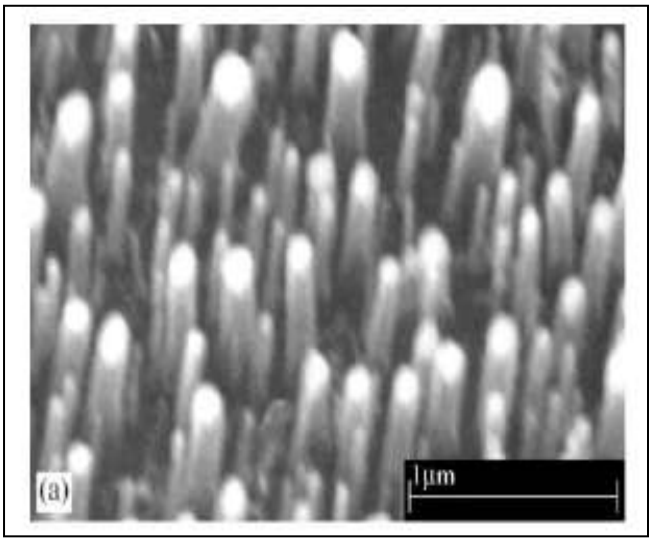


Fig. 1: VACNT (Sample-A)

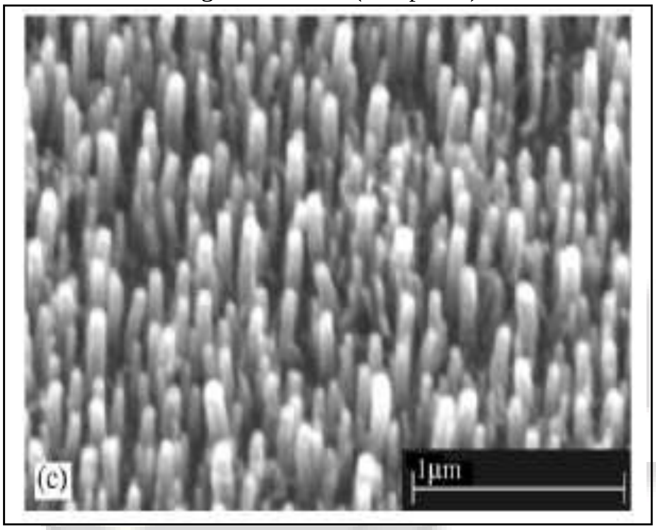
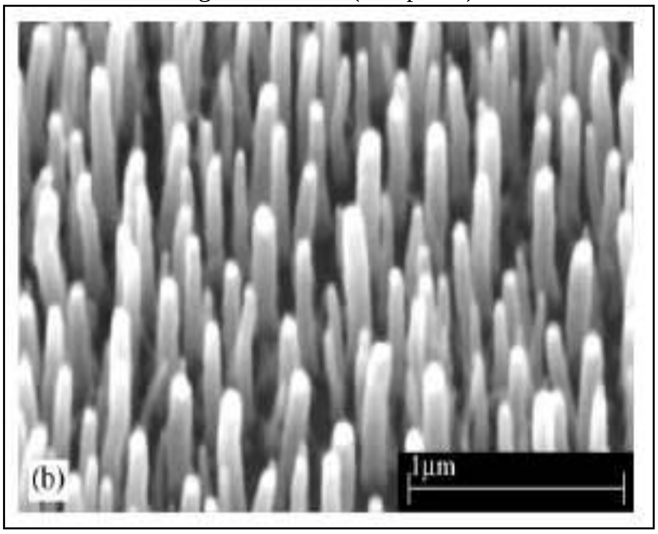


Fig. 2: VACNT (Sample-B)



(iii)
Fig. 3: VACNT (Sample-C), Qia, et al. [11]

III. FINITE ELEMENT MODELLING

The geometry and the shape of the materis and their related properties are given in Table – 1.

Sl. No.	Details of sample materials			Indenter	
	Name	Behavior	Size (Diameter & Length) in nm	Shape & Size	Material
1	Sample-A	Elastic	104 & 930	Conical & 50 nm	Diamond
2	Sample-B	Elastic	90 & 1150	Conical & 50 nm	Diamond
3	Sample-c	Elastic	55 & 570	Conical & 50 nm	Diamond

Table 1: Specifications of VACNTs [11]

A. Modeling and Simulation Process

The VACNTs are modeled as cantilever beam structures for Indentation and bending action. Therefore, a 2-D Axisymmetric solid cylindrical model that represents the cantilever beam structure has been used for modeling purposes. The geometry and the specimen details and the indenter are shown in Table-1. The Poisson Ratio for all the samples is 0.45. Finite element simulation software ANSYS is used for the modeling. 2-dimensional modeling has been carried to simulate the nanoindentation into VACNT's. 2 D structural solid four noded element PLANE 42 is used to mesh the model. The element consists of two degrees of freedom at each node. The mesh of the 2D model is shown in Figure-4. The nodes at the bottom line of the half-space are restrained to move in both X and Y directions. An indentation force is applied at the contact point in downward Y-direction and lateral force in X-direction. Ramped loading is considered starting from 20 to 60 in increments. The Input and material properties for the three samples – A, B, and C are given for Simulation. The same procedure is extended for 3D modeling. The simulation is carried out for load–displacement behavior.

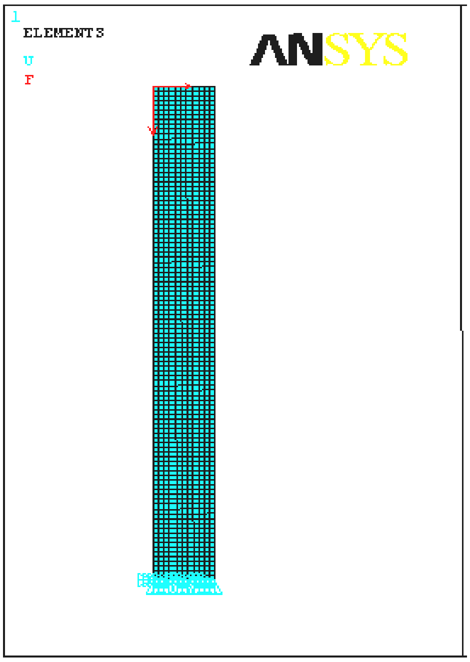


Fig. 4: 2-D Mesh of the VACNT

IV. RESULTS AND DISCUSSIONS

The results consist of Load versus indentation depth curves that are obtained by FEM for the three VACNT's samples. The corresponding stress-strain contours are also shown as output results.

The combined load-displacement curves for all the three samples are shown in Figure-5(a). It can be observed that the maximum indentation depth for the sample-A is 561 nm. Similarly, for the samples–B & C are 709 nm & 485 nm respectively and are in good correlation to experimental values available in literature as 712 and 490. Thus the results are correlated. The displacement, von mises stress and strain distributions for sample-A are shown in figure-6(a), 6(b) and 6(c) respectively. The Y-displacement,stress and contours for sample-B are shown in Figures-7(a),7(b) and 7(c) respectively.

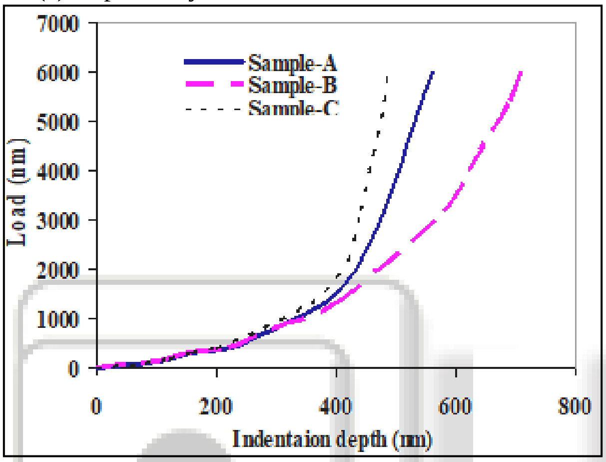


Fig. 5 (a): Load-indentation depth curves (FEM).

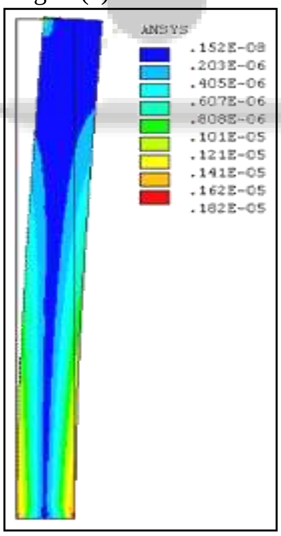


Fig. 6(a)

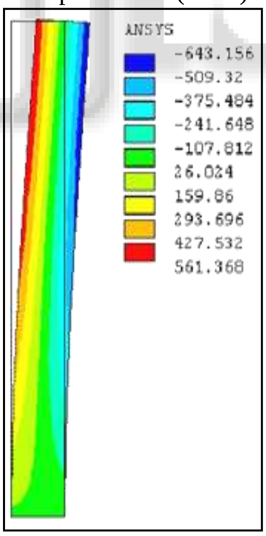


Fig. 6(b)

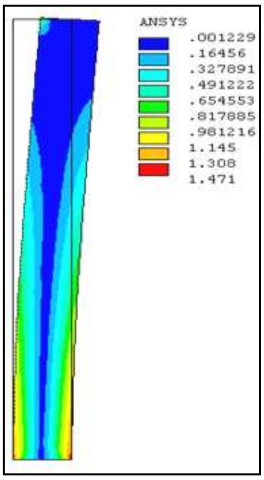
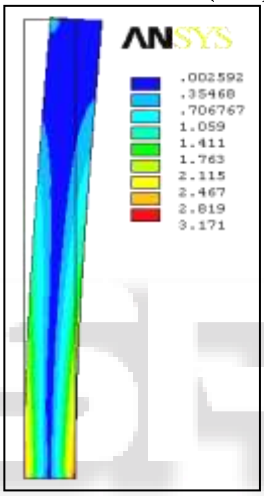


Fig. 6(c)

Fig. 6: Displacement, stress and strain contours (Sample-A)



. Fig. 7(a)

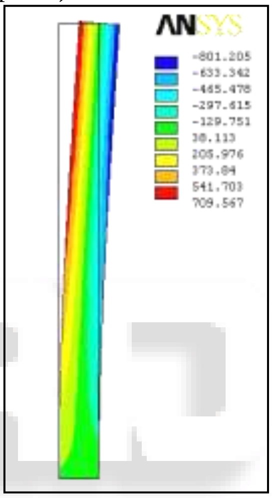


Fig. 7(b)

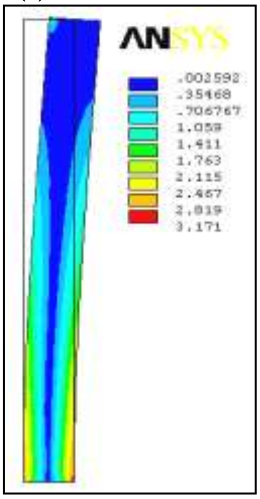


Fig. 7(c)

Fig. 7: Displacement, stress and strain contours (Sample-B)

The load-displacement behavioral curve of Sample-C shows less scatter than those of Sample-A and Sample-B since the Sample-C has the highest nanotube areal density.Sample-C is considered for three-dimensional modeling of nanoindentation. The simulation is conducted by assuming a single CNT as a continuum tube. The Von-

Mises stress distributions for 3-dimensional models are shown in Figure-8

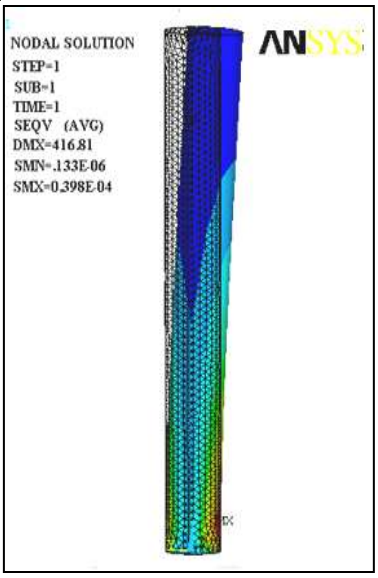


Fig. 8: Von Mises stress distribution (Sample-C)

V. CONCLUSIONS:

Finite Element Method has been used to simulate the nanoindentation process into vertically aligned carbon nanotubes; the obtained load-displacement has been used to plot the curves from which the mechanical properties can be estimated. The load-displacement data obtained by the FEM of Nanoindentation are compared and validated with the results available in the literature. The results are in good agreement. Thus the results are displayed in the form of load-displacement curves obtained from FEM data and also in the form of stress-strain contours.

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