SIZE-DEPENDENCE OF BUCKLING BEHAVIOURS IN MULTI-WALLED CARBON NANOTUBES UNDER PURE BENDING

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Abstract- Carbon nanotubes (CNTs) have very good properties such as high tensile strength and flexibility in the radial direction. Moreover, it is known that multi-walled carbon nanotubes (MWCNTs) undergo unique deformation under the application of various loads. This study examines the behaviour of MWCNTs under bending by using cylindrical shell theory. It is known that corrugation called Ripple arises in the compression side of MWCNTs under bending. In this study, we focused on the critical curvature–bending moment relationship at the point of buckling ; we found that this unique relationship depends strongly on size.

Keywords- Carbon Nanotubes, Ripple, Cylindrical Shell Theory, Bending Buckling.

I. INTRODUCTION

Carbon nanotubes (CNTs) are expected to be used as nanoscale materials because of their high tensile strength in the axial direction and remarkable bending flexibility. Another important characteristic of CNTs is their high flexibility in the radial direction. In fact, the magnitude of the radial stiffness of an isolated carbon nanotube is considerably less than that of the axial stiffness. This phenomenon allows for a reversible change in the cross-sectional shape upon the application of hydrostatic pressure or a bending moment. In addition to these significant mechanical properties, studies have shown that mechanical deformation causes considerable changes in the electronic, optical, magnetic, and chemical properties. Thus, many studies are being conducted on new technologies to utilize the correlation between deformation and properties in various fields, including electronics, biotechnology and material design.

Corrugation called Ripple is generated in the compression side of multi-walled carbon nanotubes (MWCNTs) under bending, but it behaves elastically for some types of deformation.

The purpose of this study is to examine the behaviours at the neighborhood of the buckling point logically in view of the size-dependence of bending buckling of MWCNTs under pure bending.

II. ANALYSIS MODEL

Figure 1 shows the structure of CNTs modeled by cylindrical shell theory. The thickness, length and diameter are t, L, and D respectively. Since CNTs are an elastic body (Young's modulus E) and the layer is very thin, we applied thin-shell theory and ignored the influence of Poisson ratio ν. This shell structure deforms with a constant curvature in the axial direction receiving a pure bending moment.

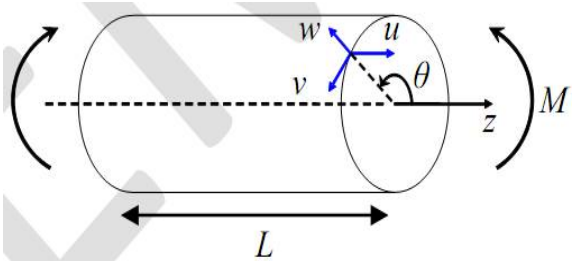


Fig.1. Structure of CNTs

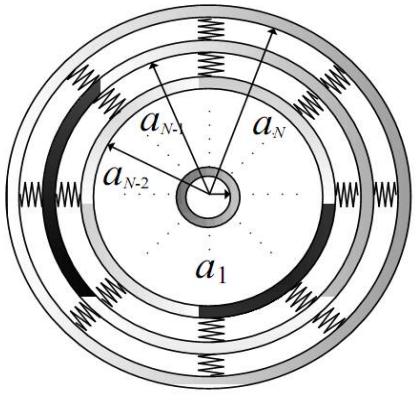


Fig.2. Cross-section of MWCNTs

Figure 2 shows the cross-section of MWCNTs (the number of layers N, interlayer distance d). Here an (=Dn/2) indicates the radius of the ith cylindrical wall of MWCNTs. MWCNTs consist of a set of concentric graphite cylindrical walls, which is an important feature of MWCNTs. These walls interact mutually via van del Waals (vdW) forces. Therefore, we modeled interlayers as a Winkler spring.

III. METHODS

The stable shape of MWCNTs under pure bending M can be evaluated by using continuum elastic theory for cylindrical shells. In the continuum approximation, the mechanical energy U of

MWCNTs in the axial direction is the sum of the strain energy Uθ in the circumferential direction, Uz in the axial direction, and interaction energy UI. All three energy terms are functions of M, and the displacements of a surface element of the ith wall are ui, vi, and wi, which denote the axial, circumferential, and radial displacements, respectively. Thus, Uθ and Uz can be written as follows [1]. Here, equations (1) and (2) respectively are differentiated by θ and z.

$$U_\theta = \sum_{i=1}^{N} \frac{1}{2} \int_0^L \int_0^{2\pi} \left[Et \left\{ \frac{v'_i + w_i}{a_i} + \frac{1}{2} \left(\frac{v_i - w'_i}{a_i} \right)^2 \right\}^2 + \frac{Et^3}{12} \left(\frac{v'_i - w''_i}{a_i^2} \right)^2 \right] a_i \, d\theta \, dz \quad (1)$$

$$U_z = \sum_{i=1}^{N} \frac{1}{2} \int_0^L \int_0^{2\pi} \left[Et \left(u'_i + \frac{1}{2} w'^2_i + \frac{1}{2} v'^2_i \right)^2 + \frac{Et^3}{12} w''^2_i \right] a_i \, d\theta \, dz \quad (2)$$

where E is Young's modulus (E = 3.83 TPa), and t is the thickness (t = 0.09 nm). The explicit form of UI is given in equation (3) [2].

$$U_I = \sum_{i=1}^{N-1} \frac{c_{i,i+1} \left[(a_i + a_{i+1})/2 \right]}{2} \int_0^L \int_0^{2\pi} (u_i - u_{i+1})^2 \, d\theta \, dz \quad (3)$$

where the vdW interaction coefficients ci,i+1 are functions of intermolecular forces.

We substitute the sum of the displacement in stable and buckling modes for equations of strain energy.

$$u_{i,0} = a_i C \left(z - \frac{L}{2} \right) \sin\theta \quad (4)$$

The cross-sectional flatness is ignored; therefore, we consider axial deformation in stable state.

In three-dimensional analysis, we can ignore the influences of deformation in the axial and circumferential directions since the deformation in the radial direction has significant influence [3]. Therefore, we only consider the radial deformation under bending. The deformation in the radial direction is given as follows by using the amplitude component Ri, Si, and Ti as

$$w_{i,1} = \left[R_i + S_i \cos\left(\theta - \frac{\pi}{2} \right) + T_i \cos 2\theta \right] \sin \frac{n\pi}{L} z \quad (5)$$

where n is the period of displacement, namely, the buckling number of corrugation.

Finally, the equations of displacement are given as

$$\begin{aligned} u_i &= u_{i,0} \\ w_i &= w_{i,1} \\ v_i &= 0 \end{aligned} \quad (6)$$

To determine the curvature in buckling, we substitute equation (6) in the equation of strain energy and calculate the second variation in strain energy.

$$\delta^2 U = \delta^2 U_\theta + \delta^2 U_z + \delta^2 U_I \quad (7)$$

We differentiate equation (7) by the displacement amplitude to derive the governing equation and determine the curvature of buckling Ccr to solve the governing equation. Here, the buckling number of corrugation is n that minimizes Ccr.

$$\begin{aligned} \partial(\delta^2 U)/\partial R_i &= 0 \\ \partial(\delta^2 U)/\partial S_i &= 0 \\ \partial(\delta^2 U)/\partial T_i &= 0 \end{aligned} \quad (8)$$

The critical bending moment Mcr is given as

$$M_{cr} = EC_{cr} \sum_{i=1}^{N} \pi r_i^3 t \quad (9)$$

We use parameter C**, which is obtained multiplying the curvature Ccr by the square of radius of external layer r.

IV. ANALYSIS RESULT

Figure 3 shows the corrugation of Ripple. The figure on the left-hand side is a general view of MWCNTs, and that on the right-hand side is a cross-sectional view in the axial direction. These figures show that the corrugations appear in the compression side, and hence, the buckling mode of Ripple can be expressed by using above the equations of displacement.

Figure 4 shows C** as a function of the number of layers N for various values of a. In the area of N ≧20, C** is almost constant. This implies that the density of the inner layers restrains deformation and the MWCNTs become close-packed CNTs; hence, the behaviour of bending correspons to MWCNTs with various value of a.

Figure 5 shows C as a function of the bending moment Mcr for various values of N. We investigate the Ccr–Mcr relationship for various MWCNTs, with the inner diameters varying from 1 to 3.5 nm in steps of 0.5 nm. 20-walled MWCNTs is only to 4.5 nm. It is shown that the point of the right-side end for 20-walled MWCNTs corresponds to the point of the left-side end for 30-walled MWCNTs. In this point, both MWCNTs have same outermost diameter. We find that the Ccr–Mcr relationship depends strongly on the outermost diameter and a group of curved lines of

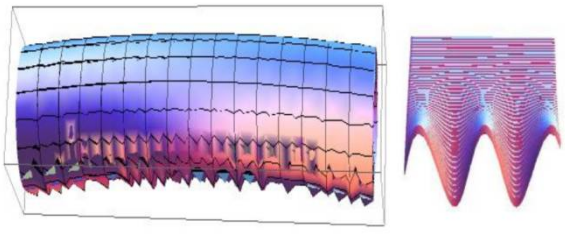


Fig.3. Buckling mode of Ripple

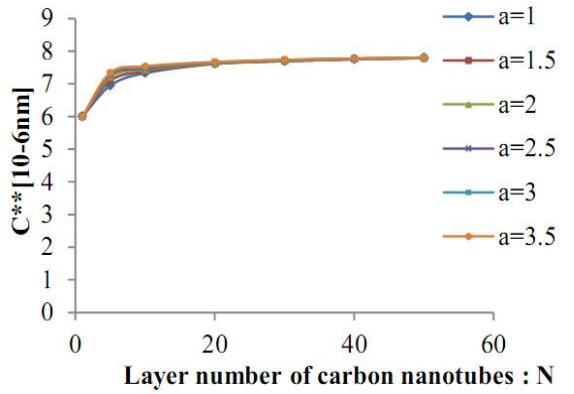


Fig.4. Graph of C vs. N for different innermost diameters**

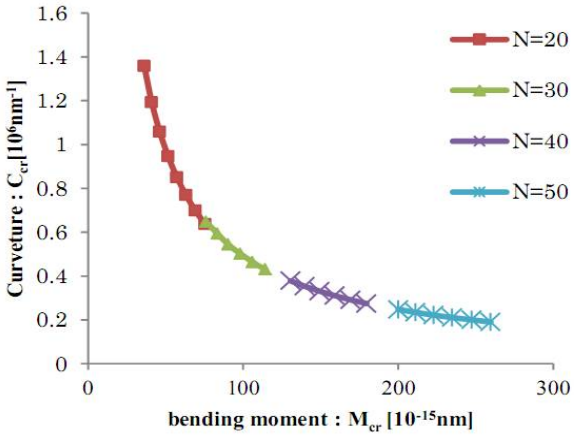


Fig.5. Graph of C vs. Mcr for different number of layers

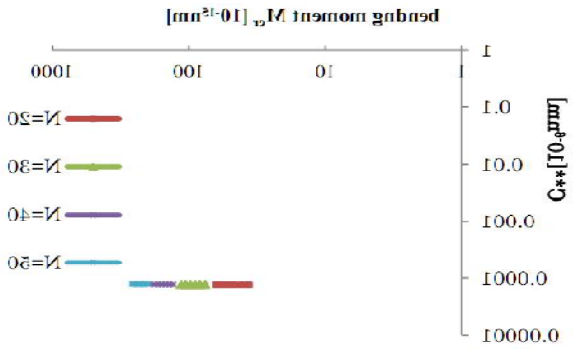


Fig.6. Graph of C vs. Mcr for different number of layers**

various MWCNTs can be approximated to one curved line. Figure 6 is a log–log plot of C** vs. Mcr for various values of N. Ccr is distributed on the curved line; however, by introducing the parameter C**, the curvature is almost constant regardless of the number of layers, innermost diameter, and bending moment.

CONCLUSIONS

The Ccr–Mcr relationship depending on the outermost diameter in MWCNTs under pure bending was studied. The main conclusions are as follows.

1. The behaviours of close-packed MWCNTs with N ≧20 correspond to each other under pure bending

2. The parameter C** of multiplying the curvature Ccr by the square of radius of external layer r is almost constant regardless of the number of layers, innermost diameter, and bending moment in close-packed MWCNTs with N ≧20.

ACKNOWLEDGMENTS

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