The 2013 World Congress on
Advances in Structural Engineering and Mechanics (ASEM13)
Jeju, Korea, September 8-12, 2013

Buckling patterns of hydrostatically pressurized multiwalled carbon nanotubes embedded in an elastic medium

*Motohiro Sato[1)], Ayako Kusano[2)] and Hiroyuki Shima[3)]

[1)] *Faculty of Engineering, Hokkaido University*
Kita 13 Nishi 8, Kita-ku, Sapporo 060-8628, Japan
[2)] *Graduate School of Engineering, Hokkaido University*
Kita 13 Nishi 8, Kita-ku, Sapporo 060-8628, Japan
[2)] *Graduate School of Engineering, Hokkaido University*
Kita 13 Nishi 8, Kita-ku, Sapporo 060-8628, Japan

[1)] *tayu@eng.hokudai.ac.jp*

ABSTRACT

We elaborate on the cross-sectional deformation of carbon nanotubes embedded into a self-contracting host medium. The continuum elastic approach is used to formulate the mechanical energy of both the embedded nanotubes and the self-contracting outer medium with finite thickness. Our formula allows us to evaluate the critical buckling pressure applied on the interface between the embedded nanotube and the outer contracting medium as well as the wavy-shaped novel buckling modes that arises immediately above the critical pressure. An interesting mechanical implication of the embedding effect is deduced by the theoretical approach established.

1. INTRODUCTION

The salient structural feature of a carbon nanotube is its self-repairing behavior that arises under high-energy beam irradiation (Shima 2013) kinetic energy transferred from the incident beam to the atoms are pushed away from the incident beam to the atoms are pushed away from the original equilibrium positions, leaving vacancies in the host hexagonal lattice (Krasheninnikov 2010 and Osv´ath 2005) .

The spontaneous shrinkage in the radial direction is a result of the knock-on collision of carbon atoms followed by annealing reconstruction of the vacancies. This experimental finding implies that when the outermost carbonwalls of an MWNT are eroded selectively by irradiation, the self-contraction of the outermost walls exert high pressure on the encapsulated, undamaged innermost walls (Guo 2007, Xu 2008 and Yang 2009) . Application of high pressure may then trigger a novel class of cross-sectional transformations of then inner walls (Shima 2010) , similar to the case of

[1),3)] Associate Professor

[2)] Graduate Student

pristine (irradiation-free) MWNTs under hydrostatic pressure (Shima 2008 and Shima 2009) .

In this article, we establish the continuum elastic approach that describes the cross-sectional deformation of carbon nanotubes surrounded by a self-contracting host medium. The mechanical energy of both the pressurized nanotubes and the contracting medium with finite thickness are formulated using thin-shell theory. The obtained formula allows as to evaluate the critical radial pressure applied on the interface between the inner nanotube and the outer medium.

2. METHODOLOGY

The stable cross-sectional shape of the embedded tube is obtained by minimizing its mechanical energy U per unit axial length (Shima 2008).

$$U = U_D + U_I + U_M + \Omega \tag{1}$$

The first term $U_D = \sum_{i=1}^{N} U_D{}^{(i)}$ with the definition

$$U_D{}^{(i)} = \frac{r_i}{2}\left(\frac{C}{1-\nu^2}\int_0^{2\pi} I_i{}^2 d\theta + D\int_0^{2\pi} B_I{}^2 d\theta\right) \tag{2}$$

where $C = Eh$, $D = \dfrac{Eh^3}{12(1-\nu^2)}$

represents the deformation energy of the embedded nanotubes. I_i and B_i are, respectively, in-plane and bending-induced strains of the *i*th wall, and θ is the circumferencial coordinate. For Eq. (2), we supposed that each *i*th wall had a radius r_i prior to cross-sectional deformation and that the deformation caused a displacement $x_i = (u_i, v_i)$ of a volume element of the *i*th wall at (r_i, θ) in the polar coordinate representation. The two strain terms I_i and B_i are described in terms of the displacement components by Shima 2009.

$$I_i = \frac{u_i + \partial_\theta v_i}{r_i} + \frac{1}{2}\left(\frac{\partial_\theta u_i - v_i}{r_i}\right)^2 \quad , \quad B_i = -\frac{\partial_\theta{}^2 u_i - \partial_\theta v_i}{r_i{}^2} \tag{3}$$

where $\partial_\theta = \partial/\partial\theta$.

The second term, $U_I = \sum_{i,j=i\pm1} U_I{}^{(i,j)}$, in Eq. (1) accounts for the vdW inter action energy, which determines the equilibrium distance between adjacent concentric walls. In accordance with the result of Lu 2009, we definite the interaction energy by

$$U_I{}^{(i,j)} = \frac{c_{ij}(r_i + r_j)}{4}\int_0^{2\pi} (u_i - u_j)^2 d\theta \tag{4}$$

The final term Ω in Eq. (1) is the negative of the work done by p during cross-sectional deformation; it can be written as (Shima 2008)

$$\Omega = p\int_0^{2\pi}\left(r_N u_N + \frac{u_N{}^2 + v_N{}^2 - v_N\partial_\theta u_N + u_N\partial_\theta v_N}{2}\right)d\theta \tag{5}$$

Our objectives are to determine (i) the optimal displacements u_i and v_i that minimize U under a given value of p and (ii) the critical pressure p_c. Applying the variation method to U with respect to u_i and v_i, we obtain a system of $2N$ linear differential equations in regard to $\delta u_i(\theta)$ and $\delta v_i(\theta)$.

$$\delta u_i(\theta) = \sum_{n=1}^{\infty} \delta \overline{u_i}^{(n)} \cos n\theta, \delta v_i(\theta) = \sum_{n=1}^{\infty} \delta \overline{v_i}^{(n)} \sin n\theta \tag{6}$$

Substituting the expansions into the differential equations results in the matrix equation $M_u = 0$. As a result, the secular equation $\det(M) = 0$ is rewritten by

$$\det(M_{n=1})\det(M_{n=2})\cdots = 0 \tag{7}$$

Solving Eq. (7) with respect to p, we obtain a sequence of discrete values of p. Among these values of p_s, the minimum one serves as the critical pressure p_c that is associated with a specific integer k.

The remaining term, U_M, in Eq. (1) is the elastic energy of the eroded medium surrounding the inner part of the nanotubes. In polar coordinates, the radial and circumferential components of normal stress in the medium are denoted by σ_r and σ_θ, respectively, and the shear stress is denoted by $\tau_{r\theta}$; all three quantities are functions of r, and θ. Then, U_m is determined by σ_r and $\tau_{r\theta}$ at $r = r_N$ as

$$U_m = U_m^{(0)} + \Delta U_m^{(n)}, U_m^{(0)} = \frac{r_N}{2}\int_0^{2\pi} \sigma_r^{(0)}\Big|_{r=r_N} u_N^{(0)} d\theta$$
$$\Delta U_m^{(n)} = \frac{r_N}{2}\int_0^{2\pi} \sigma_r^{(n)}\Big|_{r=r_N} \delta u_N + \tau_{r\theta}^{(n)}\Big|_{r=r_N} \delta v_N) d\theta \tag{8}$$

3. RESULTS AND DISCUSSIONS

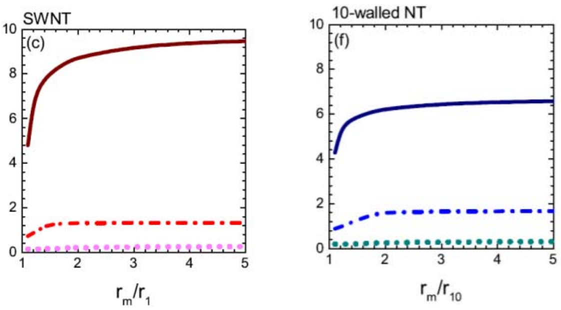

Fig. 1 Critical pressure p_c for cross-sectional deformation

Fig.1 shows the critical pressure pc required for the cross-sectional deformation of embedded carbon nanotubes. Different types of curves in the plots (dashed, dashed-dotted, and solid) correspond to different values of Young's modulus ratio E_m/E, where $E = 1$TPa is assumed to be the nanotube's modulus. We found that, independent of the E_m/E value, the p_c curves are upward convex as functions of the medium radius r_m in units of r_N . The growth of pc is rapid for $r_m/r_N < 2$, and then, is saturates for larger r_m/r_N . The rapid growth in pc indicates a „hardening effect’ caused by the surrounding medium, I.e. an enhancement in the radial stiffness of the embedded nanotube by encapsulation. This hardening effect disappears with a further increase in r_m/r_N ; the results imply that the surrounding medium with thickness $r_m > 5r_N$ no longer enhances the hardening effect and thus can be identified as a medium with infinitely large thickness($r_m \to \infty$), which is the case considered in our earlier work (Shima 2010)

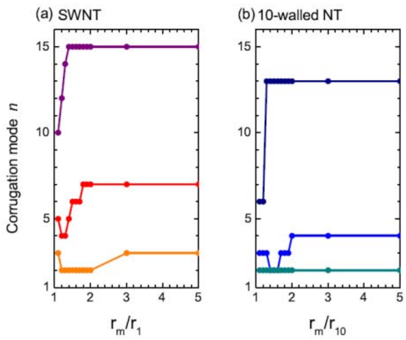

Fig. 2 Mode index n of the radial corrugation

Fig.2 provides the index of radial deformation modes observed immediately above p_c . Successive transformation of deformation modes with increasing medium thickness r_m was confirmed, as a result of the energy required to deform the surrounding medium needed to be responsible for determining the stable corrugation pattern of the embedded nanotube.

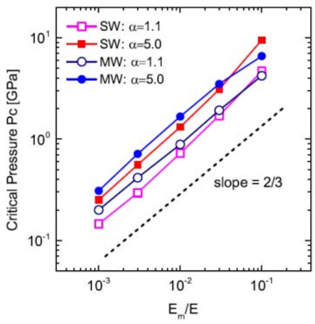

Fig. 3 Double logarithm plot of the critical pressure p_c

Fig.3 shows the p_c dependence on the modulus ratio (E_m/E) , where the radius ratio $\alpha \equiv r_m/r_N$ is fixed to be $\alpha = 1.1 or 5.0$. An unexpected result is that, for every choice of α and N , the p_c curves in this plot obey a function that is close to a power law, represented by

$$p_c \propto \left(\frac{E_m}{E}\right)^{\beta} \quad with \quad \beta \cong \frac{2}{3} \tag{9}$$

4. CONCLUSION

We have demonstrated a continuum elastic approach that describes the cross-sectional deformation of carbon nanotubes surrounded by a self-contracting host medium. The approach enables quantitative discussions of the critical pressure for radial corrugation and the stable corrugation mode of the nanotube surrounded by the contracting medium. Numerical calculations based on the established theory revealed the power-law dependence of the critical pressure on the elastic modulus of the medium, which is independent of the medium thickness.

REFERENCES

Guo Y. and Guo W. (2007), "Reassembly of single-walled carbon nanotubes into hybrid multilayered nanostructures inside nanotube exetruders," *Phys Rev B*, **76**(4), 04540 4:1-045404:6.

Krasheninnikov A. V. and Nordlund K. (2010), "Ion and electron irradiation induced effe-cts in nanostructured materials," *J Appl Phys*, **107**(7), 071301:1-071301:70

Lu. W. B., Liu. B., Wu. J. Xiao., Hwang K. C., Fu S. Y., and Huang Y., (2009), "Contiunm modeling of van der Waals interactions between carbon nanotubewalls, " *Appl Phys - Lett*, **94**(10), 101917:1-101917:3.

Osv´ath Z., V´ertesy G., Tapaszt´o L., W´eber F., Horv´ath Z. E., Gyulai J., and Bir`o L.P ., (2005), "Atomically resolved STM images of carbon nanotube defects produced by Ar+ irradiation," *Phys Rev B*, **72**(4), 045429:1-045429:6.

Shima H. and Sato M. (2013), "Elastic and Plastic Buckling of Carbon Nanotubes," *1st Ed*.

Shima H., Sato M., Iiboshi K., Ghosh S., and Arroyo M., (2010), "Diverse corrugation pa-ttern in radially shrinking carbon nanotubes," *Phys Rev B*, **82**(8), 085401:1-085401:7

Shima H. and Sato M., (2008), "Multiple radial corrugations in multiwall carbonanotube –under pressure," *Nanotechnology*, **19**(48), 495705:1-495705:8.

Shima H. and Sato M., (2009), "Pressure-induced structural transitions in mutiwalled ca-rbon nanotubes," *Phys Status Solidi (a)*, **206**(9), 2228-2233.

Xu Z., Wang L., and Zheng Q., (2008), "Enhanced Mechanical Properties of Prestresse-d Multi-Walled Carbon Nanotubes," *Sm*, **4**(6), 733-737.

Yang S. H., Feng L. L. and Feng F., (2009), "Torsional behaviour of carbon nanotubes with abnormal interlayer distances," *J. Phys. D: Appl Phys*, **42**(5), 055414:1-055414:5.