BUCKLING OF DOUBLE-WALLED CARBON NANOTUBES

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Abstract. In this note we deal with the approximate solution of the buckling problem of a clamped-free double-walled carbon nanotube. First the finite difference method is utilized to solve this case. Then this approach is verified by solving the buckling problem of a double-walled carbon nanotube that is simply supported at both ends for which the exact solution is available.

Keyword: Buckling, nanotube, finite difference method, clamped-free.

1. INTRODUCTION

The studies on buckling of carbon nanotubes (CNTs) include those of Yakobson et al. [1], Cornwell and Wille [2], Yao and Lordi [3], Garg et al. [4], Lu et al. [5], Wang et al. [6], Falvo et al. [7], Guo et al. [8], Sudak [9], He et al. [10] and Wang [11,12]. However, buckling of carbon nanotubes is not yet studied sufficiently. For example, we are not able to conclude yet if this kind of a structure exhibits the same buckling behavior as uniform beams. In their work on the buckling of double-walled carbon nanotubes (DWCNTs) Elishakoff and Pentaras [13] found, with Galerkin method, that the ratio between the critical loads of a clamped-clamped DWCNT and one simply supported at both ends is about four whereas the analogous ratio for the uniform beam equals four exactly. They did not investigate the case of clamped-free DWCNTs because of the necessity to satisfy different boundary conditions for inner and outer nanotubes. This study fills the existing gap.

Hereinafter, we use the finite difference method that has been widely used in the past for buckling analysis of various structures (see for example, works by Salvadori [14], Iremonger [15], Chajes [16], and Mikhailov [17]).

2. BUCKLING DIFFERENTIAL EQUATIONS IN FINITE DIFFERENCE FORM

The governing differential equations for buckling of the DWCNTs read [13]:

$$c\,(w_2 - w_1) = EI_1 \frac{d^4 w_1}{dx^4} + P \frac{A_1}{A_1 + A_2} \frac{d^2 w_1}{dx^2} \tag{1}$$

$$-c\left(w_2 - w_1\right) = EI_2\frac{d^4w_2}{dx^4} + P\frac{A_2}{A_1 + A_2}\frac{d^2w_2}{dx^2} \tag{2}$$

where x is the axial coordinate, $w_i\left(x, t\right)$ is the transverse displacement of the ith tube, c = 71.11 GPa^3 is the Van der Waals interlayer interaction coefficient, $E = 1$ TPa is the modulus of elasticity, inner radius R_1 is taken as 0.35 nm, whereas the outer radius R_2 is fixed at 0.7 nm, the thickness of each tube is 0.34 nm. The sought buckling load is denoted as P, I_i is the second moment of area of the ith tube, and A_i is the cross-sectional area; the indexes $i = 1,2$ pertain to the inner tube and outer tube, respectively.

In the finite difference method expressions for the derivatives of the displacement at a point are approximated by an algebraic formula through the displacements at that point and at some nearby points. In fact, the beam is divided in N segments and thus has $N + 1$ nodes for which we have to find the displacement in order to know the one of the entire DWCNT when P reaches the critical value.

For the first derivative we use the central difference expression:

$$\frac{dw}{dx}\left(x_j\right) = \Delta^c w_j = \frac{w^{(j+1)} - w^{(j-1)}}{2h} \tag{3}$$

where j is the number of the node, of coordinate x_j, where the displacement is expressed, and $h = L/N$ represents the length of a segment.

The other derivatives are expressed from the first one; thus Eqs. (1) and (2) are now written at each node j as follows

$$c\left(w_2^{(j)} - w_1^{(j)}\right) = \frac{EI_1}{h^4}\left(w_1^{(j+2)} - 4w_1^{(j+1)} + 6w_1^{(j)} - 4w_1^{(j-1)} + w_1^{(j-2)}\right) + \\ \frac{PA_1}{A_1 + A_2}\frac{1}{h^2}\left(w_1^{(j+1)} - 2w_1^{(j)} + w_1^{(j-1)}\right) \tag{4}$$

$$-c\left(w_2^{(j)} - w_1^{(j)}\right) = \frac{EI_2}{h^4}\left(w_2^{(j+2)} - 4w_2^{(j+1)} + 6w_2^{(j)} - 4w_2^{(j-1)} + w_2^{(j-2)}\right) + \\ \frac{PA_2}{A_1 + A_2}\frac{1}{h^2}\left(w_2^{(j+1)} - 2w_2^{(j)} + w_2^{(j-1)}\right) \tag{5}$$

Eqs. (4) and (5) are rewritten as follows:

$$\left(w_1^{(j+2)} - 4w_1^{(j+1)} + 6w_1^{(j)} - 4w_1^{(j-1)} + w_1^{(j-2)}\right) + \\ \alpha_1\left(w_1^{(j+1)} - 2w_1^{(j)} + w_1^{(j-1)}\right) - c_1\left(w_2^{(j)} - w_1^{(j)}\right) = 0 \tag{6}$$

$$\left(w_2^{(j+2)} - 4w_2^{(j+1)} + 6w_2^{(j)} - 4w_2^{(j-1)} + w_2^{(j-2)}\right) + \\ \alpha_2\left(w_2^{(j+1)} - 2w_2^{(j)} + w_2^{(j-1)}\right) - c_2\left(w_2^{(j)} - w_1^{(j)}\right) = 0 \tag{7}$$

where the coefficients are defined as:

$$c_i = \frac{ch^4}{EI_i} \tag{8}$$

$$\alpha_i = \frac{PA_ih^2}{EI_i\left(A_1 + A_2\right)} \tag{9}$$

The solution is found by solving the system of equations written at each node of the beam.

3. BUCKLING OF CLAMPED-FREE DWCNTS

Let us deal with the buckling load of a clamped-free DWCNT. The boundary conditions are:

$$w_i(0) = w'_i(0) = 0 \tag{10}$$

$$w''_i(L) = 0 \tag{11}$$

$$EI_i w'''_i(L) + \frac{PA_i}{A_1 + A_2} w'_i(L) = 0 \tag{12}$$

Thus there are 8 boundary conditions. The expression (10) leads in finite difference form to the following expressions

$$w_i^{(0)} = 0, \tag{13}$$

$$w_i^{(1)} = w_i^{(-1)}. \tag{14}$$

From Eq. (11) we get

$$w_i^{(n+1)} = 2w_i^{(n)} - w_i^{(n-1)} \tag{15}$$

Finally Eq. (12) provides

$$w_i^{(n+2)} = 2w_i^{(n+1)} - 2w_i^{(n-1)} + w_i^{(n-2)} - \alpha_i \left(w_i^{(n+1)} - w_i^{(n-1)} \right) \tag{16}$$

One observes that Eq. (16) constitutes a condition on $w_i^{(n+2)}$. Thus, the axis is extended over the end nodes 0 and N to introduce fictitious nodes $N+1$ and $N+2$. This is done to satisfy the equations which need the displacement values at $x = -h$, $x = L + h$, and $x = L + 2h$ (Fig. 1). We consider the equations of the displacement expressed from $j = 1$ to $j = N$ in order to have $2N$ equations and variables.
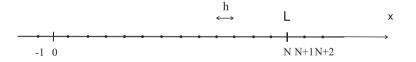

Fig. 1. Nanotube divided for finite difference analysis

In the general case when the beam is divided into N segments, we have to satisfy, at each nodal point j, the difference equations (6) and (7), which correspond, for $i = 1, 2$ to the following expression:

$$w_i^{(j-2)} - (4 - \alpha_i) w_i^{(j-1)} + (6 + 2\alpha_i + c_i) w_i^{(j)} - (4 - \alpha_i) w_i^{(j+1)} + w_i^{(j+2)} - c_i w_{1+\delta_{i,1}}^{(j)} = 0 \tag{17}$$

where $\delta_{i,1}$ is the Kronecker's delta. The latter equals unity when $i = 1$ and vanishes otherwise. The coefficients in Eq. (17) are constant and only the parameter α_i is unknown. The coefficients are sorted in a $N \times N$ matrix, and since its determinant must vanish we obtain the value of the critical load as the smallest root.

For illustration consider the cases $N = 2$ and $N = 3$ in detail. The inner nodal points are 0, 1 and 2. Thus, to facilitate satisfaction of Eq. (16) we introduce fictitious nodes -1, 3 and 4. The boundary conditions are Eqs. (13) and (14), and Eqs. (15) and (16) lead to:

$$w_i^{(3)} = 2w_i^{(2)} - w_i^{(1)} \tag{18}$$

$$w_i^{(4)} = 4w_i^{(2)} - 4w_i^{(1)} - \alpha_i \left(w_i^{(2)} - w_i^{(1)} \right) \tag{19}$$

By substitution of $j = 1$ in Eq. (17) we obtain the equation of displacement at the node 1 for the two tubes

$$w_i^{(-1)} - (4 - \alpha_i) \, w_i^{(0)} + (6 - 2\alpha_i + c_i) \, w_i^{(1)} - (4 - \alpha_i) \, w_i^{(2)} + w_i^{(3)} - c_i w_{1+\delta_{i,1}}^{(1)} = 0 \tag{20}$$

Applying the boundary conditions (13), (14), (18) and (19), we obtain:

$$(6 - 2\alpha_i + c_i) \, w_i^{(1)} - (2 - \alpha_i) \, w_i^{(2)} - c_i w_{1+\delta_{i,1}}^{(1)} = 0 \tag{21}$$

At the next node ($j = 2$) we have:

$$(-4 + 2\alpha_i) \, w_i^{(1)} + (2 - 2\alpha_i + c_i) \, w_i^{(2)} - c_i w_{1+\delta_{i,1}}^{(2)} = 0 \tag{22}$$

The coefficients of these expressions generate a matrix equation:

$$\begin{bmatrix} 6 - 2\alpha_1 + c_1 & -2 + \alpha_1 & -c_1 & 0 \\ -4 + 2\alpha_1 & 2 - 2\alpha_1 + c_1 & 0 & c_1 \\ -c_2 & 0 & 6 - 2\alpha_2 + c_2 & -2 + \alpha_2 \\ 0 & -c_2 & -4 + 2\alpha_2 & 2 - 2\alpha_2 + c_2 \end{bmatrix} \begin{pmatrix} w_1^{(1)} \\ w_1^{(2)} \\ w_2^{(1)} \\ w_2^{(2)} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{23}$$

In order this system to have a nontrivial solution, the determinant of this matrix must vanish. This requirement leads to the following equation:

$$2.261 * 10^{33} p^4 - 7.419 * 10^{23} + 2.939 * p^2 - 1.057 * 10^{16} p + 4.79 * 10^7 = 0 \tag{24}$$

The smallest root of this expression yields the critical load: $P_c r = 5.314$ nN.

The case $N = 3$ leads to 6 equations for the nodes $j = 1, 2, 3$. These are

$$(7 - 2\alpha_i + c_i) \, w_i^{(1)} - (4 - \alpha_i) \, w_i^{(2)} + w_i^{(3)} - c_i w_{1+\delta_{i,1}}^{(1)} = 0 \tag{25}$$

$$(-4 + \alpha_i) \, w_i^{(1)} + (5 - 2\alpha_i + c_i) \, w_i^{(2)} - (2 - \alpha_i) \, w_i^{(3)} - c_i w_{1+\delta_{i,1}}^{(2)} = 0 \tag{26}$$

$$2 w_i^{(1)} - (4 - 2\alpha_i) \, w_i^{(2)} + (2 - 2\alpha_i + c_i) \, w_i^{(3)} - c_i w_{1+\delta_{i,1}}^{(3)} = 0 \tag{27}$$

Eqs. (25)-(27) are equivalent to a matrix equation. Its determinant

$$\begin{vmatrix} 7 - 2\alpha_1 + c_1 & -4 + \alpha_1 & 1 & -c_1 & 0 & 0 \\ -4 + \alpha_1 & -5 - 2\alpha_1 + c_1 & -2 + \alpha_1 & 0 & -c_1 & 0 \\ 2 & -4 + 2\alpha_1 & 2 - 2\alpha_1 + c_1 & 0 & 0 & -c_1 \\ -c_2 & 0 & 0 & 7 - 2\alpha_2 + c_2 & -4 + \alpha_2 & 1 \\ 0 & -c_2 & 0 & -4 + \alpha_2 & 5 - 2\alpha_2 + c_2 & -2 + \alpha_2 \\ 0 & 0 & -c_2 & 2 & -4 + 2\alpha_2 & 2 - 2\alpha_2 + c_2 \end{vmatrix} \tag{28}$$

must vanish. This requirement yields the following sixth order polynomial equation for P:

$$4.422*10^{47}p^6-1.396*10^{43}p^5+6.67*10^{37}p^4-8.499*10^{31}p^3+9.632*10^{24}p^2-2.877*10^{17}p+1.299*10^9 = 0 \tag{29}$$

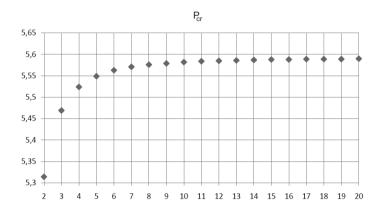The value of the critical buckling load is $P_{cr} = 5.469$ nN.

Fig. 2. Variation of the critical buckling load with the number of segments for a clamped-free DWCNT

Table 1. Critical buckling load of a clamped-free DWCNT

N	2	3	4	5	6	7	8	9	10	15	20
P_{cr}(nN)	5.314	5.469	5.524	5.549	5.563	5.571	5.576	5.579	5.582	5.588	5.590

We also conduct the evaluation of the critical load P for consecutive values of N until the convergence is reached (see Fig. 2). The results are reported in Tab. 1.

4. VERIFICATION: BUCKLING OF DWCNTS SIMPLY SUPPORTED AT BOTH ENDS

To verify the above approach we conduct a comparison with the results previously obtained by Elishakoff and Pentaras [13] for the simply supported case. Specifically, we calculate the buckling load of a DWCNT simply supported at both ends by the finite difference method. Firstly, we write the boundary conditions of this system. For each end the following expressions should be satisfied:

$$w_i(0) = w_i(L) = 0, \tag{30}$$

$$\frac{d^2w_i}{dx^2}(0) = \frac{d^2w_i}{dx^2}(L) = 0. \tag{31}$$

In finite difference setting we have:

$$w_i^{(0)} = w_i^{(N)} = 0 \tag{32}$$

Eq.(31) leads to

$$\frac{w_i^{(-1)} - 2w_i^{(0)} + w_i^{(1)}}{h^2} = \frac{w_i^{(N-1)} - 2w_i^{(N)} + w_i^{(N+1)}}{h^2} = 0 \tag{33}$$

Thus we obtain two relations:

$$w_i^{(1)} = -w_i^{(-1)} \tag{34}$$

$$w_i^{(N+1)} = -w_i^{(N-1)} \tag{35}$$

This time the equation of the displacement at $x = L + 2h$ is not needed so Eq. (17) is applied to nodes from $j = 1$ to $j = N - 1$ in order to have as many equations as the number of variables; in this case the system is of size $2(N - 1)$.

$$(4 - 2\alpha_i + c_i)\, w_i^{(1)} - c_i w_{1+\delta_{i,1}}^{(1)} = 0 \tag{36}$$

This leads to the following determinant:

$$\begin{vmatrix} 4 - 2\alpha_1 + c_1 & -c_1 \\ -c_2 & 4 - 2\alpha_2 + c_2 \end{vmatrix} = 0 \tag{37}$$

From Eq. (37) we obtain the value of the critical load as the smallest root : $P_{cr} = 18.138$ nN, whereas the Elishakoff and Pentaras [13] result is $P_{cr} = 22.63$ nN. One observes that 2 segments are not sufficient for an accurate evaluation of the buckling load.

In the case of three segments, i.e. $N = 3$, the system is composed of 4 equations which are those at nodes $j = 1$ and $j = 2$:

$$(5 - 2\alpha_i + c_i)\, w_i^{(1)} - (4 - \alpha_i)\, w_i^{(2)} - c_i w_{1+\delta_{i,1}}^{(1)} = 0 \tag{38}$$

$$(-4 + \alpha_i)\, w_i^{(1)} + (5 - 2\alpha_i + c_i)\, w_i^{(2)} - c_i w_{1+\delta_{i,1}}^{(2)} = 0 \tag{39}$$

Eqs. (38) and (39) lead to the following requirement:

$$\begin{vmatrix} 5 - 2\alpha_1 + c_1 & -4 + \alpha_1 & -c_1 & 0 \\ -4 + \alpha_1 & 5 - 2\alpha_1 + c_1 & 0 & -c_1 \\ c_2 & 0 & 5 - 2\alpha_2 + c_2 & -4 + \alpha_2 \\ 0 & -c_2 & -4 + \alpha_2 & -5 - 2\alpha_2 + c_2 \end{vmatrix} = 0 \tag{40}$$

Table 2. Critical buckling load for a DWCNT simply supported at both ends

N	2	3	4	5	6	7	8	9	10	12	15	20
P_{cr} (nN)	18.138	20.403	21.247	21.646	21.866	21.999	22.086	22.146	22.189	22.245	22.290	22.326

We obtain $P_{cr} = 20.403$ nN. The results for various values of N are listed in Tab. 2. The smallest percentage-wise difference from the Elishakoff and Pentaras [13] value is
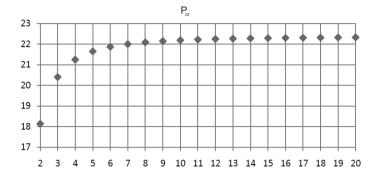
Fig. 3. Variation of the critical buckling load with the number of segments for a DWCNT simply supported at both ends

1.34%, and is achieved for $N = 20$ (see Fig. 3). Thus the finite difference method yields a result that is extremely close to the exact solution.

5. DISCUSSION AND CONCLUSION

In this study it has been demonstrated that the finite difference method can be successfully applied to buckling of double-walled carbon nanotubes since it yields extremely reliable results. The best approximation for the clamped-free DWCNT is 5.590 (Tab. 1), and the best approximation for the simply supported at both ends is 22.236 (Tab. 2). This leads to a ratio of 3.978, what tends to the ratio we expected from the beam theory. The difference comes from two reasons. First the convergence of the finite difference discretization; and second, the introduction of the boundary conditions. In the first case they are expressed with $w = 0$, $w' = 0$ at the clamped edge and $w'' = 0$ and $w''' = 0$ at the free edge (Eqs. 10-16). In the second case they are expressed with $w = 0$ and $w'' = 0$ at both edges. The examination of the finite difference formulas shows that the error level would not be the same by using the third order differentiation.

The major complexity with this method is that when the number of nodes increases substantially, the calculation time increases dramatically. Indeed this process entails the solution of a large number of simultaneous equations. As indicated by Salvadori [14], one can use the Richardson's extrapolation scheme to increase the accuracy of the result instead of increasing the number of segments. This approximation is expressed by:

$$P_{cr} = \frac{N_1^2 P_{cr_1} - N_2^2 P_{cr_2}}{N_1^2 - N_2^2} \tag{41}$$

where N_i is the number of segments into which the beam was divided to obtain an approximation of the critical buckling load denoted as $P_{cr\,i}$. To illustrate the effectiveness of Richardson's extrapolation scheme, the approximate resuls obtained for the clamped-free case with $N_1 = 4$ and $N_2 = 5$ will be substituted in Eq. (41):

$$P_{cr} = \frac{16 * 5.524 - 25 * 5.549}{16 - 25} = 5.593 \, nN \tag{42}$$

Note that this solution is nearly as accurate as can be achieved by using $N = 20$ segments of the nanotubes.

Thus, the combination of the finite difference method with the Richardson's extrapolation scheme gives an excellent tool to investigate the buckling of double-walled carbon nanotubes.

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