Buckling Temperature of a Single-Walled Carbon Nanotube Using Nonlocal Timoshenko Beam Model

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The thermal buckling of single-walled carbon nanotube (SWCNT) subjected to a uniform temperature rise is studied using Timoshenko beam model, including the effects of transverse shear deformation and rotary inertia. The governing buckling equations of SWCNT are established on the basis of nonlocal continuum theory. An analytical solution to the equations is derived for the determination of critical buckling temperature. The solution can be further reduced to obtain the results of Euler beam model. According to the analysis, for mode 4, the Euler beam model overpredicts the critical buckling temperature by 57%, 13% and 3.5% for \( L/d = 10, 30 \) and 60, respectively. The Timoshenko beam model is able to predict the buckling temperature of the SWCNT at higher-order modes with small length-to-diameter ratios. In addition, the critical buckling temperature decreases with increasing the nonlocal value.

Keywords: Single-Walled Carbon Nanotubes, Critical Buckling Temperature, Timoshenko Beam Model, Nonlocal Continuum Theory.

1. INTRODUCTION

Carbon nanotubes (CNTs) have become the most significant material in the coming nanotechnology age due to their excellent physical and chemical properties.\(^1\)\(^-\)\(^4\) A great number of researches have been made to investigate the diverse properties of them for a wide variety of applications. CNTs subjected to compression or bending are especially prone to buckling because of their high aspect ratios. The occurrence of buckling of CNTs can lead to potential applications as nanometer-sized tunnel barriers for electron transport\(^5\) and fluid-flow control nano-valves.\(^6\)\(^-\)\(^7\)

The theoretical methods, including atomistic simulations and continuum mechanics, were often applied for studying the buckling behavior of CNTs because of the difficulties encountered by experiments on the nanoscale at the current stage.\(^8\)\(^-\)\(^12\) For example, Wang et al.\(^10\) developed a continuum mechanics models to investigate the torsional buckling of CNTs with different length-to-diameter ratios and performed molecular dynamics simulations to verify the buckling results. Kumar et al.\(^12\) studied the buckling of carbon nanotubes, modeled as nonlocal one dimensional continuum within the framework of Euler–Bernoulli beams, and indicated significant dependence of nonlocal parameter on buckling load for particular types of boundary conditions.

Recently, Lee and Chang\(^13\) analyzed the buckling temperature of single-walled carbon nanotube (SWCNT) due to thermal effect. Hsu et al.\(^14\) studied similar issue that arose in the double-walled carbon nanotube. However, the effects of nonlocal parameter and elastic medium were ignored in these analyses, which may influence accuracy of the results. In this study, the critical buckling temperature of SWCNT subjected to a uniform temperature rise is analyzed based on Euler beam and Timoshenko beam models. In the analysis, the SWCNT is embedded in an elastic matrix, and the nonlocal continuum theory is introduced. In addition, the critical buckling temperature of SWCNT with different modes and nonlocal parameters for different length-to-diameter ratios is investigated.

2. ANALYSIS

A SWCNT with length \( L \) is embedded in an elastic matrix and is assumed to be a cantilever beam fixed at \( X = 0 \) and a stopper end at \( X = L \) as shown in Figure 1. The axial displacement is constrained by the stopper and that induces a thermal buckling load \( F \) due to temperature rise \( T \). The SWCNT has an equivalent Young’s modulus \( E \), shear modulus \( G \), length \( L \), average diameter \( d \) and thickness \( t \). The Timoshenko beam model, which is taken rotary inertia and transverse shear deformation into account, is employed to analyze the buckling behavior.
The governing equations of Timoshenko beam considering the nonlocal continuum theory are two coupled differential equations and the associated boundary conditions can be simplified to the following dimensionless equations and boundary conditions

\[
\frac{d^2y}{dx^2} - s^2 p \frac{d^2y}{dx^2} - s^2 wy = 0 \tag{8}
\]

\[
\frac{d^2\psi}{dx^2} - s^2 \epsilon \left( p \frac{d^3y}{dx^3} + w \frac{dy}{dx} \right) + \left( \frac{dy}{dx} - \psi \right) = 0 \tag{9}
\]

\[
\frac{d\psi(1)}{dx} - \epsilon \left( p \frac{d^2\psi(1)}{dx^2} + wy(1) \right) = 0 \tag{12}
\]

\[
\frac{dy(1)}{dx} - \psi(1) = s^2 p \frac{dy(1)}{dx} \tag{13}
\]

In order to solve the above differential system, we set the solutions to be expressed as

\[
y = Be^{yx} \tag{14}
\]

\[
\psi = Ze^{yx} \tag{15}
\]
where $B$ and $Z$ are arbitrary constants. Substituting Eqs. (14) and (15) into Eqs. (8) and (9), we find the following associated auxiliary polynomial of function $\gamma$ as:

$$
\Omega(\gamma) = (1 - p_s^2 - p_e^2)\gamma^4 + (p - w_s^2 - w_e^2)\gamma^2 + w = 0
$$

(16)

The general solutions of Eqs. (8) and (9) can be expressed as follows:

$$
\gamma = \sum_{j=1}^{4} B_j e^{\gamma_j t}
$$

(17)

$$
\phi = \sum_{j=1}^{4} Z_j e^{\gamma_j t}
$$

(18)

where $B_j$ and $Z_j$ are constants. Substituting Eqs. (17) and (18) into Eqs. (8) and (9), we obtain the following relationship as

$$
B_j = \lambda_j Z_j, \quad j = 1, 2, 3, 4
$$

(19)

where

$$
\lambda_j = \frac{s^2 \gamma_j^2 - 1}{\gamma_j (p s^2 \gamma_j^2 + s^2 w - 1)}
$$

(20)

Substituting Eqs. (17) and (18) into Eqs. (8) and (9), then applying the boundary conditions Eqs. (10)–(13), the following equation can be yielded

$$
\begin{bmatrix}
1 & 1 & 1 & 1 \\
\lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 \\
\kappa_1 & \kappa_2 & \kappa_3 & \kappa_4 \\
\xi_1 & \xi_2 & \xi_3 & \xi_4 \\
\end{bmatrix}
\begin{bmatrix}
Z_1 \\
Z_2 \\
Z_3 \\
Z_4 \\
\end{bmatrix} = 0
$$

(21)

where $\kappa_j = e^{\gamma_j} (\gamma_j \lambda_j - p s^2 \lambda_j - 1)$, $\xi_j = e^{\gamma_j} (\gamma_j - p w s^2 \gamma_j^2 - w e^2 \lambda_j)$, and $j = 1, 2, 3, 4$. Hence, the nondimensional critical buckling temperature $p_c$ can be solved from Eq. (21).

In case that $w = 0$ in Eq. (21) is assumed, the nondimensional critical buckling temperature $p_{cN}$ for the SWCNT subjected to a uniform temperature rise without an embedding medium is obtained.

Moreover, when $s = 0$ is assumed in Eq. (21), it implies that the effects of transverse shear deformation and rotary inertia are not considered. Accordingly, the critical buckling temperature based on the Euler beam model could be also obtained.

3. RESULTS AND DISCUSSION

In order to know the effect of relative parameters on the critical buckling temperature of SWCNT, we considered the geometric and material parameters as follows: $\alpha = 1.1 \times 10^{-6} ^\circ \text{C}^{-1}$, $L = 30 \mu\text{m}$, $\nu = 0.2$, $t = 0.34 \text{ nm}$. In addition, the nonlocal parameter is assumed to be $e_{0d} = 0.5 \text{ nm}$, and the Winkler constant of $w = 0.035$ which is equivalent to an elastic medium constant of $W = 0.2 \text{ MPa}$. The comparison of nondimensional critical buckling temperature of SWCNT with different length-to-diameter ratios and the nonlocal value of $e_{0d} = 0.5$ for the first ten modes based on Euler beam and Timoshenko beam models is shown in Figure 2. It can be observed that for the higher-order modes, the critical buckling temperature of the Timoshenko beam model are significantly lower than that of the Euler beam model due to the effects of shear deformation and rotary inertia. The discrepancy is large, especially at relatively small length-to-diameter ratios ($L/d < 30$) and higher-order modes. For example, for mode 4, the Euler beam model overpredicts the critical buckling temperature of SWCNT by $57\%$, $13\%$ and $3.5\%$ for $L/d = 10$, $30$ and $60$, respectively. The relative percentage difference between the two beam models increases with respect to increasing mode numbers.

Figure 3 depicts the critical buckling temperature of SWCNT with different nonlocal values and $L/d = 30$ for different modes based on Timoshenko beam model. The parameter value of $e_{0d} = 0$ implies that the nonlocal effect is neglected. It can be seen that the effect of nonlocal parameter $e_{0d}$ on the critical buckling temperature is significant, especially at higher-order modes. Increasing the nonlocal effect decreases the critical buckling temperature. This can be seen from Eq. (21).
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For comparison purposes, the variation in the ratio of buckling temperature of SWCNT with embedding medium \( p_c \) to that without embedding medium \( p_{CN} \) with different Winkler constants, for the first three modes at \( L/d = 30 \) and \( e_0a = 0.5 \) based on Timoshenko beam model has been evaluated as shown in Figure 4. It can be seen that the buckling temperature of SWCNT with embedding medium is larger than that without embedding medium due to a stiffer structure. In addition, the temperature ratio, \( p_c/p_{CN} \), increases with increasing the Winkler constant for the modes. The trend is more obvious in the lower-order modes.

4. CONCLUSIONS

The nonlocal Timoshenko beam model was applied to analyze the critical buckling temperature of SWCNT subjected to axial compression due to temperature rise. According to the analysis, the following results were obtained:

1. The effects of rotary inertia and shear deformation on the critical buckling temperature of SWCNT increased with decreasing the length-to-diameter ratio, especially at higher-order modes.
2. Increasing the value of nonlocal parameter decreased the critical buckling temperature, especially at higher-order modes.
3. The ratio of buckling temperature of SWCNT with embedding medium to that without embedding medium increased with increasing the Winkler constant. The trend was more obvious at lower-order modes.

Acknowledgment: The authors wish to thank the National Science Council of the Republic of China in Taiwan for providing financial support for this study under Projects NSC 98-2221-E-168-019 and NSC 97-2221-E-168-019-MY2.

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Received: 5 February 2010. Accepted: 30 March 2010.