Buckling Analysis of Silicon Carbide Nanotubes (SiCNTs)

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Abstract
Nanotubes have a great importance in the rising of nanotechnology. Carbon nanotubes are widely used and many works have been done about it. As the technology always need better materials with better properties, scientist have developed Carbon nanotubes to Silicon carbide nanotubes. In this work, the stability of the Silicon nanotube is investigated in the buckling case. Its stability has an important role since it is used in high-tech equipment. In this article, the buckling analysis SiCNT is investigated by using Euler-Bernoulli beam theory for different boundary conditions. Results are presented in figures and table.

Keywords: Silicon carbide, buckling, Euler-Bernoulli.

1. Introduction

Many works about the applications of carbon nanotubes (CNTs) and its durability have been done in the past decade. Due to their extraordinary mechanical and electrical properties, carbon nanotubes have been used in nano-sized devices and sensors, chemical laboratories, material engineering and even in biomechanics. The most exciting and interesting property of the CNTs is their very high mechanical strength (tensile and Young’s modulus). Many researches and analysis have been made about Carbon nanotubes by modeling it as beam and shells [16-26]. After a couple years of founding CNTs scientist have developed a new structure of carbon nanotube which is very much better in durability under high temperatures. This new structure has been called Silicon carbide nanotube (SiCNT). For example, Silicon carbide nanotubes can stay stable under 1000 °C (in air), whereas Carbon nanotubes are limited to stay stable until 600°C [1]. This specialty of SiCNTs provide to work with it under high-temperature, harsh environment nanotubes reinforced ceramics. SiCNTs obtain another kind of multiple-bilayer wall structure which allows the surface Silicon atoms to be functionalized readily with molecules. This special wall structure allows SiCNTs to undergo self-assembly and make it compatible with different kind of materials such as high-performance fiber-reinforced ceramics and biotechnological applications. In order to obtain SiCNTs, The NASA Glenn Research Center has been collaborating with Rensselaer Polytechnic Institute [2]. Researches from the collaboration have developed several methods to obtain SiCNTs. Some of those methods are chemical conversion of CNTs to SiCNTs, direct SiCNT growth on catalyst, and template-derived SiCNTs [2]. More recently, [3] have synthesized SiNTs which are considered as a kind of self-assembled SiNTs which can form crystal structures. Ansari et al. have calculated the buckling behavior of single-walled silicon carbide nanotubes by using a 3D finite element method [5].
2. Buckling analysis of silicon carbide nanotube

The demonstration of silicon carbide nanotube and its continuum model is shown in Fig.(1) and Fig.(2). In order to calculate the critical buckling load of the model, Euler-Bernoulli beam theory is used for different boundary conditions. Results are obtained for both with and without surface effect. For modeling, L is the length; \( R_{avg} \) is average radius, \( D_{avg} \) average diameter, t thickness, E Young’s modulus of the nanotube.

![Fig. 1. Demonstration of Silicon Carbide sheet](image)

Silicon (Si) is a nonmetallic chemical element from the carbon family (Group 14 of the periodic table). The name of silicon is coming from the Latin *silex* or *silicis* which means ‘flint’ or ‘hard stone’. Amorphous elemental silicon was first isolated and described as an element in 1824 by a Swedish chemist Jöns Jacob Berzelius. SiCNTs can be obtained by two different techniques. The first and the more stable one is Si atoms and C atoms are having alternating arrangement. In this structure each C atoms are bonded to three Si atoms. On the other hand in the second technique, two atoms of Si and one atom of C is bonded to each other. Studies have shown that the first technique is more effective and stable [4]. Here in Fig. 1, a single layer of SiCNT is demonstrated. Si atoms are shown in yellow color and Carbon (C) atoms are shown in grey. In order to obtain a nanotube from the sheet, similarly with graphene sheet, rolling the sheet is the basic (Fig. 2).

![Si atoms → C atoms](image)

Silicon carbide nanotubes are tubes which contain both Si and C atoms bonded each other. In this work, as it can be seen from figs. (1-2), the type of which three Si atoms are bonded to one C atoms. Calculations have been made for different types of boundary condition by employing Euler-Bernoulli classical beam theory. The mechanical continuum model of SiCNT is shown in Fig. (3). The length of the nanotube is shown with ‘L’, the average radius with ‘\( R_{avg} \)’ and the thickness with ‘t’. In continuum model, the nanotube will be modeled as a perfect cylindrical shaped tube with a constant inner and outer diameter. The average radius ‘\( R_{avg} \)’ is obtained by using the arithmetical average of the inner and outer radius. The thickness ‘t’ is the difference between the inner and outer radius.
Fig. 2. Demonstration of obtaining silicon carbide nanotube from a single layer of silicon carbide sheet

3. Euler-Bernoulli formulation

The buckling equation of a beam is:

$$E I \frac{d^4 y}{dx^4} + P \frac{d^2 y}{dx^2} = 0$$  \hspace{1cm} (1)

If setting $\alpha^2 = \frac{P}{EI}$, Eq.(1) can be simplified as:

$$y'''' + \alpha^2 y'' = 0$$  \hspace{1cm} (2)

If setting $y = e^{\alpha x}$, Eq.(2) can be simplified as:

$$Br^4 e^{\alpha x} + \alpha^2 Br^2 e^{\alpha x} = 0$$  \hspace{1cm} (3)
By reducing Eq.(3), we can obtain:

\[ r^4 + \alpha^2 r^2 = 0 \]  

Solving Eq.(4), the result is:

\[ r^2 = -\alpha^2 \]

\[ r_{1,2} = 0 \quad \text{and} \quad r_{3,4} = \pm i\alpha \]  

\( r_{1,2} \) and \( r_{3,4} \) are two pairs of single complex root of Eq.(4).

By substitution roots into Eq.(5) and solving it, we obtain:

\[ y = C_1 \sin \alpha x + C_2 \cos \alpha x + C_3 x + C_4 \]  

\( C_1, C_2, C_3, C_4 \) are constants which can be obtained from boundary conditions. The first order derivative of Eq.(6) is:

\[ y' = C_1 \alpha \cos \alpha x - C_2 \alpha \sin \alpha x + C_3 \]  

The second order derivative of Eq.(6) is:
\[ y'' = -C_1 \alpha^2 \sin \alpha x - C_2 \alpha^2 \cos \alpha x \] (8)

The third order derivative of Eq.(6) is:

\[ y''' = -C_1 \alpha^3 \cos \alpha x + C_2 \alpha^3 \sin \alpha x \] (9)

For a beam which is Clamped-Free supported, the boundary conditions would be as followed:

\[ y(0) = y'(0) = 0, \quad y''(l) = y'''(l) + \alpha^2 y'(l) = 0 \] (10)

By substituting boundary conditions into Eq.(6), Eq.(7), Eq.(8) and Eq.(9) we obtain:

\[ y(0) = C_2 + C_4 = 0 \] (11)
\[ y'(0) = C_1 \alpha + C_3 = 0 \] (12)
\[ y''(l) = -C_1 \alpha^2 \sin \alpha l - C_2 \alpha^2 \cos \alpha l = 0 \] (13)
\[ y'''(l) + \alpha^2 y'(l) = C_3 \alpha^2 = 0 \] (14)

As it is mentioned above \( C_1, C_2, C_3, C_4 \) are constants and we can obtain those constant by using Eq.(11), Eq.(12), Eq.(13) and Eq.(14). The solution is obtained as follow:

\[ \alpha^5 \cos(\alpha l) = 0 \] (15)

There are 2 possibilities which make the Eq.(15) equal to zero.

\[ \alpha^5 = 0 \] (16)
\[ \cos(\alpha l) = 0 \] (17)

By substituting \( \alpha^2 = \frac{P}{EI} \) into Eq.(17) we can obtain:

\[ \cos \left( \sqrt{\frac{P}{EI}} \right) = 0, \quad \sqrt{\frac{P}{EI}} = n \frac{\pi}{2} \] (18)

So the buckling load can be obtained via this formula:

\[ P = \frac{n^2 \pi^2 \cdot EI}{4l^2} \] (19)

The solutions are similarly obtained for other types of boundary conditions.
3.1. Numerical examples

In this study, the buckling of SiCNTs with various boundary conditions is investigated via classical Euler-Bernoulli beam theory. Some of the results which are showing the buckling loads for Clamped-Free, Simple-Simple, Clamped-Simple, Clamped-Clamped boundary conditions are in Figure 4. The elasticity modulus is $E=0.62$ TPa [1,18], the thickness is $t=0.075$ nm, the moment of inertia is $I=\pi t R_{avg}^3$. ($R_{avg}=D_{avg}/2$). As it can be seen in Fig 4, the buckling load is investigated for simply supported, clamped, propped and cantilever boundary conditions respectively. Fig. 4 shows that the buckling load is decreasing dramatically with the increasing of length.

![Buckling load plot](image)

Fig. 4. Variation of buckling load of SiCNT with different boundary conditions.

4. Concluding remarks

Buckling analysis of silicon carbide nanotube (SiCNT) is investigated for variable boundary conditions. Present equations from literature are used in order to calculate the critical buckling loads. Results are presented in a figure.

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References


