

DYNAMIC STABILITY OF EMBEDDED SINGLE WALLED CARBON NANOTUBES INCLUDING THERMAL EFFECTS^{*}

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Abstract– A nonlocal beam model based on the Bernoulli–Euler beam theory is presented to investigate the dynamic stability of embedded single-walled carbon nanotubes (SWCNTs) in thermal environment under combined static and periodic axial loads. The dynamic stability analysis is carried out by including the effects of small-scale parameter, temperature change and elastic medium. The equation of motion is reduced to the extended Mathieu-Hill equation, the stability of which is analyzed through the Floquet-Lyapunov theory as well as bounded and unbounded solution theory. The instability regions obtained from both theories are examined and compared with each other. Also, the effects of the small-scale parameter, temperature change, elastic medium, compressive static axial load and excitation frequency on the dynamic stability of SWCNTs are discussed in detail. The prediction of dynamic instability of carbon nanotubes enables one to eliminate this phenomenon in cases that may fall within the range of practical significance.

Keywords– Carbon nanotube, dynamic stability, Floquet-Lyapunov, Mathieu-Hill

1. INTRODUCTION

Since the pioneering work by Iijima [1] in 1991, leading to the discovery of carbon nanotubes (CNTs), nanotechnology has become a vibrant field of research. Like conventional fibers, CNTs are increasingly being used as extremely strong nano-reinforcements to form advanced nano-composite materials, which possess exceptionally high strength and low density. These nanostructured materials can be also used as basic elements of nano-electromechanical systems (NEMs), such as nano-probes, nanomechanical switches, nano-sensors and -actuators, to which combined static and periodic axial loads may be applied [2-12]. When a CNT is subjected to such loading conditions, failure may occur by dynamic instability at a load much smaller than that induced by static buckling. Therefore, the dynamic stability characteristics of CNTs under combined static and periodic axial loading can be of academic as well as practical interest. Mathematically, the problem is posed by the set of Mathieu –Hill equations. One of the most interesting characteristics of this kind of equations is that, for certain relationships between its coefficients, it has solutions which are unbounded. Although a vast amount of literature has been devoted to the investigation of static buckling of CNTs, the dynamic stability analysis of CNTs under the action of combined static and periodic axial loads has been far from sufficient. Wang [13] investigated the vibration and instability of tubular nano- and micro-beams conveying fluid based on a nonlocal Bernoulli–Euler elastic beam model and studied the effect of small length scale on the natural frequencies and the critical flow velocities of CNTs. The thermal effect on vibration and instability of SWCNT conveying fluid is investigated based on the classical Bernoulli–Euler beam theory by Wang [14]. It is concluded that the effect of temperature

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change on the instability of SWNTs conveying fluid is considerable. Ghavanloo [15] studied the vibration and instability analysis of SWCNTs conveying fluid and resting on a linear viscoelastic Winkler foundation. Applying the finite element method and solving a quadratic eigenvalue problem, the effects of the modulus and the damping factor of the linear viscoelastic Winkler foundation and the fluid velocity on the resonance frequencies are examined. Instability of thermally induced vibrations of SWCNTs embedded in a visco-elastic matrix under time-dependent temperature field analyzed by Tylikowski [16] and the energy-like functionals are used in the instability analysis. Making use of the radial point interpolation approximation formulated within the framework of the generalized differential quadrature method, Ansari et al. [17] studied the free vibration of double-walled CNTs based on the nonlocal Donnell shell model. It should be noted that the conventional continuum mechanics is scale free and cannot predict the size dependence of small-scale structures due to lack of intrinsic length scales. Therefore, size-dependent continuum models have been developed to describe the size-dependent behavior of nano- and micro-scale structures [17–19].

The objective of this paper is to examine the dynamic instability of SWCNTs under the effects of combined static and periodic compressive loads. A nonlocal elastic Bernoulli–Euler beam model is developed by including the effects of the small-scale parameter, temperature change and elastic medium to derive the dynamic instability equation of the Mathieu–Hill type. The Mathieu–Hill equation encountered is analyzed for stability using the theories of Floquet–Lyapunov and bounded and unbounded solutions. It is hoped that the present study stimulates and guides further experiments and molecular dynamics (MD) simulations on the subject.

2. GOVERNING EQUATION FOR ELASTIC BEAM

Consider a SWCNT of length L , Young's modulus E , density ρ , Poisson's ratio ν , cross-sectional area A , and cross-sectional moment of inertia I , embedded in an elastic medium with the spring constant \bar{k} in thermal environment. A coordinate system (X, Y, Z) is introduced on the central axis of the CNT, whereas the X axis is taken along the axial direction of the CNT, the Y axis in the tangential direction and the Z axis is taken along the radial direction. Also, the origin of the coordinate system is selected at the left end of the CNT. It is assumed that the deformations of the CNT take place in the $X - Z$ plane. Thus, assume that $U(X, \bar{t})$ and $W(X, \bar{t})$ are displacements corresponding to the axial and radial directions, respectively, in terms of the spatial coordinate X and the time variable \bar{t} [20]. The equation of motion for an embedded SWCNT considering the thermal effect and axial harmonic force according to the nonlocal Bernoulli–Euler beam theory is [21]

$$\rho A(1 - (e_0 a)^2 \nabla^2) \frac{\partial^2 W}{\partial \bar{t}^2} + EI \frac{\partial^4 W}{\partial X^4} - (\bar{F}(\bar{t}) + \bar{N}_T)(1 - (e_0 a)^2 \nabla^2) \frac{\partial^2 W}{\partial X^2} = (1 - (e_0 a)^2 \nabla^2) P(X, \bar{t}) \quad (1)$$

in which $P(X, \bar{t})$ is the interaction between the tube and the surrounding elastic medium (Fig. 1), described by the Winkler model [22–23] as follows:

$$P(X, \bar{t}) = -\bar{k}W \quad (2)$$

Also, \bar{N}_T is the axial resultant force due to the thermal loading, respectively, which is given by [24] $\bar{N}_T = -(EA/(1 - 2\nu))\alpha_x T$ and $\bar{F}(\bar{t})$ is a certain axial harmonic force. It is noted that α_x and T represent coefficient of thermal expansion and temperature change, respectively.

Applying Eq. (2) to Eq. (1), the governing equation of a SWCNT can be written in the following form

$$\rho A(1 - (e_0 a)^2 \nabla^2) \frac{\partial^2 W}{\partial \bar{t}^2} + EI \frac{\partial^4 W}{\partial X^4} - (\bar{F}(\bar{t}) + \bar{N}_T)(1 - (e_0 a)^2 \nabla^2) \frac{\partial^2 W}{\partial X^2} + \bar{k}(1 - (e_0 a)^2 \nabla^2)W = 0 \quad (3)$$

For convenience, consider the dimensionless parameters as follows:

$$w = \frac{W}{r}, r = \sqrt{I/A}, x = \frac{X}{L}, \epsilon_0 = \frac{e_0 a}{L}, t = \tilde{t} \sqrt{\frac{\rho A L^4}{EI}}, F = \frac{F L^2}{EI}, N_T = \frac{N_T L^2}{EI}, k = \frac{\bar{k} L^4}{EI} \quad (4)$$

Equation (3) can be rewritten in a dimensionless form as:

$$\frac{\partial^2 w}{\partial t^2} - \epsilon_0^2 \frac{\partial^4 w}{\partial t^2 \partial x^2} + \frac{\partial^4 w}{\partial x^4} - (F(t) + N_T) \left(1 - \epsilon_0^2 \frac{\partial^2}{\partial x^2}\right) \frac{\partial^2 w}{\partial x^2} + k \left(1 - \epsilon_0^2 \frac{\partial^2}{\partial x^2}\right) w = 0 \quad (5)$$

For SWCNT with simply-supported boundary conditions at both ends, $(w(x, t) = \partial^2 w(x, t) / \partial x^2 = 0$ at $x = 0, 1$), $w(x, t) = a(t) \sin(m\pi x)$ is considered. Assume that the dimensionless periodic axial compressive load is expressed in the following form:

$$F(t) = F_s + F_d \cos 2\Omega t \quad (6)$$

where F_s and F_d are the dimensionless static and dynamic loads and 2Ω represents the nondimensional excitation frequency. Introducing the solution and the dimensionless periodic axial compressive load into Eq. (5) gives

$$\frac{\partial^2 a}{\partial t^2} + \left[\frac{(m\pi)^4}{1 + (m\pi\epsilon_0)^2} + (N_T - F_s - F_d \cos 2\Omega t)(m\pi)^2 + k \right] a(t) = 0 \quad (7)$$

Applying the transformation $\tau = \Omega t$, Eq.(7) will take the following form

$$\frac{\partial^2 a}{\partial \tau^2} + [\omega^2 - 2\eta \cos 2\tau] a = 0 \quad (8)$$

where

$$\omega^2 = \frac{1}{\Omega^2} \left[\frac{(m\pi)^4}{1 + (m\pi\epsilon_0)^2} + (-F_s + N_T)(m\pi)^2 + k \right], \eta = \frac{F_d(m\pi)^2}{2\Omega^2} \quad (9)$$

Equation (8) represents a second order differential equation with periodic coefficient of the Mathieu–Hill type.

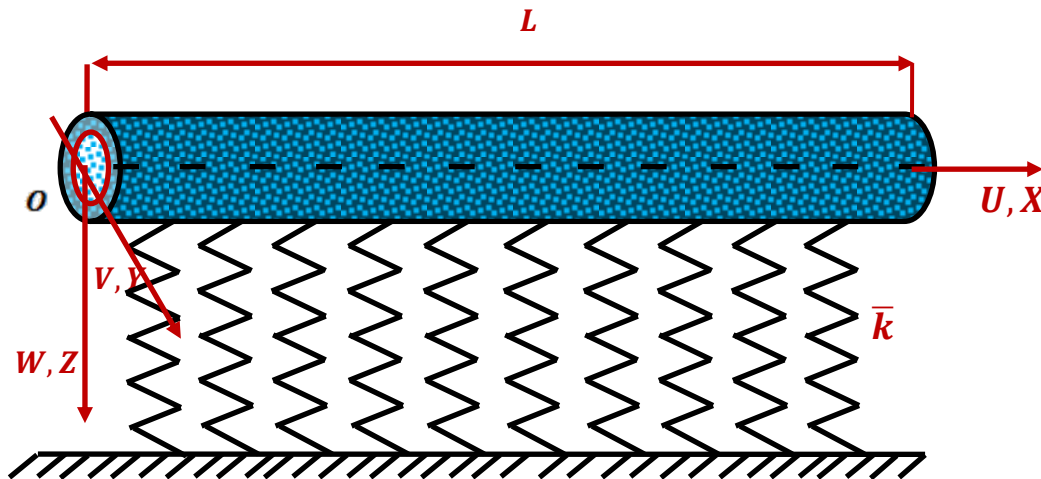


Fig. 1. Schematic of a SWCNT embedded in an elastic medium

3. SOLUTION AND STABILITY ANALYSIS

In this section, among various techniques for finding regions of stability and instability for SWCNTs, the Floquet-Lyapunov and the Bounded and unbounded solution theories are used to analyze the dynamic stability of the embedded SWCNTs in thermal environment using the obtained Mathieu–Hill type equation.

a) Floquet-Lyapunov theory for stability analysis

The theory of Floquet-Lyapunov is perhaps the most general systematic procedure for analyzing the stability of a system having differential equations with periodic coefficients. This theory provides valuable information concerning the properties of solution, without giving a solution. According to the Floquet-Lyapunov theorem, the knowledge of state transition matrix over one period is sufficient to determine the stability of a periodic system. The stability criteria can be derived from the real parts of eigenvalues of the transition matrix. An improved numerical integration scheme for computing the transition or monodromy matrix based on the fourth order Runge-Kutta method together with Gill coefficients was proposed by Friedmann and Hammond [25]. To describe the method, Eq. (8) can be written in the state space form

$$\{\dot{v}\} = [\bar{Q}(\tau)]\{v\} = \{u(\tau, v)\} \quad (10)$$

where $\bar{Q}(\tau) = \bar{Q}(\tau + T_p)$ is a periodic matrix with period T_p , which is given by

$$[\bar{Q}(\tau)] = \begin{bmatrix} 0 & 1 \\ -(\omega^2 - 2\eta \cos 2\tau) & 0 \end{bmatrix} \quad (11)$$

and v is a 2×1 vector. The fourth order Runge-Kutta scheme with Gill coefficient in the r th interval takes the form

$$v_{r+1} = v_r + \frac{h_r}{6} \left(\sigma_1 + 2 \left(1 - \frac{1}{\sqrt{2}} \right) \sigma_2 + 2 \left(1 + \frac{1}{\sqrt{2}} \right) \sigma_3 + \sigma_4 \right) \quad (12)$$

in which $\sigma_r = \sigma(\tau_r, r)$, $h_r = \tau_{r+1} - \tau_r$ is the step size and the vectors $\sigma_1, \sigma_2, \sigma_3$ and σ_4 are also given by

$$\sigma_1 = \{u(\tau_r, v_r)\} \quad (13a)$$

$$\sigma_2 = \left\{ u \left(\left(\tau_r + \frac{1}{2} h_r \right), \left(v_r + \frac{1}{2} \sigma_1 \right) \right) \right\} \quad (13b)$$

$$\sigma_3 = \left\{ u \left(\left(\tau_r + \frac{1}{2} h_r \right), \left(v_r + \left(-\frac{1}{2} + \frac{1}{\sqrt{2}} \right) h_r \sigma_1 + \left(1 - \frac{1}{\sqrt{2}} \right) h_r \sigma_2 \right) \right) \right\} \quad (13c)$$

$$\sigma_4 = \left\{ u \left(\left(\tau_r + h_r \right), \left(v_r - \frac{1}{\sqrt{2}} h_r \sigma_2 + \left(1 + \frac{1}{\sqrt{2}} \right) h_r \sigma_3 \right) \right) \right\} \quad (13d)$$

Combination of Eqs. (10) and (11)-(13d) results in

$$\sigma_1 = [\bar{Q}(\tau_r)]\{v_r\}, \quad \sigma_2 = [\bar{E}(\tau_r)]\{v_r\}, \quad \sigma_3 = [\bar{\Gamma}(\tau_r)]\{v_r\}, \quad \sigma_4 = [\bar{\Lambda}(\tau_r)]\{v_r\} \quad (14)$$

where

$$\bar{E}(\tau_r) = \bar{Q} \left(\tau_r + \frac{1}{2} h_r \right) \left(\mathbf{I} + \frac{1}{2} h_r \bar{Q}(\tau_r) \right) \quad (15a)$$

$$\bar{\Gamma}(\tau_r) = \bar{Q} \left(\tau_r + \frac{1}{2} h_r \right) \left(\mathbf{I} + \left(-\frac{1}{2} + \frac{1}{\sqrt{2}} \right) h_r \bar{Q}(\tau_r) + \left(1 - \frac{1}{\sqrt{2}} \right) h_r \bar{E}(\tau_r) \right) \quad (15b)$$

$$\bar{\Lambda}(\tau_r) = \bar{Q}(\tau_r + h_r) \left(\mathbf{I} - \frac{1}{\sqrt{2}} h_r \bar{E}(\tau_r) + \left(1 + \frac{1}{\sqrt{2}} \right) h_r \bar{\Gamma}(\tau_r) \right) \quad (15c)$$

It is noted that \mathbf{I} represents a 2×2 identity matrix. Combining Eqs. (12) and (14)-(15c) also gives

$$v_{r+1} = [\bar{\Psi}(\tau_r)]v_r \quad (16)$$

where

$$\bar{\Psi}(\tau_r) = \mathbf{I} + \frac{h_r}{6} \left(\bar{Q}(\tau_r) + 2 \left(1 - \frac{1}{\sqrt{2}} \right) \bar{E}(\tau_r) + 2 \left(1 + \frac{1}{\sqrt{2}} \right) \bar{\Gamma}(\tau_r) + \bar{\Lambda}(\tau_r) \right) \quad (17)$$

Using Eq. (16) the following expression can be written out

$$v(T_p) = \bar{\Psi}(T_p - h_r) \bar{\Psi}(T_p - 2h_r) \cdots \bar{\Psi}(0) v(0) = \left(\prod_{r=1}^N \bar{\Psi}(T_p - r h_r) \right) v(0) \quad (18)$$

b) Bounded and unbounded solution theory for stability analysis

The response of CNTs to periodic loads is considered to be dynamically stable when the solution of Eq. (8) remains bounded for all time. On the other hand, if the amplitude of displacement increases continuously with time, it is said to be dynamically unstable. The instability occurs when energy is fed into the system through self-excitation. The qualitative knowledge that all of the roots lie to the left of the imaginary axis will be sufficient to ensure that the solution remains finite (is stable). This gives rise to a condition that determines when the solution becomes unbounded.

4. RESULTS AND DISCUSSION

The material and geometric parameters of the SWCNTs are taken to be $E = 1.1 \text{ TPa}$, $\rho = 1300 \text{ Kg/m}^3$, $L = 45 \text{ nm}$, the outermost diameter $d = 3 \text{ nm}$ and the thickness $t = 0.34 \text{ nm}$. To investigate the stability characteristics of CNTs undergoing a periodic excitation, the regions of stability and instability for SWCNTs are indicated in Fig. 2. By making use of the Floquet-Lyapunov theory, the (ω^2, η) plane is divided into shaded and unshaded regions. The points that lie inside the shaded region denote unstable conditions, whereas the points inside the unshaded region represent stability. Each point belonging to the transition borderline between stability and instability represents a periodic response of the system. It can be clearly understood from the figures drawn for various η that the unshaded region grows as the magnitude of ω^2 increases. Therefore, by increasing the natural frequency of carbon nanotubes because of increasing the stiffness, it is expected that the system will become more stable.

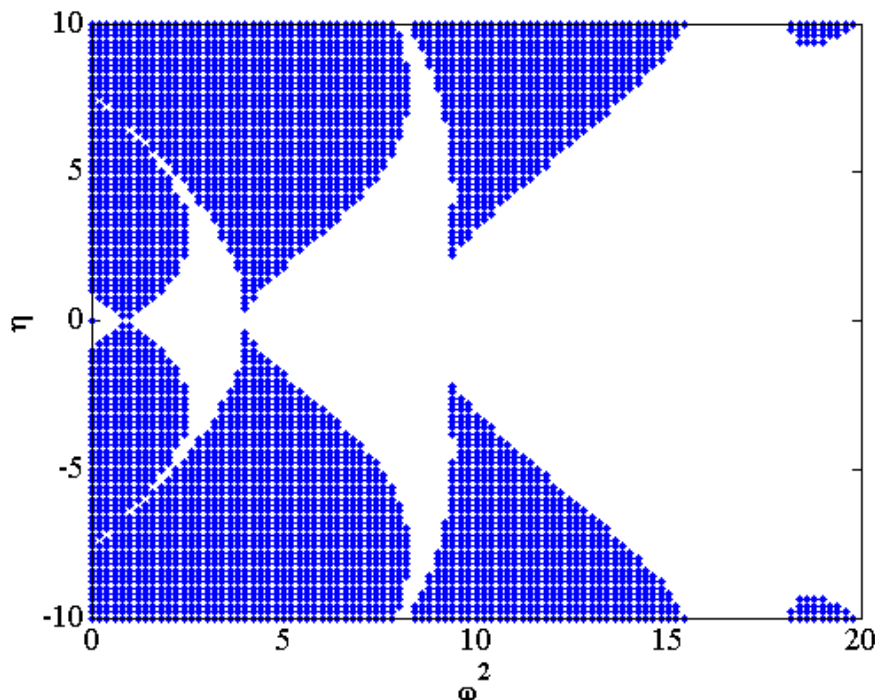


Fig. 2. Lyapunov theory: Regions of instability (shaded regions) and stability (white regions) for a SWCNT

Parameters such as the small-scale parameter, temperature change, the spring constant of elastic medium and compressive static axial load affect the stability region of CNT. The effect of each parameter on the dynamic stability of CNT is discussed here. Considering the dependence of ω^2 on the small-scale parameter (Eq. (9)), it can be clearly noted that the natural frequencies of SWCNTs generally decrease when the small-scale parameter increases. Hence, as it can be seen from Fig. 2, the unstable region for SWCNTs increases. In other words, the classical Bernoulli–Euler beam model has an overestimated

prediction for the instability region of the SWCNT. The other important point is the influence of the spring constant of the elastic medium on the dynamic stability of SWCNTs. It is well known that the natural frequencies of a system generally increase when its stiffness increases. Hence, as it can be seen from Fig. 2, the stable region of SWCNTs increases when the spring constant of Winkler foundation increases.

In addition to the above mentioned cases, the temperature changes also affect the dynamic stability of the CNTs. Since the coefficient of thermal expansion in carbon nanotubes is negative ($\alpha_x = -1.6 \times 10^{-6} \text{K}^{-1}$) at low temperatures and is positive ($\alpha_x = 1.1 \times 10^{-6} \text{K}^{-1}$) at high temperatures, both cases are discussed here [14, 24, 26]. At high temperatures, increasing in the temperature change leads to a negative value of the axial resultant force due to the thermal loading. Thus, by considering Eq. (9), the value of ω^2 decreases with increasing the temperature change in high temperatures. Therefore, the system tends to become unstable with increasing the temperature change in high temperatures. Unlike, at low temperatures, increasing the temperature change causes an increase in the natural frequency of SWCNT and leads to more stability of the system.

The amount of static axial compressive load also influences the dynamic stability of SWCNTs. Increasing the static compressive load leads to the decrease of the natural frequency and the dynamic instability region of the system. Additionally, the excitation frequency also affects the dynamic stability of the system. Increasing the excitation frequency decreases the value of ω^2 . Therefore, the possibility of instability in the system will increase.

Similar figures obtained from the bounded and unbounded solutions are also plotted in Figs. 3. The coincidence of the Floquet-Lyapunov theory with the bounded and unbounded solutions is seen from these figures. The Floquet-Lyapunov theory is found to be more conservative than the bounded and unbounded solution theory in predicting the regions of stability and instability for SWCNTs.

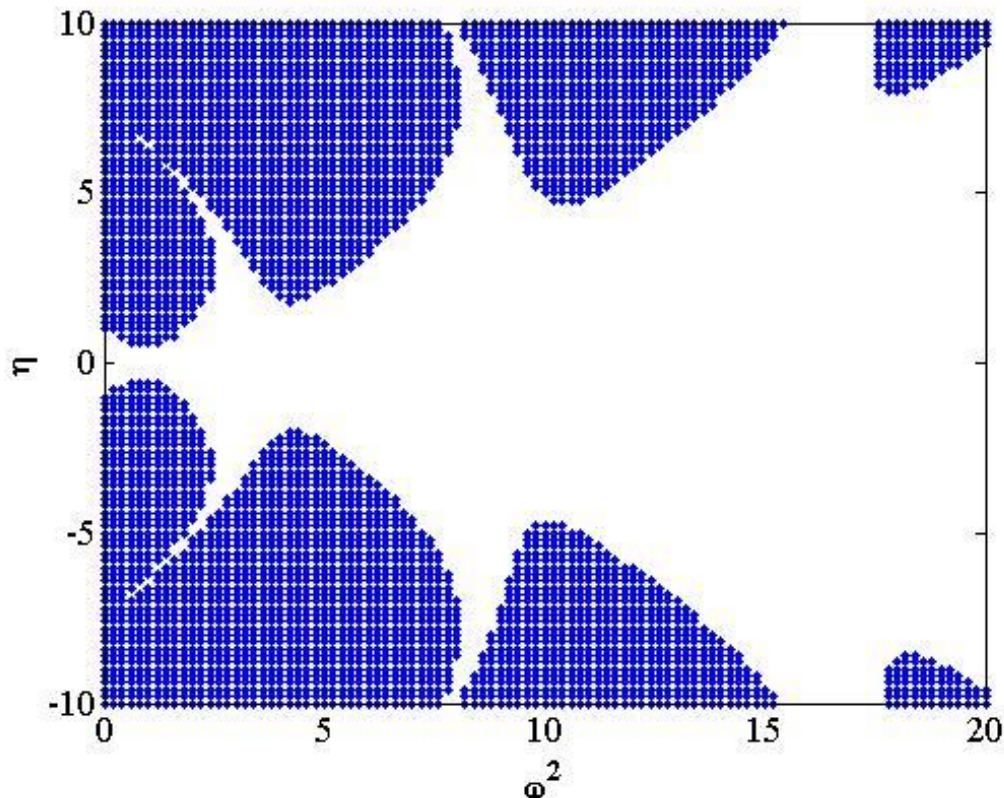


Fig. 3. Bounded and unbounded solutions: Regions of instability (shaded regions) and stability (white regions) for a SWCNT

As mentioned above, increasing the natural frequency leads to the improvement in the stability of carbon nanotubes. To quantitatively show how the parameters such as neighbor elastic medium, temperature rise and nonlocal parameter could affect the system stability, Tables 1-2 are given. Tables 1 and 2 show the influences of elastic medium constant, temperature rise and nonlocal parameter on the dimensionless natural frequencies ($\bar{\omega}\sqrt{\rho AL^4/EI}$) of SWCNTs at low and high temperatures, respectively. $\bar{\omega}$ denotes the natural frequency of SWCNT. In low temperature environment, increasing the temperature change leads to increasing the natural frequency of SWCNTs. It means that at low temperatures, the temperature change increases the stiffness of SWCNTs and leads to improvement in the stability of the system. On the other hand, in high temperature environment, an increase in temperature change leads to decreasing the natural frequency due to thermal loading. Thus, an increase in the temperature change decreases the stiffness and the embedded SWCNT tends to become unstable when the temperature change increases at high temperatures. Moreover, it can be found that an increase in the elastic medium constant leads to an increase in the dimensionless natural frequencies and improvement in the stability of SWCNTs.

Table 1. Effects of elastic medium constant, temperature rise and nonlocal parameter on the dimensionless natural frequencies at low temperatures ($L = 20 \text{ nm}, h = 0.34 \text{ nm}$)

Elastic medium constant (\bar{k})	Temperature rise (T)	$e_0 a \text{ (nm)}$				
		0	0.5	1.0	1.5	2.0
$\bar{k} = 0$	0	9.8696	9.8393	9.7501	9.6065	9.4159
	100	9.9582	9.9282	9.8397	9.6975	9.5087
	200	10.0460	10.0163	9.9286	9.7877	9.6006
	300	10.1331	10.1036	10.0167	9.8770	9.6917
$\bar{k} = 10^8$	0	10.1540	10.1246	10.0379	9.8985	9.7136
	100	10.2402	10.2110	10.1250	9.9869	9.8036
	200	10.3256	10.2966	10.2114	10.0744	9.8928
	300	10.4103	10.3816	10.2970	10.1613	9.9812
$\bar{k} = 10^9$	0	12.4242	12.4001	12.3294	12.2163	12.0669
	100	12.4947	12.4708	12.4005	12.2880	12.1395
	200	12.5648	12.5410	12.4711	12.3592	12.2116
	300	12.6345	12.6109	12.5413	12.4301	12.2833

Table 2. Effects of elastic medium constant, temperature rise and nonlocal parameter on the dimensionless natural frequencies at high temperatures ($L = 20 \text{ nm}, h = 0.34 \text{ nm}$)

Elastic medium constant (\bar{k})	Temperature rise (T)	$e_0 a \text{ (nm)}$				
		0	0.5	1.0	1.5	2.0
$\bar{k} = 0$	0	9.8696	9.8393	9.7501	9.6065	9.4159
	100	9.8082	9.7777	9.6879	9.5435	9.3515
	200	9.7465	9.7158	9.6254	9.4800	9.2867
	300	9.6843	9.6534	9.5624	9.4161	9.2215
$\bar{k} = 10^8$	0	10.1540	10.1246	10.0379	9.8985	9.7136
	100	10.0944	10.0648	9.9775	9.8373	9.6512
	200	10.0344	10.0046	9.9168	9.7758	9.5885
	300	9.9740	9.9440	9.8557	9.7138	9.5253
$\bar{k} = 10^9$	0	12.4242	12.4001	12.3294	12.2163	12.0669
	100	12.3755	12.3513	12.2804	12.1667	12.0168
	200	12.3266	12.3024	12.2311	12.1170	11.9664
	300	12.2775	12.2532	12.1816	12.0671	11.9158

The other more important issue is the effect of nonlocal parameter on the stability of SWCNT. As indicated in Tables 1 and 2, an increase in $e_0 a$ leads to decrease the stiffness and consequently the natural frequency of SWCNT. Thus, the stability of embedded SWCNT diminishes with increasing the nonlocal

parameter. This fact reveals that the classical beam models have an overestimated prediction for the stability of the nanotubes.

5. CONCLUSION

In this letter, the dynamic response of embedded SWCNTs to combined static and periodic axial loads was studied. The nonlocal Bernoulli–Euler beam theory taking into consideration the small-scale effect, thermal effect and elastic medium effect was adopted to investigate the dynamic stability characteristics of SWCNTs. The equation of motion was reduced to an extended Mathieu-Hill equation whose stability was analyzed via the Floquet-Lyapunov theory as well as bounded and unbounded solution. The instability regions obtained from both theories were shown to be in reasonable agreement with each other, proving the validity of the present approaches. The structural instability of carbon nanotubes in some cases that may fall within the range of practical significance can be suppressed or even eliminated by putting the nanotubes in a compliant surrounding elastic medium (such as a polymer matrix). Among the conclusions and observations, the important results may be listed as follows:

The surrounding elastic medium significantly affects the dynamic stability of SWCNTs. By increasing the spring constant of the surrounding medium, the dynamic stability of CNTs increases.

At high temperature, increasing the temperature change leads to a decrease in the dynamic stability of CNTs, whereas at low temperature, the system tends to become more stable by increasing the temperature change.

The dynamic stability region of CNTs decreases by increasing the static compressive load. The dynamic instability of SWCNTs increases as the excitation frequency increases.

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