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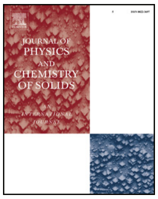

Investigation of affecting parameters on the effective modulus and natural frequency of wavy carbon nanotubes

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ABSTRACT

Wavy carbon nanotubes (CNTs) are ubiquitously present in high-aspect-ratio CNT arrays used in advanced device applications. This paper investigates the effective modulus and natural frequency of wavy CNTs that have random, sinusoidal, or helical structures. Parameters such as loading deviation angle, boundary condition, and low shear modulus are considered. It was found that loading deviation could cause 3–4 orders modulus reduction for sinusoidal and helical CNTs at small waviness ratio. In contrast, there is slight modulus enhancement by a small loading deviation for randomly wavy CNTs. By applying pined or fixed boundary condition at the loading end, the moduli of wavy CNTs may be enhanced by up to 4 orders in magnitude. As another critical parameter, low shear modulus (~50 MPa) may cause significant modulus reduction only for helical CNTs, about 2 orders of magnitude due to large shear and torsional deformation. The natural frequencies of wavy CNTs were also computed, showing that helical CNTs generally have lower frequency than other wavy CNTs. Furthermore, very low shear modulus could result in significant frequency reduction for helical CNTs, but has limited effect on random or sinusoidal CNTs. With the high sensitivity to shear modulus, helical CNTs are thus more desirable in the electric-field-induced resonance testing used for CNT property characterization. The findings on the properties of wavy CNTs can provide fundamental guidelines for the design of CNT arrays or CNT-based composites.

1. Introduction

Owing to their extraordinary thermal, electrical and mechanical properties, carbon nanotubes (CNTs) have been widely used in the design of high-performance and multifunctional materials [1–3]. Examples of CNT applications include ultralight and strong nanocomposites [4,5], high-performance electromagnetic wave absorbers, heat dissipation, field emission sources, and biosensors [6–12]. With photolithographically defined patterns, scientists have also produced high-aspect-ratio, vertically aligned CNT arrays that can be used as advanced interconnects for next-generalization microelectronics [13–16].

However, the extremely high elastic modulus of a single and short CNT (i.e., ~100 GPa to ~1.7 TPa) may not be fully utilized in vertically aligned CNT arrays. The effective modulus of a CNT array (E_{array}) can be several orders of magnitude lower than a single CNT (E_{eff}), and as indicated by the summary of several experimental works in Table 1, the effective modulus of typical CNT arrays ranges from 0.1 MPa to 1 GPa and generally decreases when the CNT porosity (V_f) increases. Depending on the manufacturing configuration, CNT porosity may vary from 80% to 99%. Based on the rule of mixture, the relation between these two moduli and porosity is $E_{eff} = E_{array}/(1-V_f)$, but this can only account for a maximum of 2 orders of magnitude in modulus reduction. The actual modulus of a CNT array, nonetheless, could be reduced by up to 6 orders of magnitude, as indicated in Table 1.

One identified factor for low modulus of CNT arrays is the intrinsic CNT waviness produced during the manufacturing process. Ginga et al. [17] showed that CNTs with sinusoidal waviness could have 4–6 orders of magnitude modulus reduction in comparison to the straight CNT [20]. Stein et al. [18] modeled stochastically wavy CNTs and concluded that low shear modulus may further reduce the effective modulus of CNT arrays by about 2 orders of magnitude. Poelma et al. [19] also considered CNT waviness based on the sinusoidal geometry when evaluating the effect of conformal coating on vertically aligned CNT arrays. In addition to vertically aligned CNT arrays, waviness has also been shown to reduce the elastic stiffness of carbon nanotube-reinforced composites [20,21].

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Table 1
A summary of effective moduli of vertical aligned CNT arrays.* V_f = 95% if unknown.

Ref.	Testing Method	Measured Modulus (E_{array}, GPa)	Porosity (V_f)	Individual CNTs (E_{eff}, GPa)	Orders of Modulus Reduction
[22]	Nanoindention, Berkovich	0.0015 ~ 1.109	80%~99%	0.15~ 5.5	3~4
[22]	Nanoindention, spherical	0.008~.89	80%~99%	0.08~4.4	3~5
[17]	Nanoindention, Berkovich	0.00012~0.00027	~95%	0.0024~0.0054	~6
[23]	Electrical-Mechanical Tester	~0.05	~87%	~0.38	~4
[19]	Nanoindentation, flat punch	< 0.3	~99%	< 30	> 2
[24]	Nanoindentation, Berkovich	0.4 ~ 0.8	*	8~16	~2
[25]	Nanoindention, Berkovich	0.03 ~ 0.3	*	0.6~6	2~3
[26]	Nanoindention, spherical	~0.058	~98%~99%	2.9~5.8	~2

Furthermore, intrinsic CNT waviness may change the natural frequency and thus affects the applications of CNTs in nanorobotics, nanoinductors, and impact protection coatings. Based on the fact that the natural frequency of a CNT is linked to its elastic moduli, researchers have developed electric-field induced resonance technique to characterize CNT properties [27]. With similar technique, Saini, et al. [28] studied the properties of helically coiled CNTs. The effect of CNT waviness on the vibrational behavior of CNT-reinforced composite beams were also studied and shown to have a significant effect [29]. Nevertheless, a systematic study is still limited on the natural frequency of wavy CNTs with different structures.

This paper provides a comprehensive investigation on the properties of wavy CNTs. Section 2 defines various structures of wavy CNTs and presents the computational method based on continuum beam theory. Section 3 provides the results of effective modulus and natural frequency of wavy CNTs, where several critical design parameters such as loading deviations, boundary conditions, and low shear modulus are considered. The overall findings are summarized and discussed in Section 4.

2. CNT morphologies and computational methods

This paper investigates three representative structures of wavy CNTs, as shown in Fig. 1. The first structure is a randomly wavy CNT segment extracted from the SEM image of a CNT array [17]. In its original form (Fig. 1a), the loading position slightly deviates from the growing axis, forming an angle of 5.6°. The effect of deviation angle (denoted as θ) was not investigated in the literature, but will be systematically evaluated in this study. The second and the third structure are sinusoidal and helical CNTs, as shown in Fig. 1b and c, respectively. The degree of waviness for both structures is controlled by the parameter of waviness ratio defined as $w = a/l$, where a is amplitude and l is wavelength. The mathematical models of sinusoidal and helical CNTs are given in Appendix A. In this study, l is assumed as 1 μm, while w = 0.015, 0.1, and 0.33 to cover the low and high waviness regime. The total length of 7 μm is chosen for the distance between the two ends of each CNT (or the chord length denoted as L). Multi-walled CNTs are assumed according to the literature [17], with an outer radius of R_O = 7.5 nm and inner radius of R_i = 5.0 nm. The effect of loading deviation angle θ is considered for all the structures and ranges from $-10 \sim +10°$.

Both the effective modulus and natural frequency are calculated by continuum beam theory that has been validated against atomistic models of CNTs [30]. Furthermore, Timoshenko beam theory allows considerations of anisotropic behavior of CNTs with very low shear modulus [27,31]. In this study, commercially available finite element software package (ABAQUS) is used to calculate the effective modulus and natural frequency of wavy CNTs. The intrinsic modulus of CNT chosen is E_O = 100 GPa, whereas the shear modulus varies from 50 GPa to 50 MPa to consider the anisotropic behaviors of wavy CNTs. The density of CNT is assumed to be ρ = 2.1 g/cm^3 [27].

To compare wavy CNTs to an ideally straight CNT, the relative modulus (E_r) is calculated based on the following equation:

$$E_r = \frac{E_{eff}}{E_0} = \frac{\sigma_{eff}}{\varepsilon_{eff} E_0} = \frac{F/A_0}{(\delta/h)E_0} = \frac{F}{\delta}\cdot\frac{h}{A_0 E_0} = \frac{1}{C}\cdot C_0 = \frac{1}{C_r} \tag{1}$$

where E_0 is Young's modulus of CNT, F is the applied force, δ is the calculated displacement, σ_{eff} is effective stress on the cross-sectional area A_0, ε_{eff} is the effective strain defined on CNT height h, C is CNT compliance, C_0 is the compliance for ideally straight CNT, and C_r is the relative compliance. To further compare wavy CNTs with a straight CNT, Eq. (2) is used to normalize the frequency results, as

$$f_r = f(w, G, L)/f_0(w = 0, G, L) \tag{2}$$

where *L is CNT chord length*. Implementing a method from a previous work, the effect of CNT length is considered by shortening or cutting the original CNT to a length from 7 μm to 1 μm [27].

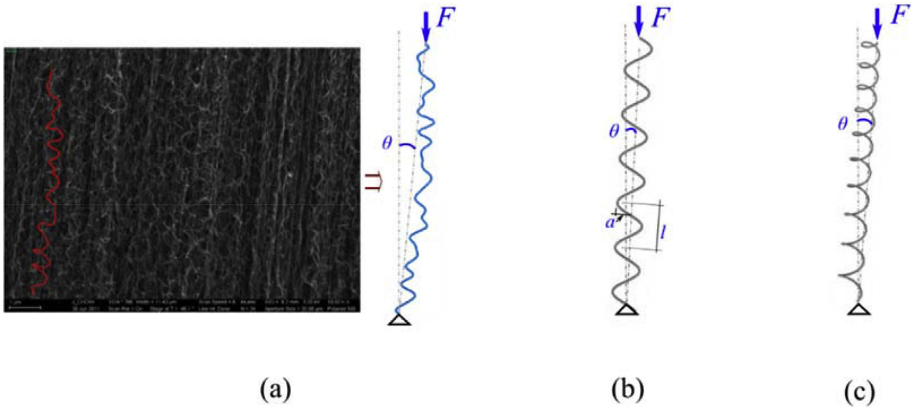

Fig. 1. (a) SEM image of CNT arrays with wavy CNTs and extracted CNT structure with an initial deviation angle θ (≈5.6 °) [17]; (b) Sinusoidal CNT with arbitrary deviation angle θ; waviness ratio $w = a/l$; and (c) Helical CNT with arbitrary deviation angle θ. The values of w range from 0.015 to 0.33 and θ from −10–10°.