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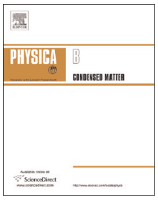

Vertically aligned carbon nanotubes for sensing unidirectional fluid flow

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ABSTRACT

From applied mechanics points of view, potential application of ensembles of single-walled carbon nanotubes (SWCNTs) as fluid flow sensors is aimed to be examined. To this end, useful nonlocal analytical and numerical models are developed. The deflection of the ensemble of SWCNTs at the tip is introduced as a measure of its sensitivity. The influences of the length and radius of the SWCNT, intertube distance, fluid flow velocity, and distance of the ensemble from the leading edge of the rigid base on the deflection field of the ensemble are comprehensively examined. The obtained results display how calibration of an ensemble of SWCNTs can be methodically carried out in accordance with the characteristics of the ensemble and the external fluid flow.

1. Introduction

As an innovative material, carbon nanotubes (CNTs) have revealed outstanding sensing properties [1–3]. These characteristics have accelerated their usage as gas sensors [4–6], temperature sensors [7,8], humidity sensors [9–11], pressure sensors [12,13], biosensors [14–16], and fluid flow sensors [17–20]. In fact, such possible applications for CNTs are devoted to their unprecedented physical and chemical properties [21–23]. In the present work, the latter above-mentioned application of CNTs is of interest from applied mechanics points of view.

Shortly, CNTs could be exploited as fluid flow sensors since researchers draw on electro-kinetic phenomena and slip boundary conditions that suggest a detailed insight to both inside and outside nanofluidic flows. To date, vibrations of CNTs due to inside nanofluidic flow have been widely investigated in the context of the classical continuum theory (CCT) [24–30] as well as nonlocal elasticity [31–36]. Both linear vibrations and nonlinear dynamic response of CNTs have been covered. Further, nonlocal vibrations of CNTs for nanoparticle delivery have been addressed in some detail [37–43]. However, the necessity for further studies to realize their nonlinear dynamic responses due to the moving inside fluid flow or nanoparticles is still highly demanded. Concerning the influence of an outside flow on a group of CNTs as well as their ensembles and bundles, there exist a number of experimental works [18,20,44–47]. Such works propose CNTs as fluid flow sensors. However, the theoretical aspects of CNTs acted upon by moving fluid flows have not been methodically examined yet. Further, the roles of geometry properties of CNTs' ensembles and those of the moving fluid on nanomechanical sensing mechanics of such nanostructures have not been disclosed. To bridge this scientific gap, this work has been devoted to examine the static behavior of CNTs' ensembles due to unidirectional fluid flows in the context of the nonlocal continuum theory.

Application of atomistic-based methodologies to nanostructures under externally applied loads commonly requires considerable labor and time costs. To reduce such expenditures, appropriate continuum-based theories would be a good alternative. In the framework of the CCT, the information regarding the interatomic bonds is not incorporated into the equations of motion. As a result, such a theory cannot factually capture the vibration behavior of nanostructures as well as the characteristics of the propagated waves within them. To overcome such a deficiency of the CCT, some advanced theories of elasticity have been developed during the past century. One of the most well-known theories is the nonlocal continuum theory of Eringen [48–51]. Its popularity may be related to its simplicity in taking into account the atomic bond effect in its formulations through the so-called small-scale parameter. So far, such a theory has been frequently used for a diverse range of problems pertinent to vibrations of CNTs [52–58] and nanowires [59–64]. Through comparisons of the obtained results by the nonlocal models and those of suitable atomistic methods, a reasonably good agreement has been achieved in most

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of the cases. Herein, for modeling the flexural behavior of CNTs' ensembles subjected to unidirectional fluid flows, an appropriate nonlocal beam model is exploited.

Since seeking closed-form solutions to the governing equations of the elastic solid problems would be a difficult job in most of the cases, application of efficient numerical methodologies would be very helpful. Concerning the problem at hand, when the thickness of the boundary layer would be comparable with the length of the CNTs, the drag force would be a function of velocity profile of the moving fluid, arrangement of the CNTs on the substrate, and diameter of the CNTs. Thereby, evaluation of the drag force and the resulting deflection field would not be an easy task. For such a case, a numerical approach based on the reproducing kernel particle method (RKPM) is proposed. RKPM is one of the most powerful and efficient methods in the family of meshless methods which was initiated by a group of scientist at Northwestern University [65,66]. To date, such a numerical technique has been applied to many structural problems of CNTs [67–69,57,70–72] and reasonably good results have been reported.

In this paper, novel nonlocal mathematical models are developed for predicting static response of ensembles of SWCNTs subjected to unidirectional fluid flows. The derivation of the applied nonlocal drag force on the ensemble, extraction nonlocal equations of motion of the ensemble, and suggestion of novel numerical and analytical solutions to the governing equations are among the new features of the present study. The deflection of the ensemble at its tip is considered as a crucial factor for sensing the external fluid flow. The predicted deflections of the ensemble of SWCNTs due to the fluid flow are compared with those of experimentally observed data, and a reasonably good agreement is achieved. Thereby, the proposed models can be successfully employed for detecting any fluid flow by SWCNTs' ensembles. In order to realize the sensing mechanisms of the ensembles well, the role of length and radius of the SWCNT, intertube distance, fluid flow velocity, and distance of the ensemble from the leading edge of the rigid base on the maximum static response of the ensemble due to the fluid flows are comprehensively examined.

2. Definition of the nanomechanical problem

Consider an array of vertically aligned SWCNTs subjected to a steady fluid flow as shown in Fig. 1. The cantilevered SWCNTs have similar geometrical properties. The SWCNTs have been uniformly placed perpendicular to the y–z plane (see Fig. 1(a)), and they have been connected to a rigid base at the bottom. The length of SWCNTs, center-to-center distance of SWCNTs along the y and z directions (i.e., intertube distance), and the dimension of the square ensemble are represented by l_b, d, and a_s, respectively. The SWCNTs are acted upon by a steady unidirectional fluid flow of velocity profile $v(x)$ (see Fig. 1(b)). For continuum-based modeling of the SWCNTs of the ensemble, each SWCNT is replaced by its equivalent continuum structure (ECS). The ECS associated with a SWCNT is a circular cylindrical shell of thickness 0.34 nm whose length and mean radius are identical to those of the SWCNT.

By impacting the molecules of the fluids to the outer surface of the SWCNTs, a tiny interaction force would be exerted on them. Since the fluid flow moves along the z-axis, the resultant applied force on the SWCNTs of the ensemble would have only one component along the z-axis. From molecular dynamics points of view, evaluation of such forces is a difficult job. Further, implementation of such methods is commonly accompanied with high cost of time and labor. Thereby, application of suitable elasticity models would be very helpful.

3. Characteristics of the unidirectional fluid flow

3.1. Velocity profile of the fluid flow

Through the thickness of the boundary layer, a parabolic variation of the fluid flow velocity is assumed, whereas outside of the boundary layer zone, the fluid velocity is constant. Therefore,

$$\frac{v(x)}{v_{peak}} = \begin{cases} 2\left(\dfrac{x}{\delta}\right) - \left(\dfrac{x}{\delta}\right)^2, & x \le \delta \\ 1, & x \ge \delta \end{cases} \tag{1}$$

where v_{peak} denotes the peak fluid velocity expressed by $v_{peak} = \big(1 + (0.722/\log(Re/6.9))\big) v_{ave}$ in which v_{ave} is the average velocity of the fluid, Re is the Reynolds number which is expressed by $Re = \rho_f v l / \mu_f$. In this relation, ρ_f and μ_f are the density and dynamic viscosity of the fluid flow, respectively, and l is the characteristic length. Regarding the parameter l, its magnitude relies on the problem at hand. For instance, in the case of the fluid flow inside the micropipe, over the ensemble, and through the vertically aligned SWCNTs, l is set equal to the inner diameter of the micropipe, the distance of the ensemble from the leading edge, and the outer diameter of the SWCNT, respectively [45]. In Eq. (1), δ is the thickness of the boundary layer. By assuming a laminar flow, the Blasius relation [73] is employed for predicting the boundary layer thickness: $\delta(z) = 5\,Re^{-0.5}\,z$ where z is the distance from the leading edge of the rigid base.

3.2. Evaluation of the exerted hydrodynamic force on SWCNTs of the ensemble

The externally applied drag force on all SWCNTs of the ensemble is calculated by

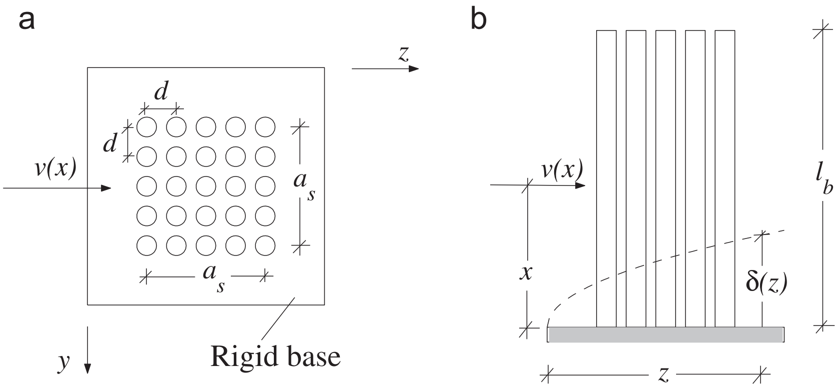

Fig. 1. Schematic representation of a vertically aligned ensemble of SWCNTs on a rigid base subjected to a unidirectional fluid flow: (a) top view and (b) side view.