An All-in-One Nanomechanical Bio-nanofluidic System for Possible Applications as Sensor and Actuator in Precise Drug Delivery

M. M. S. Fakhrabadi*

*School of Mechanical Engineering, College of Engineering, University of Tehran, Tehran, Iran, mfakhrabadi@ut.ac.ir

ABSTRACT

The paper presents the physical design and mathematical formulation of a bio-nanofluidic device for possible applications in nanoengineering in general and bio-nanoengineering in particular such as in precise drug delivery. The drug or any other fluid flows through a carbon nanotube and its stream is controlled by the electrostatic actuation technique. The fluid flow affects the mechanical characteristics of the nanosystem including its stiffness and damping. In order to have a model with higher compatibility with the experiment, the recently developed consistent couple stress theory is used to capture the size effects for both solid and fluid parts of the model. The effects of the fluid velocity, viscosity, density, temperature and pressure on the results are investigated via the mentioned size-dependent theory.

Keywords: consistent couple stress theory, bio-nanofluidics, carbon nanotube

1 INTRODUCTION

Bio-nanoengineering in general and bio-nanofluidics in particular have attracted researchers to work on different aspects of these multi-disciplinary research areas. One of the main applications of the bio-nanofluidics categorized as a field in *wet nanotechnology* is in drug delivery. Many attempts have been done to precise this process in order to avoid side-effects of the chemical drugs applied to cure diseases. Such side-effects can be potentially causes of some other health problems such as in chemical treatment of the cancer therapy. Thus, it is very important to explore effective methods to reduce these effects, substantially. In addition, some diseases such as HIV grow increasingly and unfortunately, no effective remedy has been found to cure them yet. Thus, it seems that a revolution is a must in medicine to combine the ideas of engineering with the concepts of medicine to invent novel techniques to cure hard diseases and to precise the drug delivery. Among various ideas, smart molecular machines can be an effective one for this purpose. If such machines come to use, they can detect accurately the target cells and antigens to cure or annihilate them. Since such machines have extremely tiny sizes, they or their parts can enter the cell membrane and rehabilitate the internal cell components. They can carry the medicine near the target cells and deliver it with predefined values with minimum side effects. In this paper, a nano-mechanism for the mentioned drug delivery process is presented and mathematically modeled. Other utilizations of the nanosystem studied in this paper are in many nanofluidic applications as the nanosensors and nanoactuators.

2 SYSTEM DESCRIPTION

The nanosystem under study composes of a single-walled CNT separated from some graphene sheets with a nanometer gap under an electrical voltage. The CNTs are able to carry the fluid and this capability was proved and analyzed in the literature using both experimental and theoretical investigations [1-3]. As shown in Fig. 1, the applied voltage distributes positive and negative charges on the CNT and graphene sheets. The charge distribution, accompanying the van der Waals (vdW) interaction, produces an attractive force deflecting the CNT towards the fixed graphene sheets. If the attractive force exceeds the elastic tolerance of the CNT, the tip of the cantilevered and the center-point of the doubly clamped CNTs suddenly drop down on the graphene sheets that is called pull-in instability. The molecular dynamic simulation of this pheneomenon was studied by the author before [4]. The results showed that in case of pull-in instability, there is a critical cross section deforming from the initial circular shape to oval and then closes. If the fluid flows through the nanotube, this deformation can confine or block the flow stream working as the nanoactuator with exteremely high precison in dosage rate. In addition to the mentioned application as a nanoactuator in bio-nanofluidics, the nanosystem can be applied in other nanofluidic systems as nanosensors, described in detail below.

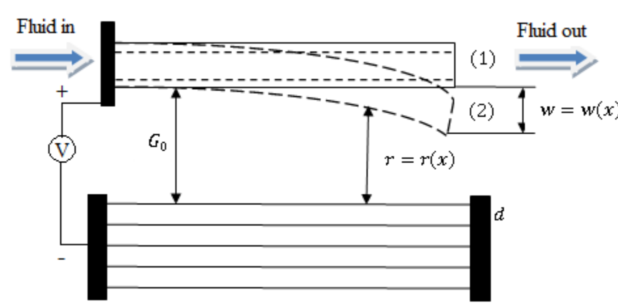


Fig. 1. Schematic view of analyzed nanosystem

2.1 Mathematical formulation

In this paper, the recently developed consistent couple stress theory (CCST) is applied [5,6]. This is a size-dependent theory to capture the small-size effects. The detailed desciption of the formulations were reported before in author's paper [7] and here, just the final reults are presented.

$$(EI+4GAl_1^2)\frac{\partial^4 w}{\partial x^4}-\left(N+\frac{EA}{2L}\int_0^L\left(\frac{\partial w}{\partial x}\right)^2dx\right)\frac{\partial^2 w}{\partial x^2} \tag{1}$$
$$+m_c\frac{\partial^2 w}{\partial t^2}+c\frac{\partial w}{\partial t}=q(x)$$

where E, I, G, A, l_1, w, x, N, m_c, t, c and $q(x)$ are elastic modulus, moment of inertia, shear modulus, cross sectional area, size-dependent parameter, deflection, longitudinal coordinate, axial force, mass per unit length, time, damping coefficient and externally distributed force, respectively. In this paper, the effects of external axial force, N, is disregarded for the cantilevered CNTs but it is supposed to represent the axial force due to the temperature variations and fluid pressure for the doubly clamped CNTs.

$$N=-\frac{EA}{1-2\nu}\alpha_x\Delta T-p^*A \tag{2}$$

where ν, α_x and ΔT are respectively the Poisson's ratio, coefficient of longitudinal thermal expansion and temperature variation. The minus signs are for the compressive nature of the forces.

The external force is due to electrostatic actuation, van der Waals interaction and fluid flow. The latter is formulated by consideration of small-scale effects [6] in Eq. (3) and the other two terms can be found in [7].

$$q_{fluid}=-m_f\left[\frac{\partial^2 w}{\partial t^2}+2v_{av}\frac{\partial^2 w}{\partial t\partial x}+v_{av}{}^2\frac{\partial^2 w}{\partial x^2}\right] \tag{3}$$
$$+\mu^*A_i\left[\frac{\partial^3 w}{\partial x^2\partial t}+v_{av}\frac{\partial^3 w}{\partial x^3}\right]$$
$$-\mu^*A_il_2^2\left[\frac{\partial^5 w}{\partial x^4\partial t}+v_{av}\frac{\partial^5 w}{\partial x^5}\right]$$

where $m_f=\rho A_i$ is the mass of the fluid per unit length.

3 RESULTS AND DISCUSSION

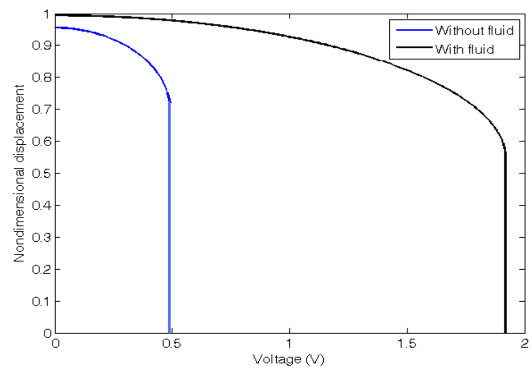
In this section, the effects of the fluid flow on pull-in instabilities of the CNTs with cantilever and doubly clamped boundary conditions are investigated. The numerical values of the applied parameters are presented in Table 1. They are fixed unless stated otherwise.

Table 1. Numerical values of the parameters.

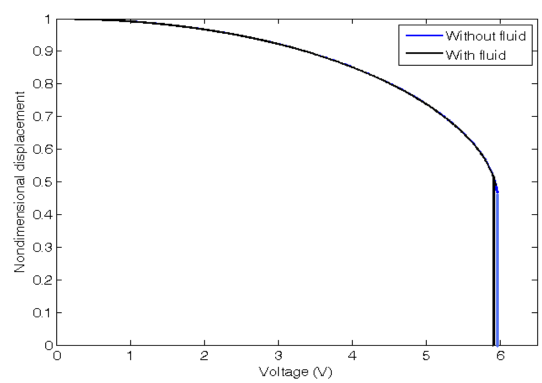
Parameter	Numerical value
Length	L= 50 nm
Chirality	(10,10)
Reference fluid velocity	$v^*={L}/{t^*}$
Dynamic viscosity	$\mu=1$ Pas
Pressure	$P=1$ kPa
Nondimensional velocity	$\bar{v}_{av}={v_{av}}/{v^*}=1$
Mass ratio	$m_r={m_f}/{m_c}=0.1$
Small-scale parameter	$l_1=0.2$ nm
Temperature	300 K

The calculated results prove that, for the current case with the mentioned assumption, the small-scale effects on fluid part can be disregarded. Thus, $l_2=0$ nm. However, the small scale has remarkable influences on the structural part of the nanosystem to be scrutinized in the following paragraphs. So, all of the results will be presented considering CCST.

The static deflections of the critical points of the CNT with both cantilever and doubly clamped boundary conditions are illustrated in Fig. 2 (a) and (b). The figure reveals that with increasing the applied voltage the deflection increases until the CNT cannot tolerate the attractive. In this case, the static pull-in instability occurs. This kind of pull-in phenomenon corresponds to the nano-valve application of the bio-nanofluidic device, described before. The effects of fluid flow on the static pull-in voltages of the nanotubes are illsutrated in Fig. 2 (a) and (b) with two different colors.



(a)



(b)

Fig. 2. Static pull-in voltages of (a) cantilver, (b) doubly clamped CNT

3.1 Sensor application of the nanodevice

The variation of the the pull-in voltages can be used for sensor applications of the fluid flow. Although both of the static and dynamic pull-in behaviors can be analyzed, this paper covers only the static mode. In order to better have a comparison, the pull-in voltages are normalized by the voltages presented in Table 2, obtained from the classical elasticity theory. The results are presented for two low, $\mu_{low} = 1$ mPas, and high, $\mu_{high} = 1$ Pas, viscosities.

Table 2. Normalized pull-in voltages

Conditions	Pull-in voltage
Static pull-in of cantilever boundary conditions: (a) $\mu = 1$ mPas, (b) $\mu = 1$ Pas	(a) 0.39 V, (b) 1.9 V
Static pull-in of doubly clamped boundary conditions: (a) $\mu = 1$ mPas, (b) $\mu = 1$ Pas	(a) 5.46 V, (b) 5.46 V

The variations of the pull-in voltages of the fluid-conveying CNT under electrostatic actuation with cantilever boundary conditions vs. the fluid viscosity are shown in Fig. 3.

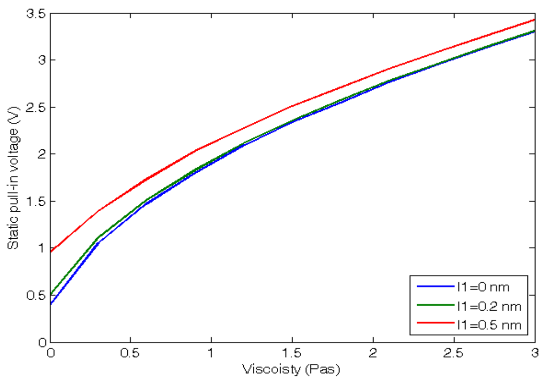
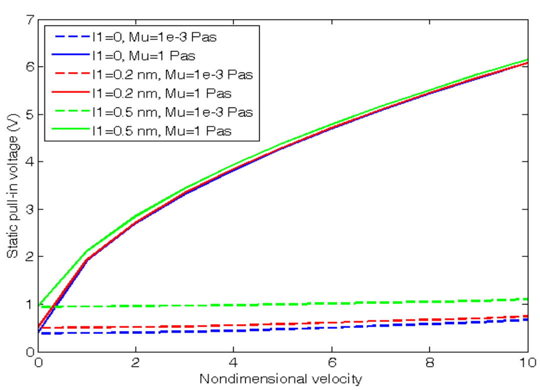


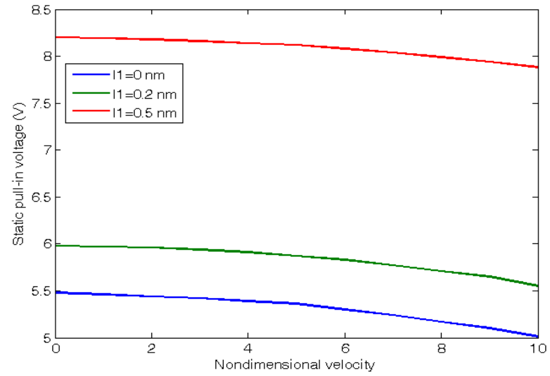
Fig. 3. Static pull-in volateg of cantilevr CNT vs. fluid viscosity

The figure shows that the static pull-in voltage of the CNT with the cantilever boundary conditions increases with increasing the viscosity. However, the calculations show no effects of the viscosity variation on the static pull-in volatages of the doubly clamped CNT. So, the mentioned results can be used in viscometer application of the studied bio-nanofluidic sensor in different conditions.

The pull-in voltages of the bio-nanosystem vs. the fluid velocity are analyzed in Fig. 4.



(a)

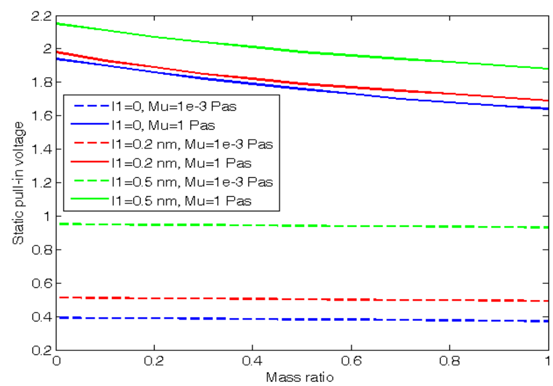


(b)

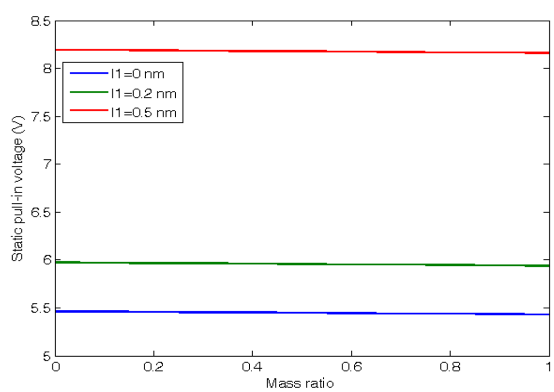
Fig. 4. Static pull-in voltages of (a) cantilevr, (b) doubly clamped CNT vs. fluid viscosity

According to this figure, the static pull-in voltages of the cantilever CNT possess different values for low and high viscosities where the other case does not. This figure reveals that the static pull-in voltages of the cantilever CNT increase with increasing the fluid velocity but decrease for the doubly clamped one. So, Fig. 4 proves the possibility of the application of this nanosystem as the flowmeter in precise drug delivery.

The variation of static pull-in voltages of the nanosystem vs. the changes of the mass ratio is shown in Fig. 5.



(a)



(b)

Fig. 5. . Static pull-in voltages of (a) cantilevr, (b) doubly clamped CNT vs. mass ratio

Fig. 5 (a) and (b) reveals that increasing mass ratio decreases the static pull-in volatges of the CNTs with both considered boundary conditions. Although, the calculations prove that increasing mass ratio does not affect the static pull-in voltage of the fixed-fixed CNT, drastically. Fig. 5 (a) shows that gradient of variation for the cantilvered CNT increases with increasing the fluid viscosity.

The effects of the temperature changes on the static pull-in voltages of the nanosystem are demonstrated in Fig. 6. The results are presented just for the doubly clamped boundary condition due to its confined structure. The 0-point on horizontal axis corresponds to temperature equaling 300K.

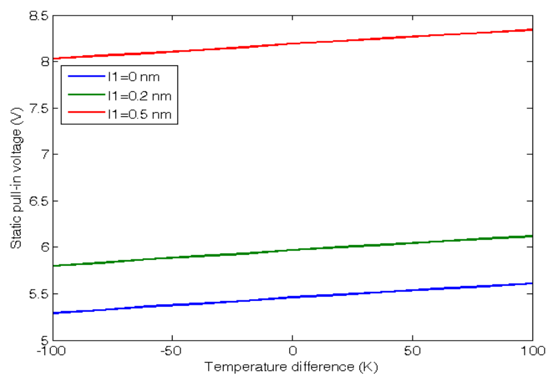


Fig. 6. Static pull-in voltages of doubly clamped CNT vs. temperature

According to the figure, increasing temperature increases the static pull-in voltages. This might seem strange because increasing temperature commonly should increases the length of the nanotube and this, due to the doubly clamped boundary conditions, induces a compressive force resulting in smaller pull-in voltages. However, the fact is that the longitudinal expansion coefficient of the CNT is negative in the considered temperature range. It means that its length decreases with increasing temperature.

Finally, the calculations show that changes of the fluid pressure, in the considered applicable region, does not affect the pull-in voltages of neither cantilever nor fixed-fixed CNT. Weakening the nanostructure with increasing its length may yield a nanosystem with higher sensitivity to the variation of the fluid pressure.

4 CONCLUSION

The paper discussed the physical design and mathematical modeling of an electrostatically actuated CNT-based bio-nanofluidic system. The fluid-conveying CNT was considered as an Euler-Bernoulli beam model formulated using the recently developed CCST. Its static deformation under electrostatic actuation were investigated. The CCST theory was applied to investigate the size effects in both solid and fluid parts of the model. The influences of various fluidic parameters including fluid velocity, viscosity, mass ratio and temperature on the static pull-in voltages of the cantilever and doubly clamped CNTs were analyzed. Most of them had different effects on the pull-in voltages. For example, increasing the fluid velocity increased the pull-in voltages of the cantilever nanotubes but decreased them for the fixed-fixed ones. The nanosystem can have many applications in different aspects of the nanofluidic and bio-nanofluidic devices. Its nano-valve application in some nanofluidic processes such as precise drug delivery or other processes requiring accurate measurement of the injected nano-flow was studied. In addition, the possible application of the nanosystem in nanofluidic sensing was analyzed via variation in the static pull-in voltages.

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