Modeling carbon nanotube as a real-time mass sensor in viscous fluid

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Summary In this work, we derived simple analytical formulas for mass detection from the resonant frequency shift and Q-factor of the carbon nanotube based resonators operating in viscous fluid. It is found that Q-factor allows one to detect the attached mass without knowing a-priori fluid properties. We show how the nanotube`s dimension should be chosen in order to measure the resonant frequencies in fluid and to detect particle in fluid. The bridge configuration is found to have higher Q-factor then the bridge configuration.

INTRODUCTION

Due to their small dimension (submicron in length) and ultralight mass, carbon nanotube based resonators (CNT) have been found to detect up to a mass resolution of zeptogram (10^{-21} g) in air and yottagram (10^{-24} g) in vacuum [1]. For detecting binding molecules it is useful to operate nanotube mass sensors in various fluids [2]. However, a nanotube that operates in viscous fluid is complicated by the energy dissipation of the surrounding fluid, which can have the same magnitude as the total energy stored in resonator. This results either in very low Q-factors or even in a loss of the nanotube resonant frequencies in fluid.

The purposes of this paper are to elucidate the impact of fluid properties and CNT dimensions on the Q-factor in bridge and cantilever configurations, and to provide theoretically-guided selection of parameters to enable one to detect particle or molecule mass in fluid.

THEORY

The governing equation for a vibrating CNT in viscous fluid is well known [3], and reads

$$w_{tt}(x, t) + 2\delta w_t(x, t) + a^2 w_{xxxx}(x, t) - c^2 w_{xx}(x, t) = F_E(t), \quad (1)$$

where $2\delta = C_f/(\rho_\Sigma A)$, $a = [EI/(\rho_\Sigma A)]^{0.5}$, $c = [F_T/(\rho_\Sigma A)]^{0.5}$, $F_E(t) = F_e(t)/(\rho_\Sigma A)$, $\rho_\Sigma = \rho(1 + \chi)$, $\chi = \rho_l/\rho$, $w(x, t)$, ρ, A, E, I and F_T are the traverse displacement, the density, the cross sectional area, the Young`s modulus, the moment of inertia, and the axial tension of the nanotube (e.g. from an applied electric field [4]), respectively; $C_f = (4\pi^3 D^2 \rho_l \mu_l)^{0.5}$ is the drag coefficient [5], f_d is the external driving frequency, D_o is the outer diameter of the nanotube, ρ_l is the density, μ_l is the viscosity of the surrounding fluid and $F_e(t)$ is the driving force caused by an external periodic electrical field (i.e. $F_e(t) = F_o \sin 2\pi f_d t$, where F_o is the maximum force per length).

The displacement of the CNT in fluid can be found by an eigenfunction method $w(x, t) = \sum_{n=1}^{\infty} w_n(t) X_n(x)$, where $X_n(x)$ are the eigenfunctions of the corresponding homogeneous problem and $w_n(t) = B_n \sin(\omega_d t - \varphi_n)$, $B_n = F_{An}/[(\omega_n^2 - \omega_d^2)^2 + (2\delta\omega_d)^2]^{1/2}$, $\tan \varphi_n = 2\delta\omega_d/(\omega_n^2 - \omega_d^2)$, $F_E(x,t) = \sum_{n=1}^{\infty} F_{An}(t) X_n(x)$, $\omega_d = 2\pi f_d$, l is the CNT length and ω_n are the fundamental resonant frequencies of the CNT in vacuum with and without accounting for an attached mass [6, 7].

If $\omega_n >> \delta$, then the nanotube resonant frequencies in fluid can be identified and consequently single-molecule measurements in fluid can be realized. This lead to a very important inequality between the nanotube`s properties (E, ρ, l, D_o; for simplicity we set innermost diameter $D_{in} = 0$) and the fluids properties (ρ_l, μ_l)

$$D_o^3/l^2 >> 32\mu_l\chi/[\gamma_{on}^2(E\rho)^{0.5}(1 + \chi)^{3/2}], \quad (2)$$

where γ_{on} are the eigenfunctions. For $F_T = 0$, the unloaded cantilever or bridge $\gamma_{o1} = 1.88…$ and $\gamma_{o1} = 4.73…$, respectively. For CNT of mass M loaded by an attached mass (m) and for the small mass ratio ($\varepsilon << 1$, $\varepsilon = m/M$), the eigenfunctions can be expressed through known values of an unloaded one [7]: $\gamma = \gamma_{on}[1 - \varepsilon\alpha_i(h^*, \gamma_{on})]$. The exact forms of the $\alpha_i(h^*, \gamma_{on})$ are given in Fig. 1 and subscript $i = c, b$ stands for cantilever and bridge. The resonant frequencies and the Q-factor of the vibrating CNT in viscous fluid are

$$\omega_{fn} = (\omega_n^2 - 2\delta^2)^{1/2}, \; Q = f_{fn}/\Delta f_n \approx \omega_{fn}/(2\delta), \quad (3)$$

where $f_{fn} = \omega_{fn}/(2\pi)$ and Δf_n is the bandwidth.

In vacuum, the attached mass causes an increase of total mass of the nanotube and it results in the lower values of the resonant frequencies [7]. Similarly, it can be expected that this will cause a frequency shift and also a change of Q-factor in fluid. Mathematically, the frequency shift and Q-factor change in fluid, which can be easily obtained from Eq. (3) by accounting for $\gamma = \gamma_{on}[1 - \varepsilon\alpha_i(h^*, \gamma_{on})]$ given by

$$\Delta f_n/f_{fn} = 2\varepsilon\alpha_i(h^*, \gamma_{on})/[1 - 2(\delta/\omega_{fn})^2], \quad (4a)$$

$$\Delta Q_n/Q_n = \varepsilon\alpha_i(h^*, \gamma_{on}). \quad (4b)$$

For example, let us consider CNT of $l = 200$ nm, $D_o = 30$ nm and mass ratio $\varepsilon = 0.1$ in th ebridge configuration and operating in DI water. The the frequency shift and Q-factor caused by attached molecule mass at $x = 0.5l$ are: $\Delta f_1/f_{f1} = 0.1$ and $\Delta Q_1/Q_1 = 0.06$, respectively.

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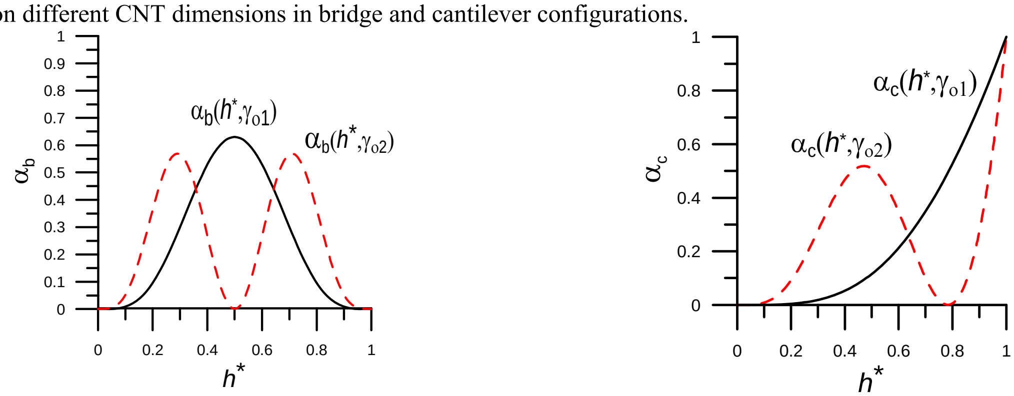
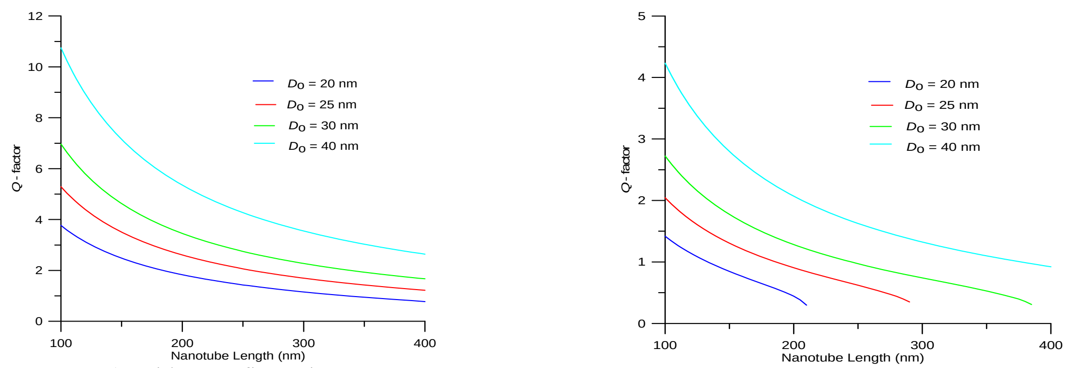
RESULTS AND DISCUSSIONS

It is evident from inequality (2) that the dimension of the CNT must be chosen based on the consideration of the fluid properties (i.e. DI water, alcohol, etc.). Moreover, inequality (2) also implies: I) if the resonator`s dimension is uniformly reduced, the fluid damping will increase and the Q-factor decreases; II) for same CNT dimension the bridge configurations provides higher *Q*-factor then cantilever. To illustrate these findings, Fig. 2 shows the dependency of the *Q*-factor on different CNT dimensions in bridge and cantilever configurations.



a) Bridge configuration b) Cantilever configuration

Fig. 1. The variation of the coefficients $\alpha_i(h^*, \gamma_{on})$ for (a) bridge and (b) cantilever configurations. Solid and dashed lines stand for the first and second vibrational modes, respectively.



a) Bridge configuration b) Cantilever configuration

Fig. 2. The relationship between *Q*-factor and CNT dimensions for: a) bridge at middle position (x = 0.5l) and b) cantilever at free end ($x = l$). Density and Young`s modulus of the resonator are: ρ = 2300 kg/m^3, E = 0.3 TPa, respectively and $D_{in} = 0$.

In contrast to a CNT operating in vacuum, attached mass can be detected in fluid either from the resonant frequency shift or from the broadening of *Q*-factor.

The use of *Q*-factor may be preferred because its change due to an attached mass is independent of the fluid properties (ρ_l, μ_l).

CONCLUSIONS

Simple analytical formulas [Eqs. (4a) and (4b)] for mass detection by CNT in viscous fluid have been derived. It has been found that an attached mass can be detected not only from the frequency shift but also from the *Q*-factor broadening. The advantage of using the *Q*-factor is that the attached single-molecule mass can be detected without knowing the fluid properties. In addition, a criterion for CNT dimension is found for detection in fluid. The present results can be applied to future nanotube based sensors for single-molecule detection in physiological environments.

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