Mass and rotary inertia sensing from vibrating cantilever nanobeams

S. Adhikari and H. H. Khodaparast[1]

[1]Zienkiewicz Centre for Computational Engineering, College of Engineering, Swansea University, Bay Campus, Swansea SA1 8EN, Wales, UK

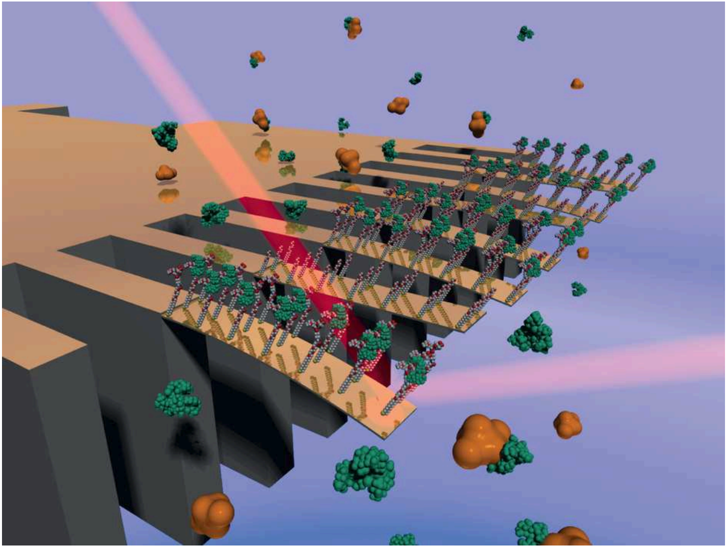
SPIE Smart Structures/NDE 2016, Las Vegas, NV, USA

Outline

Nano mechanical sensors

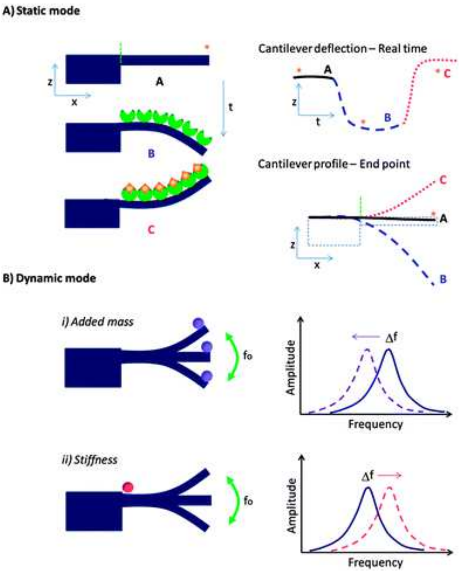
- Progress in nanotechnologies has brought about a number of highly sensitive label-free biosensors.
- These include electronic biosensors based on nanowires and nanotubes, optical biosensors based on nanoparticles and mechanical biosensors based on resonant micro- and nanomechanical suspended structures.
- In these devices, molecular receptors such as antibodies or short DNA molecules are immobilized on the surface of the micro-nanostructures. The operation principle is that molecular recognition between the targeted molecules present in a sample solution and the sensor-anchored receptors gives rise to a change of the optical, electrical or mechanical properties depending on the class of sensor used.
- These sensors can be arranged in dense arrays by using established micro- and nanofabrication tools.

Cantilever nano-sensor



Array of cantilever nano sensors (from http://www.bio-nano-consulting.com)

The mechanics behind nanomechanical sensors



(From Tamayo et. al.)

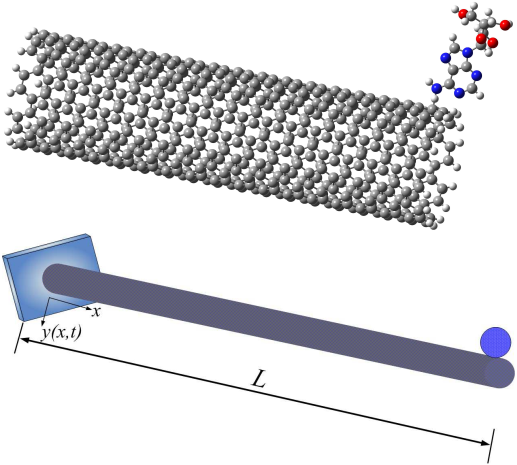
The need for identifying rotary inertia

- Vibrating nano-mechanical cantilevers have received wide attention due to the possibility of obtaining resonance frequency very accurately.
- Existing approaches mainly focus on sensing of an attached mass to a cantilever sensor by exploiting the shift in the first mode of vibration
- The magnitude of the mass gives the basic information of an attached object. But it gives no information about the shape of and size of such objects.
- Rotary inertia can give some further insights into its shape and size.
- This work proposes a novel way by which both the mass and rotary inertia of an object can be obtained simultaneously from frequency shifts.
- With the additional information of the rotatory inertia, it may be possible to infer more about the attached object to a cantilever nanosensor, which is a key motivation for this work.

Mass and rotary inertia sensing - an inverse problem

- This talk will focus on the detection of mass and rotary inertia based on shifts in frequency.
- Mass and rotary inertia sensing is an inverse problem.
- The “answer” in general in non-unique. An added mass and rotary inertia at a certain point on the sensor will produce unique frequency shifts. However, for a given frequency shifts, there can be many possible combinations of mass and rotary inertia values and locations.
- Therefore, predicting the frequency shifts - the so called “forward problem” is not enough for sensor development.
- Advanced modelling and computation methods are available for the forward problem. However, they may not be always readily suitable for the inverse problem if the formulation is “complex” to start with.
- Often, a carefully formulated simplified computational approach could be more suitable for the inverse problem and consequently for reliable sensing.

Single-walled carbon nanotube based sensors



A cantilevered carbon nanotube resonator with attached mass. The inertia effect arises from 'height' of the attached object (DeOxy Thymidine used as an example). (a) Original configuration with a point mass at the tip; (b) Mathematical idealisation with a point mass at the tip.

Euler-Bernoulli beam thoery

- The equation of motion of free-vibration using Euler-Bernoulli beam bending theory can be expressed as

$$EI\frac{\partial^4 y(x,t)}{\partial x^4} + \rho A\frac{\partial^2 y(x,t)}{\partial t^2} = 0 \tag{1}$$

  where x is the coordinate along the length of the cantilever oscillator, t is the time, $y(x,t)$ is the transverse displacement of the cantilever oscillator, E is the Young's modulus, I is the second-moment of the cross-sectional area A and ρ is the density of the material. Suppose the length of the cantilever oscillator is L.

- For the cantilevered oscillator without any attached mass, the resonance frequencies can be obtained from

$$f_{0_j} = \frac{c_0}{2\pi}\lambda_j^2, \quad c_0 = \sqrt{\frac{EI}{\rho A L^4}} \tag{2}$$

Free vibration of a cantilevered oscillator

- The constants λ_j should be obtained by solving the following transcendental equation

$$\cos\lambda\cosh\lambda + 1 = 0 \tag{3}$$

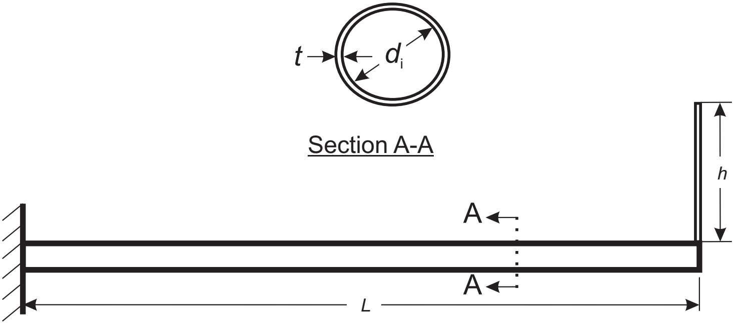
- The vibration mode shape can be expressed as

$$Y_j(\xi) = (\cosh\lambda_j\xi - \cos\lambda_j\xi) - \left(\frac{\sinh\lambda_j - \sin\lambda_j}{\cosh\lambda_j + \cos\lambda_j}\right)(\sinh\lambda_j\xi - \sin\lambda_j\xi) \tag{4}$$

  where $\xi = \frac{x}{L}$ is the normalised coordinate along the length of the cantilever oscillator.

- The values of λ arising from the solution of equation (3) are be given by $\lambda_1 = 1.8751$, $\lambda_2 = 4.6941$, $\lambda_3 = 7.8547$, $\lambda_4 = 10.9954$ and $\lambda_5 = 14.1371$. For $j > 5$, in general $\lambda_j = (2j-1)\pi/2$.
- For sensing applications, we are interested in the first few modes of vibration only. In this paper the first two modes of vibration will be used.

Cantilevered oscillator with attached mass and rotary inertia



Illustrative diagram of a cantilevered nanotube resonator with an attached mass and rotary inertia at the tip.

Boundary conditions

- Deflection at $x = 0$:

$$y(0, t) = 0 \tag{5}$$

- Slope at $x = 0$:

$$\frac{\partial y(x, t)}{\partial x} = 0 \tag{6}$$

- Bending moment at $x = L$:

$$EI \frac{\partial^2 y(x, t)}{\partial x^2} + J \frac{\partial \ddot{y}(x, t)}{\partial x} = 0 \Big|_{x=L} \tag{7}$$

- Shear force at $x = L$:

$$EI \frac{\partial^3 y(x, t)}{\partial x^3} - M \ddot{y}(x, t) = 0 \Big|_{x=L} \tag{8}$$

Here $(\dot{\bullet})$ denotes derivative with respective to t.

Cantilevered oscillator with attached mass and rotary inertia

- Assuming harmonic solution we have

$$y(x,t) = Y(\xi)\exp[\mathrm{i}\omega t] \tag{9}$$

where i is the unit imaginary number $\mathrm{i} = \sqrt{-1}$ and ω is the frequency.

- Substituting this in the equation of motion and the boundary conditions

$$\frac{\partial^4 Y(\xi)}{\partial \xi^4} - \Omega^2 Y(\xi) = 0 \tag{10}$$

$$Y(0) = 0,\ Y'(0) = 0,\ Y''(1) - \beta\Omega^2 Y'(1) = 0 \quad \text{and} \quad Y'''(1) + \alpha\Omega^2 Y(1) = 0 \tag{11}$$

- Here $(\bullet)'$ denotes derivative with respective to ξ and

$$\Omega^2 = \omega^2/c_0^2 \quad \text{(nondimensional frequency parameter)} \tag{12}$$

$$\alpha = \frac{M}{\rho A L} \quad \text{(mass ratio)} \tag{13}$$

$$\text{and} \quad \beta = \frac{J}{\rho A L^3} \quad \text{(inertia ratio)} \tag{14}$$

Equation governing the natural freqnecues

- Assuming a solution of the form

$$Y(\xi) = \exp\{\lambda\xi\} \tag{15}$$

and substituting in the equation of motion (10) results

$$\lambda^4 - \Omega^2 = 0 \quad \text{or} \quad \lambda = \pm \mathrm{i}\Omega, \quad \pm\Omega \tag{16}$$

- In view of the roots in equation (16), the solution $Y(\xi)$ can be expressed as

$$\begin{aligned} Y(\xi) &= a_1 \sin\lambda\xi + a_2 \cos\lambda\xi + a_3 \sinh\lambda\xi + a_4 \cosh\lambda\xi \\ \text{or} \quad Y(\xi) &= \mathbf{s}^T(\xi)\mathbf{a} \end{aligned} \tag{17}$$

- Here the vectors

$$\mathbf{s}(\xi) = \{\sin\lambda\xi, \cos\lambda\xi, \sinh\lambda\xi, \cosh\lambda\xi\}^T \tag{18}$$

$$\text{and} \quad \mathbf{a} = \{a_1, a_2, a_3, a_4\}^T. \tag{19}$$

Equation governing the natural freqnecues

- Applying the boundary conditions in equation (11) on the expression of $Y(\xi)$ in (17) we have
$$\mathbf{Ra} = \mathbf{0} \tag{20}$$
where **R** is a 4×4 matrix.
- The natural frequencies is given by
$$\det\{\mathbf{R}\} = 0 \tag{21}$$
- Simplifying this we have:
$$((1 - \cos(\lambda)\cosh(\lambda))\lambda^3\beta - \sin(\lambda)\cosh(\lambda) + \cos(\lambda)\sinh(\lambda))\lambda\alpha \\ - (\cos(\lambda)\sinh(\lambda) + \sin(\lambda)\cosh(\lambda))\lambda^3\beta + [\cos(\lambda)\cosh(\lambda) + 1] = 0 \tag{22}$$
Due to the nonlinearity of this transcendental equation, it needs to be solved numerically.

Approximation based on assumed mode

- The exact analytical frequency equation is complex enough so that a simple relationship between the change in the mass and rotary inertia and the shift in the frequency is not available.
- As we have two unknowns α and β, two frequency shifts are necessary to identify them.
- An arbitrary j-th natural frequency of a cantilever oscillator can be expressed as

$$f_j = \frac{1}{2\pi}\sqrt{\frac{k_{eq_j}}{m_{eq_j}}}, j = 1, 2, 3 \cdots \tag{23}$$

  Here k_{eq_j} and m_{eq_j} are respectively equivalent stiffness and mass of the cantilever oscillator in the j-th mode of vibration.
- The equivalent mass m_{eq_j} changes depending on the mass and inertia of the attached object.
- Suppose Y_j is the assumed displacement function for the j-th mode of vibration. We consider this to be the vibration mode of the cantilever only.

Kinetic and potential energy of the system

- The kinetic energy of the system contributes to m_{eq_j} while the potential energy contributes to k_{eq_j}.
- The total kinetic energy comes from three components, namely, the kinetic energy of the cantilever, kinetic energy of the attached mass due to linear velocity and kinetic energy of the attached mass due to rotational velocity.
- Assuming harmonic motion, the overall equivalent mass m_{eq_j} can be expressed as

$$m_{eq_j} = \rho AL \int_0^1 Y_j^2(\xi)\mathrm{d}\xi + MY_j^2(1) + J \left(\frac{\partial Y_j}{\partial x} \right)^2 \bigg|_{\xi=1} \quad (24)$$

$$= \rho AL \int_0^1 Y_j^2(\xi)\mathrm{d}\xi + MY_j^2(1) + \frac{J}{L^2} {Y_j'}^2(1) \quad (25)$$

$$= \rho AL \left[\underbrace{\int_0^1 Y_j^2(\xi)\mathrm{d}\xi}_{I_1} + \alpha Y_j^2(1) + \beta {Y_j'}^2(1) \right] \quad (26)$$

Kinetic and potential energy of the system

- From the potential energy, the equivalent stiffness k_{eq_j} can be obtained as

$$k_{eq_j} = \frac{EI}{L^3} \underbrace{\int_0^1 Y_j^{''2}(\xi) \mathrm{d}\xi}_{I_2} \tag{27}$$

- From these equations we have

$$\frac{k_{eq_j}}{m_{eq_j}} = \left(\frac{EI}{\rho A L^4} \right) \frac{I_2}{I_1 + \alpha Y_j^2(1) + \beta Y_j'^2(1)} \tag{28}$$

- Using the expression of the natural frequency we have

$$f_j = \frac{1}{2\pi} \sqrt{\frac{k_{eq_j}}{m_{eq_j}}} = \frac{c_0}{2\pi} \frac{\gamma_{1_j}}{\sqrt{1 + \gamma_{2_j}\alpha + \gamma_j \beta}}, \quad j = 1, 2, 3, \cdots \tag{29}$$

Approximate frequency equation

- The mode dependent constants can be evaluated exactly as

$$\gamma_{1_j} = \sqrt{\frac{I_2}{I_1}} = \sqrt{\frac{\int_0^1 Y_j''^2(\xi)\mathrm{d}\xi}{\int_0^1 Y_j^2(\xi)\mathrm{d}\xi}} = \lambda_j^2$$

$$\gamma_{2_j} = \frac{Y_j^2(1)}{I_1} = \frac{Y_j^2(1)}{\int_0^1 Y_j^2(\xi)\mathrm{d}\xi} = 4 \text{ (for all } j) \tag{30}$$

$$\text{and} \quad \gamma_j = \frac{Y_j'^2(1)}{I_1} = \frac{Y_j'^2(1)}{\int_0^1 Y_j^2(\xi)\mathrm{d}\xi}$$

- In view of the above expressions we have

$$f_j = \frac{1}{2\pi}\sqrt{\frac{k_{eq_j}}{m_{eq_j}}} = \frac{c_0}{2\pi}\frac{\lambda_j^2}{\sqrt{1+4\alpha+\gamma_j\beta}}, \quad j = 1, 2, 3, \cdots \tag{31}$$

- Since we have two parameters to identify, only the first two modes are necessary. For these two modes $\gamma_1 = 7.579069394$ and $\gamma_2 = 91.42336885$.

Sensor equations

- Combining equation (2) and (31) the relationship between the resonance frequencies with and without the attached mass can be obtained as

$$f_j = \frac{f_{0_j}}{\sqrt{1 + 4\alpha + \gamma_j \beta}} \tag{32}$$

- The frequency-shift can be expressed using Eq. (32) as

$$\Delta f_j = f_{0_j} - f_j = f_{0_j} - \frac{f_{0_j}}{\sqrt{1 + 4\alpha + \gamma_j \beta}} \tag{33}$$

- From this we can obtain the relative frequency shift as

$$\delta_j = \left(\frac{\Delta f_j}{f_{0_j}} \right) = 1 - \frac{1}{\sqrt{1 + 4\alpha + \gamma_j \beta}} \tag{34}$$

- Rearranging gives the expression

$$\frac{1}{\sqrt{1 + 4\alpha + \gamma_j \beta}} = \left(1 - \delta_j\right) \quad \text{or} \quad \left(1 + 4\alpha + \gamma_j \beta\right) = \frac{1}{\left(1 - \delta_j\right)^2}, \quad j = 1, 2 \tag{35}$$

Sensor equations

- These two equations arising for two values of j completely relate the change in mass and rotary inertia with the two relative frequency-shifts. Solving these equations and after some simplifications we have

$$\beta = \frac{(2-\delta_1-\delta_2)(\delta_2-\delta_1)}{(1-\delta_1)^2(1-\delta_2)^2(\gamma_2-\gamma_1)} \tag{36}$$

$$\text{and} \quad \alpha = \frac{1}{4}\left[\frac{1}{(1-\delta_1)^2} - 1 - \gamma_1\beta\right] \tag{37}$$

- These are the general equations which completely relate the added mass and rotary inertia and the frequency shifts. In the special case, when the rotary inertia is neglected, substituting $\beta = 0$, expanding in a Taylor series and keeping only the linear term, we have

$$\alpha \approx \frac{\delta_1}{2} \quad \text{or} \quad \frac{M}{\rho AL} \approx \frac{1}{2}\left(\frac{\Delta f_1}{f_{0_1}}\right) \tag{38}$$

  which is the widely-used classical relationship between the added tip mass and the frequency-shift.

Cantilevered SWCNT with mass at the tip

- A zigzag (7, 0) SWCNT with Young's modulus $E = 1.0$ TPa, $L = 20$nm, density $\rho = 9.517 \times 10^3$ kg/m^3 and thickness t = 0.08nm is uses as example.
- The diameter of the SWCNT is 0.55nm. Using these, the cross-sectional area A and area moment of inertia I can be obtained as

$$A \approx \pi d_i t \quad \text{and} \quad I \approx \frac{\pi}{8} d_i^3 t \tag{39}$$

- To consider realistic values of the rotary inertia, we assume that the attached mass is a straight vertical linear object of height h. The mass moment of inertia of such an object is given by

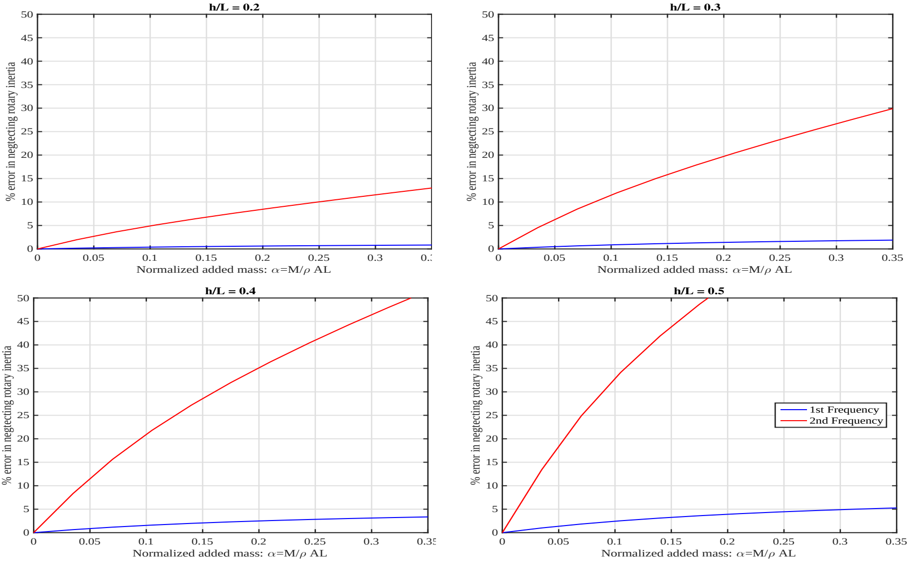
$$J = Mh^2/3 \tag{40}$$

- Therefore

$$\beta = \frac{J}{\rho A L^3} = \frac{Mh^2/3}{\rho A L^3} = \frac{M}{\rho A L} \frac{1}{3} \left(\frac{h}{L}\right)^2 = \frac{\alpha}{3} \left(\frac{h}{L}\right)^2 \tag{41}$$

- This implies that for physically realistic objects, α and β are not independent quantities.

Error due to neglecting the rotary inertia effect



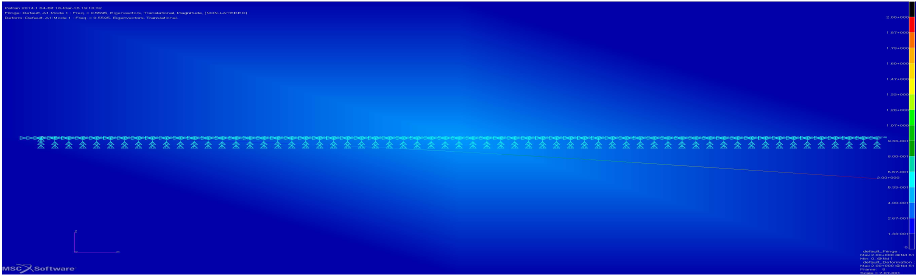
Finite element model

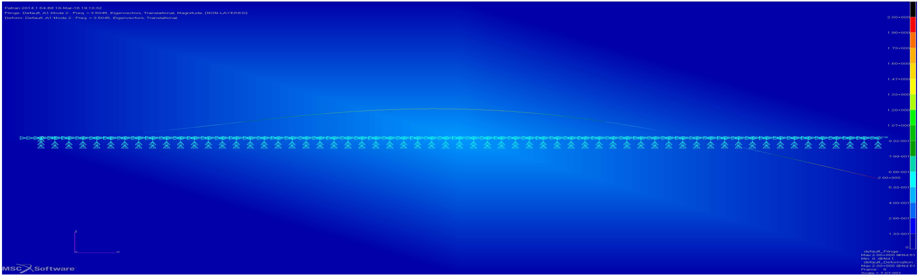
- Equations (36) and (37) give closed-form expression to detect added mass and rotary inertia from the first two frequency shifts.
- Consider that the frequency shifts corresponding to the two modes, namely

$$\delta_1 = \left(\frac{\Delta f_1}{f_{0_1}}\right) = \left(\frac{f_{0_1} - f_1}{f_{0_1}}\right) \quad \text{and} \quad \delta_2 = \left(\frac{\Delta f_2}{f_{0_2}}\right) = \left(\frac{f_{0_2} - f_2}{f_{0_2}}\right) \tag{42}$$

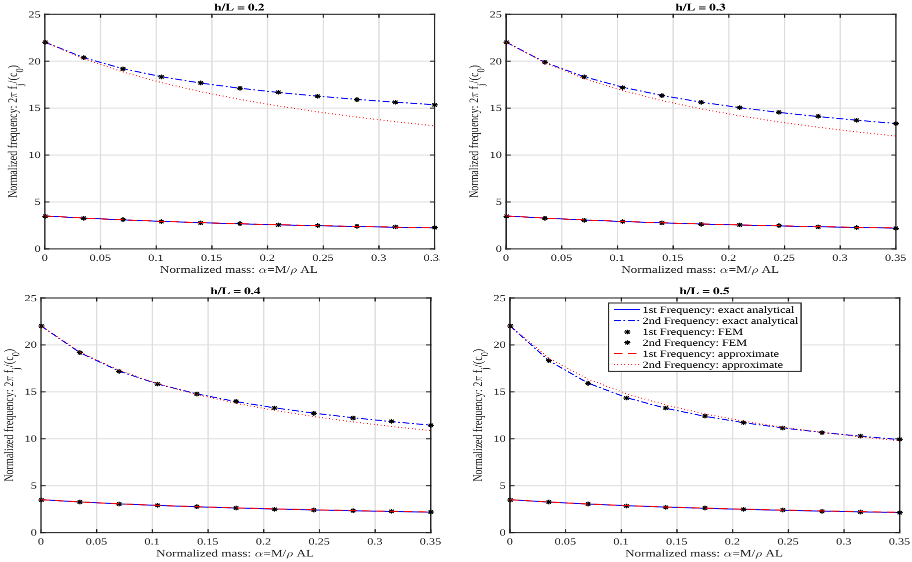
  are available from experiment.
- These quantities can then be used as an 'input' to equations (36) and (37) to identify the added mass and rotary inertia.
- In the absence of experimental results in this work, we generate the 'experimentally measured frequencies' from a completely independent finite element model (in `Nastran`)

Finite element modes

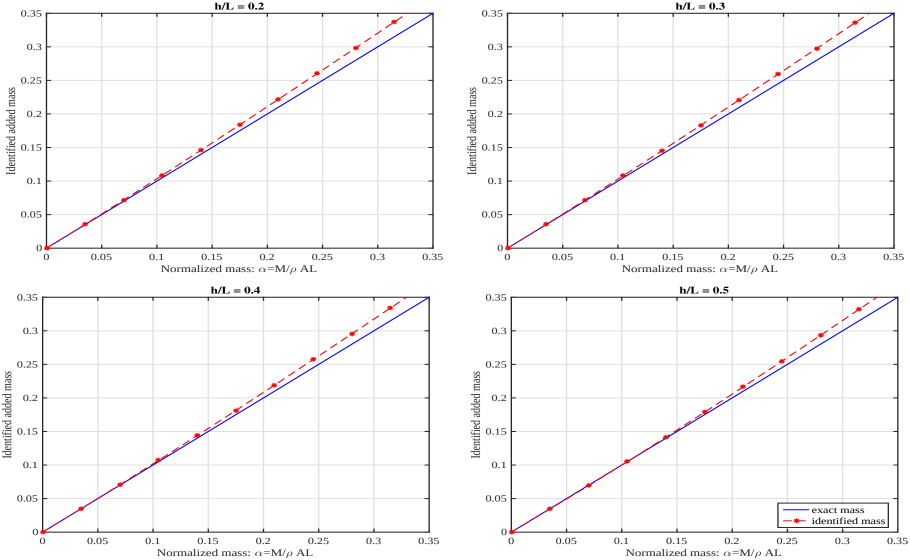




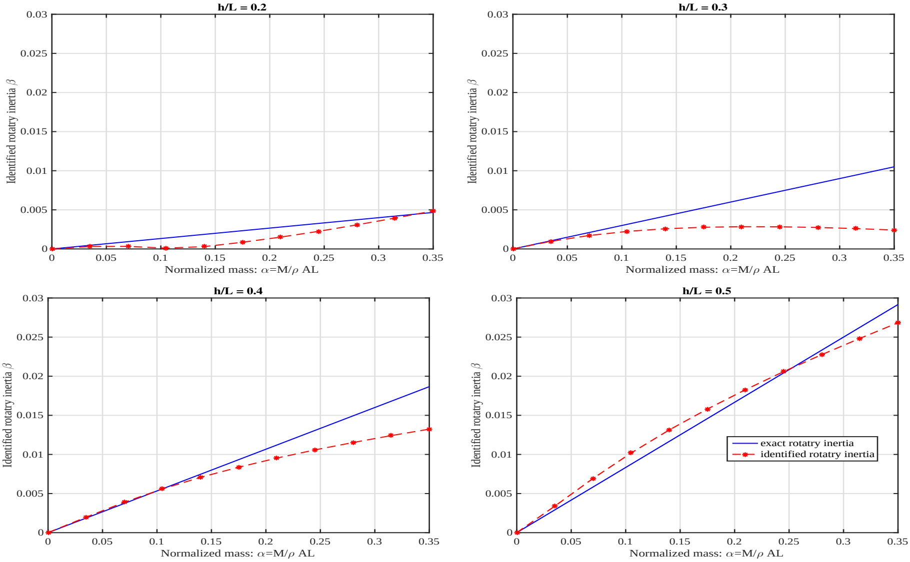
Comparisons of the frequencies



Error is mass indetification



Error is rotary inertia indetification



Summary of the main derivations

Exact equation governing the frequencies

$$\left(\left(1-\cos(\lambda)\cosh(\lambda)\right)\lambda^3\beta - \sin(\lambda)\cosh(\lambda) + \cos(\lambda)\sinh(\lambda)\right)\lambda\alpha$$
$$-\left(\cos(\lambda)\sinh(\lambda) + \sin(\lambda)\cosh(\lambda)\right)\lambda^3\beta + \left[\cos(\lambda)\cosh(\lambda) + 1\right] = 0$$

Approximate frequency equation

$$f_j = \frac{1}{2\pi}\sqrt{\frac{k_{eq_j}}{m_{eq_j}}} = \frac{c_0}{2\pi}\frac{\lambda_j^2}{\sqrt{1+4\alpha+\gamma_j\beta}}, \quad j = 1, 2, 3, \cdots$$

Sensor equations

$$\beta = \frac{(2-\delta_1-\delta_2)(\delta_2-\delta_1)}{(1-\delta_1)^2(1-\delta_2)^2(\gamma_2-\gamma_1)}$$

and $$\alpha = \frac{1}{4}\left[\frac{1}{(1-\delta_1)^2} - 1 - \gamma_1\beta\right]$$

Main conclusions

- The sensing of mass and rotary inertia of an attached object in the context of cantilever nano-mechanical sensors has been considered.
- Using Euler-Bernoulli cantilever beam theory, the exact equation governing the natural frequencies of the sensor with the attached mass and its rotary inertia effect has been derived.
- Therefore, using an energy approach, approximate simple closed-form expressions for the identified mass and rotary inertia from the first two frequency shifts have been derived.
- It was proved that the classical equation to obtain the attached mass from the first frequency shift is a special case of the general equations derived in this paper. Some of the highlights of this paper are:
  1. Prediction of the second natural frequency can be very inaccurate if the rotary inertial effect is completely ignored.
  2. The proposed approximate closed-form expression for both the natural frequencies give acceptable numerical accuracy when compared to the exact analytical solution.
  3. The new sensor equations expressed in terms of the first two frequency shifts gives an excellent estimate for the attached mass and relatively less accurate estimate for the rotary inertia.