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ON THE ROLE OF ADSORBATE POSITION, GEOMETRY, AND BINDING CHARACTERISTICS ON THE MULTI-MODAL RESPONSE OF CANTILEVER-BASED RESONATORS FOR HIGHER-ORDER DISCRETE-MASS DETECTION

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INTRODUCTION

Recent work [1-3] has indicated the potential for higher-order mass detection, or inertial imaging, using micro/nanobeam resonators to quantify not only the mass of a discrete adsorbate (e.g., particle, cell, molecule) that binds to the resonator, but also higher-order inertial characteristics related to its mass distribution and how these attributes evolve over time. These approaches are predicated on the ability to accurately quantify the perturbing effect of the adsorbate on the resonant frequencies of the micro/ nanobeam-based sensor. As device dimensions become smaller, the size of a given adsorbate increases relative to the sensor, thereby suggesting the possibility that the resonator can serve as more than just a device to weigh small entities; it may also "see" the size and/or shape of the adsorbate by virtue of higherorder inertial characteristics (e.g., rotational inertia) affecting the sensor's resonant response. In most earlier theoretical studies the adsorbate is assumed to be either a point mass [4,5] or a rigid body that is rigidly attached to the vibrating beam [3]; however, in applications in which the adsorbate size approaches the same order of magnitude as that of the device, the adsorbate geometry and the binding/adherence characteristics between the adsorbate and the beam may also influence the frequency response of the beam/ particle system. Therefore, in the present study we develop a theoretical model in an attempt to understand how the resonant frequencies and mode shapes of a cantilever/adsorbate system are influenced by the position, mass, and rotational inertia of the adsorbate and a "rotational adherence" parameter (elastic rotational stiffness, k) defining how effectively the adsorbate binds to the resonator (Fig. 1).

MATHEMATICAL FORMULATION & SOLUTION We assume that the adsorbate is rigid but attached elastically to the beam (in the rotational sense) at $\xi_0=x_0/L$ with an eccentricity H+h/2 as shown in Fig. 1. Beam mass and flexural rigidity are denoted by mand EI, while M and J are the mass and rotational inertia (w.r.t. center of mass G) of the adsorbate. Beam deflection is denoted by $w(\xi,t)$, where $\xi=x/L$ and t is time, and $\theta(t)$ is the angle of spring deformation. The boundary value problem (BVP) is identical to that appearing in the rigid-attachment case [3] except for a different moment discontinuity condition and an additional equation governing $\theta(t)$:



Fig. 1. Idealized system and notation: rigid adsorbate elastically attached to cantilever.

$$w''(\xi_0^+, t) - w''(\xi_0^-, t) = \frac{ML^3}{FL} \frac{\overline{JH}^2 \overline{h}^2}{\overline{L} + \overline{H}^2} \ddot{w}'(\xi_0, t) - \frac{\overline{J} + \overline{H}^2 (1 + \overline{h})}{\overline{L} + \overline{H}^2} \overline{k} L \theta(t),$$
(1)

$$\ddot{\theta}(t) + \frac{\bar{k}}{\bar{J} + \bar{H}^2} \frac{EI}{ML^3} \theta(t) = \frac{\bar{J} + \bar{H}^2}{\bar{J} + \bar{H}^2} \frac{\ddot{w}'(\xi_0, t)}{L} .$$
(2)

Above and in what follows, we use the notation

$$\overline{k} = \frac{kL}{EI}$$
, $\overline{J} = \frac{J}{ML^2}$, $\overline{M} = \frac{M}{m}$, $\overline{H} = \frac{H}{L}$, $\overline{h} = \frac{h}{2H}$. (3)

To determine the resonant frequencies and mode shapes, we assume a solution of constant shape:

$$w(\xi,t) = A\varphi(\xi)e^{i\omega t} = \begin{cases} A\varphi_1(\xi)e^{i\omega t} , & 0 \le \xi \le \xi_0 , \\ A\varphi_2(\xi)e^{i\omega t} , & \xi_0 \le \xi \le 1 , \end{cases}$$
(4)

$$\theta(t) = \alpha w'(\xi_0, t) / L = A \alpha \varphi'_1(\xi_0) e^{i\omega t} / L , \qquad (5)$$

in which the mode shape is characterized by the beam shape $\varphi(\zeta)$ and the constant α , the latter describing the particle's rotation w.r.t. that of the beam. Placing (4) and (5) into the BVP permits the problem to be reduced to an 8-by-8 eigenvalue problem from which the resonant frequencies and mode shapes are found.

NUMERICAL RESULTS AND OBSERVATIONS

Figure 2 shows the resonant frequency shifts predicted by the new model for modes 1-3 as functions of adsorbate position and for various \overline{k} values. Also shown are FEA results at $\zeta_0=0.8$. We note: (1) results of the model show excellent agreement with FEA; (2) dependence on \overline{k} is *not* monotonic; (3) the adsorbate may cause a frequency *increase*; (4) the threshold values of \overline{k} , corresponding to $\overline{k}=0$ or $\overline{k}=\infty$ behavior, increase as mode number *n* increases, indicating that larger rotational velocities result in more relative rotation potential at the binding site; (5) higher-order effects due to the adsorbate's rotational inertia and eccentricity are more prominent at larger \overline{k} values.

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Fig. 2. Frequency shift predictions (modes 1-3) for varying values of rotational adherence: present model and FEA. (M/m=0.1, J/ML²=0.0051, H/L=0.071, h/H=0.7)

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