DESIGN OF BIOLOGICAL SENSORS UTILISING MODE-LOCALISATION IN ELECTROSTATICALLY COUPLED MICRORESONATORS

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Abstract **— In this paper we present the initial stages of research aimed at developing a microscale sensor based on the mode-localisation effect seen in electrostatically coupled microresonators. Mathematical and finite-element method (FEM) models have been set up and used to analyse a proposed device design. Biological functionalisation of the proposed device is discussed.**

Keywords: **Mode localisation, MEMS, Resonators, Biological sensors**

I – Introduction

There are many sensors that utilise microelectromechanical systems (MEMS) components for various applications. Mass, force, stress, strain and acceleration can be measured by exploiting the mechanical properties of microscale structures such as cantilevers, bridges and rings, which are typically made of silicon. Thus far, one of the most researched areas of MEMS sensors has been the development of systems that can detect a change in the resonant frequency of a microstructure caused by the measurand, as has been demonstrated previously [1].

The future development of microsensors will focus on increasing their sensitivity. One application is biological sensing, which requires increased sensitivity in order to discriminate between various viruses, bacteria and other pathogens. In addition, MEMS-based sensors are currently being developed that can detect DNA strands [2, 3].

However, while frequency-shift resonant sensors have been widely researched and developed, another resonator sensing technique has emerged that utilises two microstructures that are weakly coupled together with an electric field [4]. As yet, mass detection with an electrostatically coupled microresonators system has not been demonstrated. In this paper, we report on research that aims to exploit the properties of electrostatically coupled microresonators to create ultra-sensitive biological sensors.

II – Theory

Mode-localisation is a phenomenon that occurs in arrays of resonant structures that are coupled together. When disorder in the form of a change in the stiffness or mass is introduced to a previously balanced system, oscillation energy becomes confined or "localised" to one of the resonators.

Consider a lumped-element representation of a two degree-of-freedom (DOF) system with two coupled resonators (shown in figure 1). Each resonator is represented by a mass, m_1 or m_2, and a stiffness, k_1 or k_2. The two resonators are coupled together with a coupling element represented by a spring k_c. The displacement of each resonator is given by x_1 and x_2.

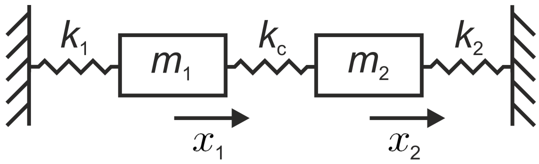

Figure 1: *Lumped element model of a 2-DOF system consisting of two coupled resonators*

To describe the vibration response of the system the equations of motion can be written as

$$m\ddot{x}_1 + kx_1 + k_c(x_1 - x_2) = 0$$
$$m\ddot{x}_2 + kx_2 + k_c(x_2 - x_1) = 0 \qquad (1)$$

where $m_1 = m_2 = m$ and $k_1 = k_2 = k$ for a balanced system.

To obtain the mode frequencies and the mode shapes, the following eigenvalue problem must be solved.

$$Ku_i = \lambda_i M u_i \qquad (2)$$

where K and M represents the stiffness and mass matrices respectively and are given by

$$K = \begin{bmatrix} k+k_c & -k_c \\ -k_c & k+k_c \end{bmatrix}$$
$$M = \begin{bmatrix} m & 0 \\ 0 & m \end{bmatrix} \qquad (3)$$

and λ_i and u_i (i = 1, 2) represent the eigenvalues and eigenvectors, respectively.

If the eigenvalue problem in (2) is solved, the following eigenvalues and eigenvectors are calculated

$$\lambda_1 = \frac{k}{m}, u_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$
$$\lambda_2 = \frac{k+2k_c}{m}, u_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \qquad (4)$$

The eigenvalues give the mode frequencies ($\lambda_i = \omega_i^2$) and the corresponding eigenvectors give the mode shapes. If the mass of one of the resonators is increased by Δm, an imbalance is created and mode-localisation will occur, as shown in the expression [4]

$$\frac{|u_n - u_{0n}|}{|u_{0n}|} = \left| \frac{\Delta m}{4k_c} \left(\frac{k}{m} \right) \right| \quad (5)$$

where u_n and u_{0n} represents the perturbed and unperturbed eigenvectors, respectively. Therefore, the left side of equation 5 represents the shift in the eigenvectors relative to the unperturbed state. The shift in the eigenvectors is deduced from the change in the ratio of the oscillation amplitudes of the two resonators, x_1 and x_2.

Mode-localisation has been demonstrated previously in microscale resonators that are coupled with both mechanical [5] and electrostatic [4] elements. A main advantage of forming the coupling element by applying DC bias to the two resonators is that the strength of the coupling can be easily varied.

It has been shown previously [4] that when the stiffness of one of a pair of coupled resonators is varied, the percentage change in mode shape ratio can be up to four or five orders of magnitude higher than the corresponding shift in resonant frequency of a single resonator. Therefore, microscale sensors based on the mode-localisation effect have the potential to be successful in biological sensing applications.

III – 2-DOF Model Simulation Details

A mathematical analysis of a coupled resonator system has been performed. The model consists of two rectangular silicon beams that are fixed at both ends, with a length of 400 μm, width of 20 μm and a thickness of 25 μm. The beams are spaced 1 μm apart and fixed electrodes (for actuation) are positioned with a 1 μm spacing on either side of the two beams. Next, the values detailed in figure 1 have been calculated. The effective value for m_1 and m_2 has been calculated as follows [6]

$$\begin{aligned} m_{1,2} &= 0.4\rho AL \\ &= 0.4 \times 2331 kg/m^3 \times 20\mu m \times 25\mu m \times 400\mu m \\ &= 186ng \end{aligned} \quad (6)$$

where ρ is the density of silicon (2331 kg/m^3), A is the beam cross section and L is the beam length. The effective spring constants of the beams, k_1 and k_2, are given by

$$k_{1,2} = \omega_0{}^2 m \quad (7)$$

where the resonant frequency, ω_0, of each individual beam, is given by

$$\omega_0 = 4.73^2 \sqrt{\frac{EI}{\rho AL}}$$

$$I = \frac{1}{12} t w^3 \quad (8)$$

E is the Young's modulus and I is the moment of inertia of the beam. For our model of silicon beams, with the dimensions specified, the mechanical spring constant is calculated

$$\begin{aligned} k_{1,2} &= \frac{16.7Etw^3}{L^3} \\ &= \frac{16.7 \times 130GPa \times 25\mu m \times (20\mu m)^3}{(400\mu m)^3} \\ &= 6784N/m \end{aligned} \quad (9)$$

The coupling spring, k_c, is electrostatic and is induced by applying DC voltages of -5 V and 5 V to the two beams and is calculated by

$$\begin{aligned} k_c &= \frac{(\Delta V)^2 \varepsilon_0 A}{g^3} \\ &= \frac{(10V)^2 \times 8.85 \times 10^{-12} \times 400\mu m \times 25\mu m}{(1\mu m)^3} \\ &= 8.85N/m \end{aligned} \quad (10)$$

These values have been used with equation 5 to plot the resulting change in eigenvectors for an increase in mass on one of the resonators. The effect of adding an additional mass of up to 46 pg to the beam has been plotted and the result can be seen in figure 2. For the observed region of small mass change (< 0.01%), an approximately linear relationship can be seen. Also, the eigenvectors can be used to derive the ratio of the vibration amplitudes (x_1 / x_2) of the two resonators, which is an alternative method of measuring the perturbation.

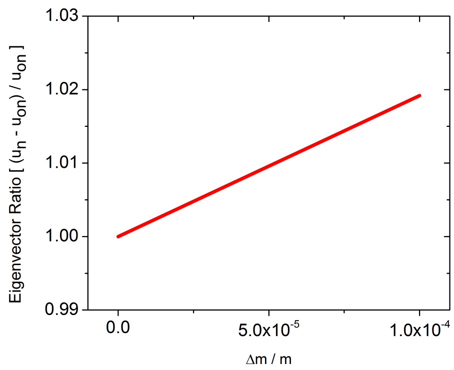

Figure 2: *Theoretical change in mode shape for a mass perturbation*

Finite-element method (FEM) simulations have been performed in *CoventorWare* for the two coupled beams model. A modal analysis of the two coupled rectangular beams model has been performed. The mode shapes (ratio of the amplitudes x_1 and x_2) have been extracted as shown in figure 3 and the change in the shape has

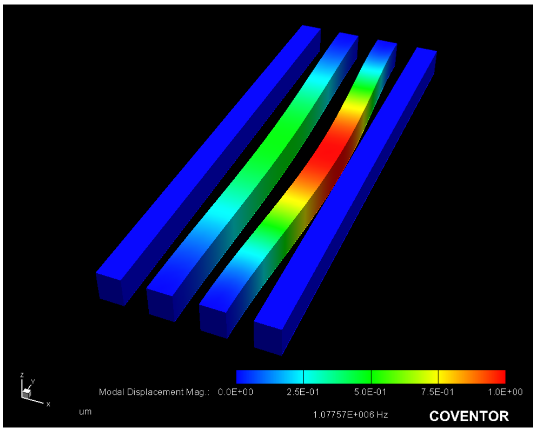

Figure 3: *FEM simulation of normalised mode-shape of disordered electrostatically coupled beams*

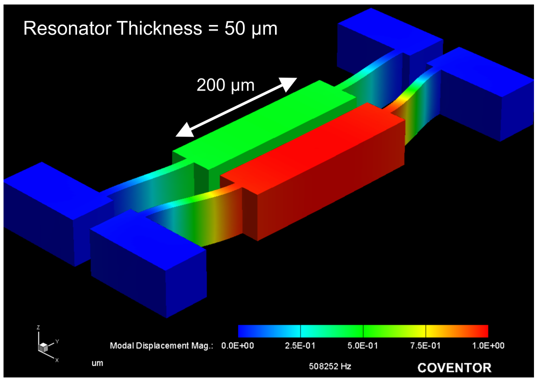

Figure 5: *FEM simulation of normalised mode-shape of disordered coupled resonators of proposed fabrication design*

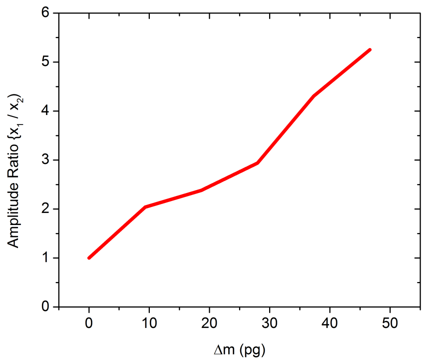

Figure 4: *FEM simulation change in mode shape for a mass addition to one resonator in 2-DOF system*

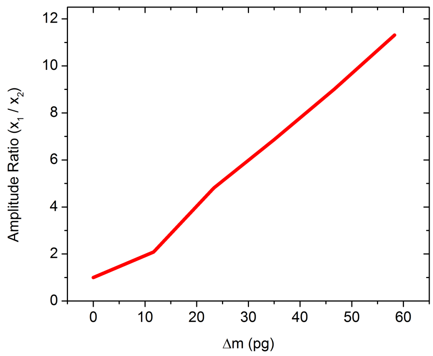

Figure 6: *FEM simulation change in mode shape for a mass addition to one resonator in proposed fabrication model*

been plotted as a function of the added mass up to 46 pg, as shown in figure 4

The results show that *CoventorWare* can be used effectively to model the mode-localisation effect. FEM simulations more accurately model the changing shape of the coupling gap as the beams bend during oscillation, yielding a more accurate result that can guide real-world design and fabrication.

A further model has been used for FEM simulations with a design that has a larger surface area for functionalisation (Figure 5). It is our intention to fabricate a device of this design. The mode shape variation as a function of the added mass, up to 58 pg, is shown in figure 6.

To compare with a previous result [7], which used a resonant shift sensor and showed a sensitivity of 50 pg/Hz (a percentage change in frequency of 0.003%), our simulation shows that an additional mass of 50 pg should cause a variation in the ratio of the modal amplitudes from 1:1 up to approximately 10:1, a ten-fold increase. The fabrication of actual devices of the design in figure 5 is planned and the measurement set-up will be optimised to achieve the best measurement resolution possible in order to detect the smallest possible mass.

IV – 4-DOF Coupled Resonator Sensor

As a further improvement to the coupled resonator system, a 4-DOF system has been considered for mass sensing. The lumped mass model of the system is shown is figure 7, and in this case each resonator is coupled to two other adjacent resonators.

For the symmetric case where all the masses $m_{\mathrm{i}} = m$, $k_{\mathrm{i}} = k$ and $k_{\mathrm{cij}} = k_{\mathrm{c}}$, the mass and stiffness matrices are given by

$$M = \begin{bmatrix} m & 0 & 0 & 0 \\ 0 & m & 0 & 0 \\ 0 & 0 & m & 0 \\ 0 & 0 & 0 & m \end{bmatrix}$$

$$K = \begin{bmatrix} k+k_c & \frac{k_c}{2} & 0 & \frac{k_c}{2} \\ \frac{k_c}{2} & k+k_c & \frac{k_c}{2} & 0 \\ 0 & \frac{k_c}{2} & k+k_c & \frac{k_c}{2} \\ \frac{k_c}{2} & 0 & \frac{k_c}{2} & k+k_c \end{bmatrix} \tag{11}$$

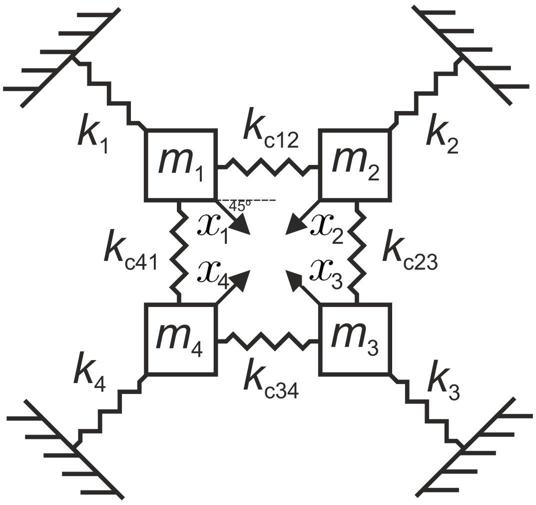

Figure 7: *4-DOF lumped-element model*

Introducing a mass perturbation to resonator 1 and taking $m = k = 1$, the amplitude ratios of the resonators are shown in figure 8. It is observed that a general improvement in terms of the system sensitivity can be obtained for the 4-DOF system versus the 2-DOF system.

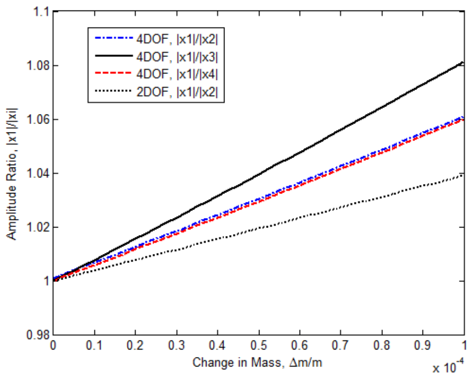

Figure 8: *Amplitude ratio versus mass perturbation*

V – Functionalisation for Biological Sensing

In a practical bio-sensor, the microstructure needs to be functionalised so that the biological element is attracted to and binds with the surface [8]. A previous study [9] describes a silicon cantilever resonator that has been functionalised to attract the bacteria *Listeria innocuous*. The cantilever has been functionalised by dispensing the bacteria antibody over the resonator surface using micropipettes. Another study [10] showed a cantilever array functionalised to detect the growth of *Escherichia coli*. The cantilevers have a length of 500 μm, a width of 100 μm and a thickness of 7 μm. They have been coated in the hyroxyl group Agarose using microcapillaries.

For coupled microresonators, only one of the two structures needs to be functionalised. To do this, it is proposed to use micropipettes to precisely coat one of a pair of closely spaced resonators with functional material. A device of the design in figure 5 will be used as the large surface area at the centre of the resonator will aid successful functionalisation.

VI – Conclusion and Future Work

The behaviour of electrostatically coupled microresonators has been investigated as the first stage in the design process of novel biological sensors. Mathematical and FEM models have been set-up to analyse these microresonator sensors.

The authors intend to fabricate actual coupled-resonator devices and characterise them. Both 2-DOF and 4-DOF coupled resonator sensors will be implemented using a silicon-on-insulator (SOI) process. Techniques will be developed to enable the functionalisation of the device so that a biological element is attracted to only one of the coupled resonators, allowing for the realisation of a bio-sensor based on the mode-localisation effect.

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