Optimal Design of Coupled Microelectromechanical Resonating Arrays for Mass Sensing

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Abstract: Microelectromechanical coupled resonating arrays are being used for detecting biological and chemical analytes through mass sensing. Such arrays of perfectly identical resonators can be considered as periodic, ordered, non-localized systems. The change in the eigen parameters of the system upon mass or stiffness perturbation is a measure of the amount of perturbation. An attempt has been made in this article to investigate the dependence of mass sensitivity on the number of resonators in the system and whether it depends on the resonator which is perturbed and the eigenfrequency which is observed. Its dependence on the coupling strength was also observed. Using first order perturbation techniques, an approximate expression for eigenvalue sensitivity values was derived. Based on this expression, the authors predict an optimal configuration to be used for mass sensing. In the end it was observed that the eigenvector sensitivity values for weakly coupled resonating arrays far surpass the eigenvalue sensitivity values for strongly coupled resonating arrays. All numerical results were subsequently verified by performing FEM analysis in COMSOL Multiphysics.

Keywords: Coupled Resonating Array (CRA), Eigenvalue, Eigenvector, Perturbation, Sensitivity

1. Introduction

Recently, there has been considerable interest in the use of micro- and nanoscale structures as sensing devices. The research has especially focused on micro- and nano-cantilevers and their arrays. Due to their small size, these devices have increased resonance frequencies and an increased sensitivity to external inputs or changes in the system. The superiority of dynamic devices such as micro- and nano-resonators over static devices has already been established. Such resonating devices have found applications as pressure sensors, mass sensors, charge sensors, force sensors etc. These devices either measure the change in resonance frequency [1] or the change in mode shapes [2] upon perturbation. This change is a direct measure of the level of perturbation.

Some researchers have successfully used coupled resonating arrays (CRAs) as sensing devices. Most of these techniques involve perturbing one of the resonators and sensing the change in the system resonance frequency. A pre-condition to this approach is that perturbation of a single element must result in significant change in the system resonance frequency. This is possible when eigenmodes are fully localized, such that each mode shape is dominated by the motion of a single array element. The changes in other modes of the system are negligible only if the inter-coupling strength is sufficiently small. However, we consider the case of non-localized (or at least incompletely localized) CRA with strong inter-coupling, as this offers distinct advantages as far as eigenvalue sensitivity is concerned. Some techniques also focus on observing the change in eigenmodes of a weakly coupled array, which is initially non-localized.

The current research focuses on increasing the sensitivity of these devices. Davis *et al.* [3] showed that nanocantilevers based on aluminum had higher potential mass sensitivity than silicon nanocantilevers, when used as dynamic sensors. Sharos *et al.* [4] showed that mass sensitivities of the torsional and lateral mode frequencies are an order of magnitude greater, and their *Q* factors significantly higher, than that of the conventionally used fundamental bending mode. Spletzer *et al.* [2] suggests that observing the relative changes in mode shapes of weakly coupled resonating arrays may prove to be more beneficial than observing the eigenfrequencies. Zhao *et al.* [5] reported a 3DOF resonator array used as a stiffness sensing device with the change in modal amplitude ratio being used as the output sensing parameter. He claimed an increased sensitivity (49 times increase) in the stiffness sensitivity compared to existing state-of-art 2DOF resonator arrays.

This article tries to answer some fundamental questions. For instance, an increase or decrease in the mass of one array element results in a change in all natural frequencies and mode shapes of the system. However, which of the array element should be perturbed with mass and which of these frequencies should be observed in order to detect the mass is the question. Another question which might strike the reader is, whether there are an optimal number of elements to be used in the array. The authors also investigate the dependence of eigenvalue and eigenvector sensitivity values on inter-coupling strength.

The article begins with a theoretical model of the multi-DOF (degree-of-freedom) resonator model. Numerical simulation results are presented next. Finite element method (FEM) simulations were performed in COMSOL Multiphysics and the results for the same are presented in the next section.

2. Mathematical Model

A coupled resonating system can be modeled as a mass-spring-damper system. However, the mass used in the model is not the actual mass of the resonator, but the dynamic, effective mass of the resonator. For instance, the effective mass of each resonator in case of coupled resonating cantilevers is usually taken to be 1/4th of the actual mass of the cantilever resonator. Mass-spring-damper representation of a 2-DoF CRA is shown in figure 1. k_1 represents the effective stiffness of the first resonator and k_2 represents the effective stiffness of the second resonator. k_c represents the stiffness of the coupling beam. We consider a system which is identical. This means that the effective mass, effective stiffness of all resonators in the array is same. Further, the effective stiffness of all coupling elements in the system is also same. Thus,

$$k_1 = k_2 = k$$
$$m_1 = m_2 = m$$

In our hypothesis, we have considered the damping to be negligible. Hence, the damping coefficients are considered to be zero. However, this may not be always true. For instance, squeeze film damping may be a major problem in some cases. For a multi-DOF system,

$$k_{c1} = k_{c2} = ... = k_c$$

Coupling coefficient is defined as the ratio of stiffness of the coupling element to the stiffness of the resonating element. It is thus non-dimensional in nature.

$$\alpha = \frac{k_c}{k} \tag{1}$$

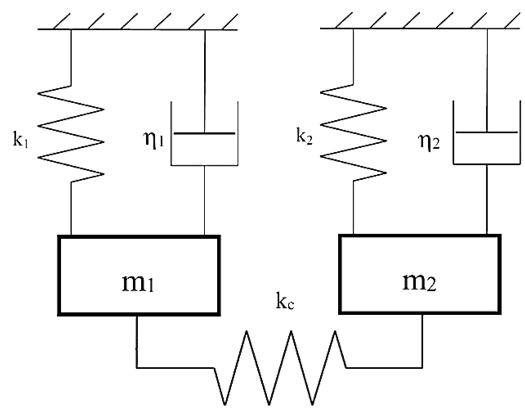

Figure 1. Mass-spring-damper representation of a 2DOF coupled resonating array

The vibratory motion of the CRA can be modeled as an eigen problem. In practice, the vibrations would be forced vibrations. The resonators would be electrostatically actuated by an AC voltage of the same frequency as the natural frequency of the structure. However, here the eigen analysis has been performed for free vibrations of the CRA. For a CRA consisting of *n* identical resonators, equations of motion may be written as:

$$\begin{aligned}
&m_1\ddot{x}_1 + kx_1 + k_c(x_1 - x_2) = 0\\
&m_2\ddot{x}_2 + kx_2 + k_c(x_2 - x_1) + k_c(x_2 - x_3) = 0\\
&.\\
&.\\
&m_{n-1}\ddot{x}_{n-1} + kx_{n-1} + k_c(x_{n-1} - x_{n-2}) + k_c(x_{n-1} - x_n) = 0\\
&m_n\ddot{x}_n + kx_n + k_c(x_n - x_{n-1}) = 0
\end{aligned}$$

Employing a harmonic solution of the form $x_n = X_n \sin \omega t$, these differential equations can be reduced to the following eigenvalue problem,

$$[K]\{X\} = \lambda[M]\{X\} \quad (2)$$

Here, M denotes the effective mass matrix.

$$[M] = diag(m, m, ..., m) \quad (3)$$

Also, K denotes the tri-diagonal stiffness matrix.

$$K = \begin{bmatrix} k+k_c & -k_c & . & 0 \\ -k_c & k+2k_c & -k_c & 0 \\ . & . & . & . \\ 0 & 0 & -k_c & k+k_c \end{bmatrix} \quad (4)$$

$\lambda = \omega_n^{\ 2}$ are defined as the eigenvalues of the system and $\{X\}$ are defined as the corresponding eigenvectors. ω_n itself is known as the fundamental frequency of the system and is given by the following expression:

$$\omega_n = \sqrt{\frac{k}{m}} \quad (5)$$

Thus, the multi-resonator vibration is characterized by a set of n eigenvalues, $\lambda_r, (r = 1, 2, ..., n)$ and n eigenvectors $\{X\}_r, r = 1, 2, ..., n$. The set of eigenvalues form a spectrum, and it can be shown that:

$$\frac{k}{m} \le \lambda_r < \frac{k}{m}(1 + 4\frac{k_c}{k}) \quad (6)$$

To study eigenspectrum characteristics and its dependence on resonator parameters, the eigenvalue problem is normalized as:

$$\begin{bmatrix} 1+\alpha & -\alpha & . & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ . & . & . & . \\ 0 & 0 & -\alpha & 1+\alpha \end{bmatrix} \{\phi\} = \bar{\lambda}[I]\{\phi\} \quad (7)$$

Here, $\bar{\lambda} = \lambda \frac{m}{k}$ is the non-dimensional eigenvalue. As stated before, α is a measure of inter-coupling strength. $\alpha \ll 0.1$ can be considered as weak coupling and $\alpha \ge 0.1$ can be categorized as strong coupling. A coupled resonating array is a periodic ordered system. Disorder can be introduced in this ordered system either as a perturbation in mass or a perturbation in stiffness. We consider perturbation in mass here. The above eigen analysis was for an unperturbed system. Suppose a mass, Δm (say of a bio-molecule) is added to one of the array elements. The eigenvalues of the system will now change. If the k^{th} resonator is perturbed and the i^{th} eigenvalue is observed, the corresponding eigenvalue sensitivity is defined as:

$$s_{ki} = \frac{1}{\delta_k} \frac{\left|\bar{\lambda}_i - \lambda_i\right|}{\lambda_i} \quad (8)$$

Here, $\bar{\lambda}_i$ is the new system eigenvalue. We define another parameter δ as,

$$\delta = \frac{\Delta m}{m}$$

The eigenvalue problem after mass perturbation is shown below. It is assumed that the mass has been added to the last array element. As you can notice, the symmetry of the problem has broken due to the added mass.

$$\begin{bmatrix} 1+\alpha & -\alpha & . & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 \\ . & . & . & . \\ 0 & 0 & -\alpha & 1+\alpha \end{bmatrix} \{\bar{\phi}\} = \bar{\lambda} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & . & . \\ 0 & 0 & . & 1+\delta \end{bmatrix} \{\bar{\phi}\}$$

We can expand the modified eigenvalues as a perturbation expansion of δ [6,7]. Assuming δ to be very small, we can neglect the higher order terms of this expansion. It has also been assumed that eigenvectors of the system do not change by a large factor upon being perturbed by a small mass element. Thus we arrive at the following expression.

$$\bar{\lambda}_i = \lambda_i + \lambda_i \delta_k \phi_{ki}^{\,2}$$

Upon rearranging the terms of the above expression, we arrive at the following result.

$$\frac{1}{\delta_k}\frac{\left|\bar{\lambda}_i - \lambda_i\right|}{\lambda_i} = \phi_{ki}^{2} = s_{ki} \qquad (9)$$

If the resonating array is an *n*-DOF system, any of the *n* resonators may be perturbed and any of the *n* eigenvalues may be measured. This gives rise to *n* x *n* possibilities, which are represented in an *n* x *n* eigenvalue sensitivity matrix. What the above expression means is that the eigenvalue sensitivity matrix may be approximated by the square of the original eigenvector matrix. This conclusion has another far-reaching consequence. We know that for a particular value of *k*, i.e. for mass addition on a particular resonator,

$$\sum_{i=1}^{n} \phi_{ki}^{2} = 1$$

Hence, the summation of all eigenvalue sensitivity values for mass addition on a particular resonator would also be equal to a constant (theoretically equal to unity). In actuality, the constant would not equal unity since the expression is a theoretical approximation. Thus, we can conclude that, if the number of elements in CRA increases, the maximum eigenvalue sensitivity will reduce, in order to keep the summation constant.

3. Numerical Simulation

The CRA was modeled as a mass-spring system in the previous section. The eigen problem for the system was numerically solved in MATLAB and the results and the conclusions which were derived are presented in this section. Each resonator was mass perturbed and change in each of the *n* eigenvalues was found out. Thus, the *n* x *n* eigenvalue sensitivity matrix was successively populated. A theoretical eigenvalue sensitivity matrix was also found out, based on the expression derived in the previous section. The eigenvalue sensitivity matrix is represented as a gray scale checkerboard plot. The row number in the checker-board representation represents the resonator which is perturbed and the column number denotes the eigenvalue which is examined. White color represents highest value of sensitivity and black color represents the lowest value of eigenvalue sensitivity. The sensitivity matrix for a 3DOF system has been shown in figure 2.

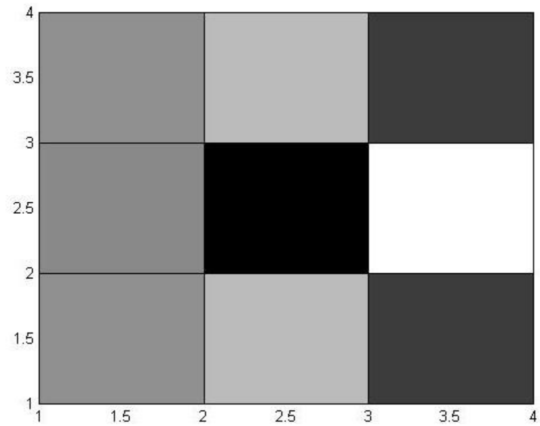

Figure 2. Eigenvalue sensitivity matrix for a 3DOF system

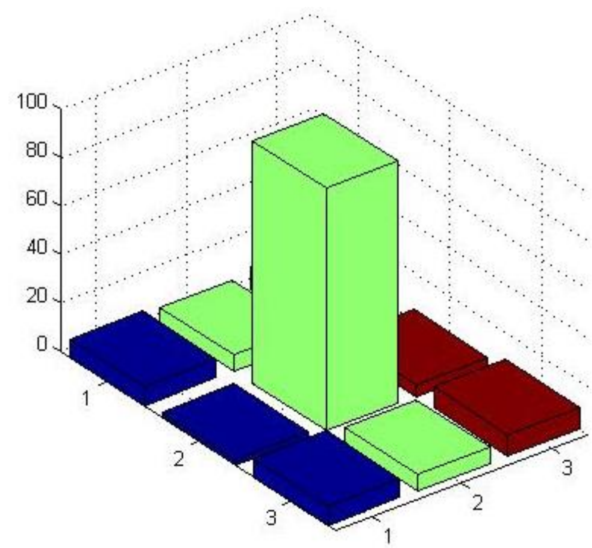

Figure 3. Error matrix for a 3DOF system

The theoretical eigenvalue sensitivity matrix has been represented in figure 2. This would be used in calculating the mass. This differs from the actual eigenvalue sensitivity matrix. Hence, the calculated mass would be different than the actual mass. The error matrix is defined as the relative difference between theoretical and actual eigenvalues. Lower the error of the configuration used, more accurate is the estimate of the added mass. This error maybe modeled as the measurement noise. Hence, the selected configuration should have high eigenvalue sensitivity, which is as close to the actual eigenvalue sensitivity as possible.

The authors also varied the number of the elements in the array. Highest value of eigenvalue sensitivity was found for a single DOF system. However, coupling the resonator offers many distinct advantages. When a single resonator is used, actuation, mass addition, sensing have to be performed on that resonator only. This is practically cumbersome. Further, coupling reduces the motional impedance of the structure, and thus the phase noise. The next best sensitivity (equal to 0.67) is achieved for a 3DOF coupled resonator array when the second resonator is perturbed and the third eigenvalue is examined. After $n=3$, the eigenvalue sensitivity goes on decreasing as the number of resonators in the CRA increases, as can be deduced from figure 4. For a given value of α, error increases as n increases. Hence, this proves that increasing the number of elements in the array offers no significant advantage as far as sensitivity is considered.

As α increases above 0.1, sensitivity increases and error decreases. As α decreases below 0.1, error increases. The measurement error can thus be said to be inversely proportional to α. For performing eigenvalue measurements, it is important that the system should be strongly coupled. Weak coupling of arrays affects the mode shapes drastically, and the previous assumption made by the authors does not hold. The measurement error was also found to be proportional to the added mass. Thus, the following relation has been derived.

$$e \propto \frac{\delta}{\alpha} \tag{10}$$

The authors also investigated the change in eigenvectors of a weakly coupled resonating array on addition of mass to one of the array elements. For a 3DOF system, the maximum value of eigenvector sensitivity was found to be 383.95. This represents an increase of three orders of magnitude compared to its eigenvalue counterpart.

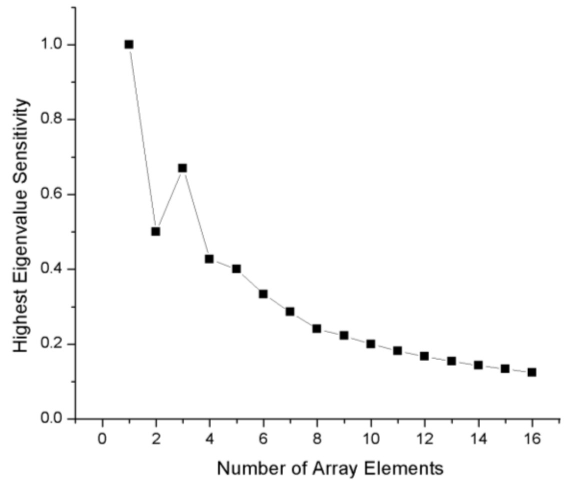

Figure 4. Variation of eigenvalue sensitivity with number of elements in the resonator array

4. FEM Simulation

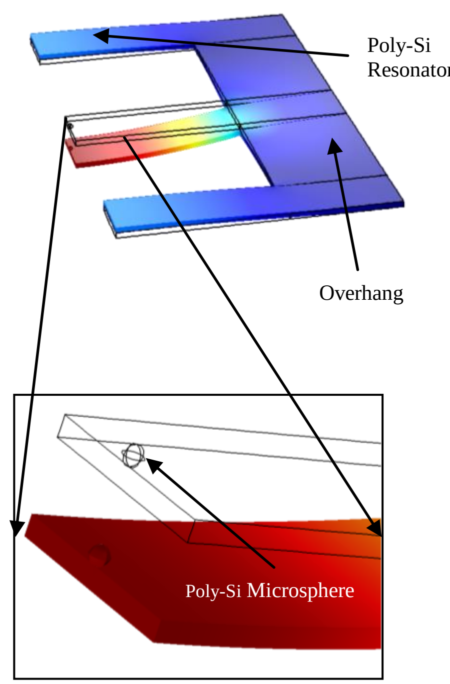

Figure 5. Mode shape of the 3DOF array after mass perturbation

As stated previously, the second best eigenvalue sensitivity was observed for the 3DOF system for the (2,3) configuration. FEM analysis of a poly-Si overhang coupled cantilever array was performed in COMSOL Multiphysics for validating this. The length, width and thickness of each resonator were 300 μm ,100 μm and 10 μm respectively. The edge to edge separation between two elements is 250 μm and the width of the overhang is 200 μm . A poly-Si microsphere weighing 1.22 ng, was used for perturbing the array. The microsphere may be of any composition, since the main concern here is its mass. The reader should take note, that for the mass-spring-damper model to be applicable, the perturbation should be at a single point, preferably at the tip of the cantilever resonator. The third eigenmode was considered and the second resonator was perturbed as shown in figure 5. As one can see, the mode shape is highly localized, due to the mass disorder introduced. Figure 6 shows the frequency response function of the 3DOF system before and after mass perturbation.

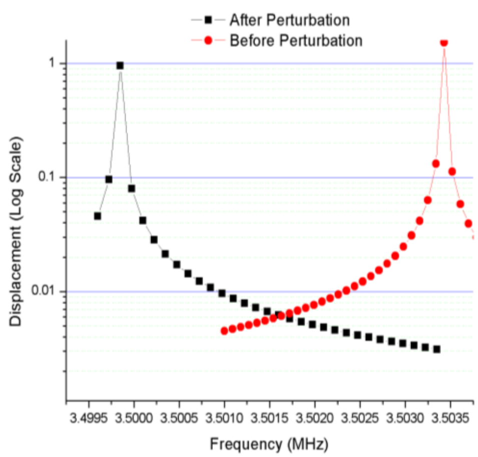

Figure 6. Frequency response function, before and after mass perturbation

The perturbation results in a frequency shift of 3584 Hz. Thus, the mass responsivity for the 3DOF system is 338.94 fg/Hz. This experiment was repeated for the 2DOF system, with all parameters remaining the same. The frequency shift observed in this case was 2037 Hz, and the resulting mass responsivity was 596.34 fg/Hz. For the 4DOF array, the frequency shift was a mere 1355 Hz, with the mass responsivity being 896.49 fg/Hz.

The eigenvalue sensitivity also depends upon the strength of inter-element coupling. In an overhang coupled cantilever array, the coupling strength depends on the width of the overhang. In the case of 4DOF system, when the width of overhang was halved, the frequency shift dropped to a mere 5 Hz, from the earlier 1355 Hz. The mass responsivity was found to be 242.95 pg/Hz, as opposed to the earlier figure of 896.49 fg/Hz.

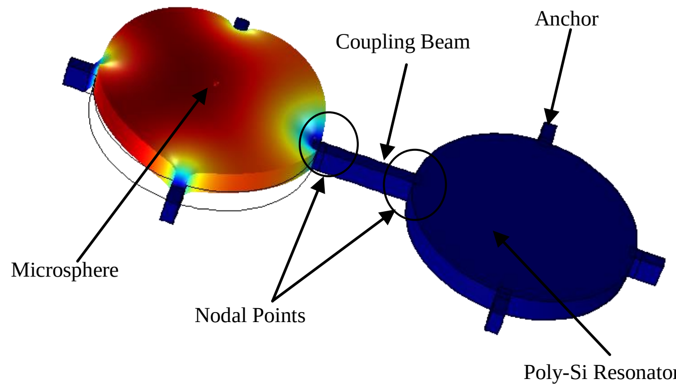

Figure 7. Poly-Si disk resonators, coupled at nodal points

Next, we consider two Poly-Si disk resonators, coupled together with a coupling beam, at nodal points. The radius of each disk is 5 μm , and the microsphere weighs 1.22 fg. The coupling coefficient is extremely high in this case, compared to the 2DOF overhang coupled cantilever array considered previously. Figure 7 depicts the first eigenmode of the array, after mass adsorption. As one may expect, the mode shape is highly localized. The frequency shift observed on adsorption of mass is 326.9 KHz. Compared to the 2DOF overhang coupled cantilever array, the frequency shift is orders of magnitude higher. The mass responsivity in this case is found to be 3.716 zg/Hz.

Change in the eigenmodes can also be a measure of level of perturbation. It was found that the change in eigenmodes is more pronounced when the array elements are weakly coupled to each other. This is due to the resonance localization effect, observed in weakly coupled systems. Electrical coupling is comparatively weaker than mechanical coupling. Corner coupled square plate resonators vibrating in Lamé mode, are another example of resonators weakly coupled to each other. Figure 8 shows two clamped-clamped poly-Si beams, electrically coupled to each other, through a minute air-gap between them. This 2DOF system is subjected to a potential difference of 10 V, by means of two rigidly bound electrodes on either side of the resonators. Here too, a poly-Si microsphere was used for perturbing the system. The authors consider the displacement amplitudes of the C-C beam, as an approximation of eigenvectors. For one of the observed modes, the relative change in system eigenfrequency was found to be 0.000383 %, while the relative change in the approximated eigenvector was found to be 1.6064 %. Thus, the relative change in eigenvector of this system was orders of magnitude higher than the relative change in system eigenfrequency.

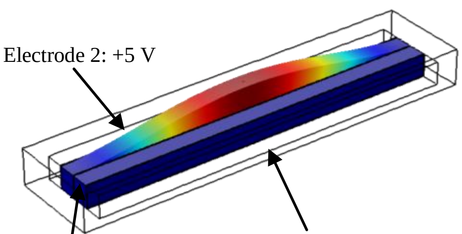

Figure 8. Electrically coupled C-C beams

5. Conclusions

The coupled resonating array was modeled as a mass-spring system. Based on first order perturbation techniques, an expression for eigenvalue sensitivity was derived. Based on this expression, the authors endeavor to predict an optimal configuration of the array. For a fixed value of coupling coefficient, eigenvalue sensitivity goes on decreasing, and error goes on increasing, with increasing number of elements in the array. Highest sensitivity for a 4DOF overhang coupled cantilever array was found to be comparatively lower than that for the 3DOF array. Apart from the number of elements in the array, eigenvalue sensitivity is also highly dependent on inter-element coupling strength. The eigenfrequency sensitivity of a 2DOF poly-Si disk resonator array (having a higher value of coupling coefficient) is found to be orders of magnitude higher than the sensitivity of a 2DOF overhang coupled cantilever array. The change in eigenvectors may also be examined, in order to gauge the level of perturbation. It is found that the relative change in eigenvector is many times higher than the relative change in the system eigenfrequency for a 2DOF system of electrically coupled C-C beams. All numerical simulations were performed in MATLAB, which were then substantiated by FEM simulations, performed in COMSOL Multiphysics.

In future, the authors would like to extend these ideas for stiffness sensing. In addition, the authors would like to fabricate these devices using 2D materials such as transition metal dichalcogenides which have unique mechanical properties.

6. References

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