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ON MASS SENSING USING MICRO/NANO RESONATORS - APPROACHES, CHALLENGES AND DIRECTIONS

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Abstract- Micro/Nano electromechanical systems based Mass sensors are being increasingly used for detecting very low masses, with significant applications in bio-sensing as well as environmental sensing. A number of different shapes, excitation mechanisms as well as materials have been suggested for these sensors. In addition, with reducing dimensions due to improvement in fabrication, these sensors have the potential to measure bacterial level masses. This paper reviews some of the research directions in this field. Various sensing and actuation strategies for these resonators are discussed. In addition, three important challenges, which have the potential of providing new directions of research are also explored. These include quality factor, increasing nonlinearity and coupling. Coupling of sensors can provide a unique opportunity to build several resonant sensors on the same chip and reduce the number of contacts required as well as the potential bandwidth

Index Words - Microelectromechanical systems, Mass sensors, damping, nonlinearity, coupled systems

I. Introduction

There has been an increased interest in making sensors, which utilise micoelectromechanical systems for measuring very low levels of mass or mass change [1, 2, 3, 4]. This has been further advanced by improvements in nano-fabrication processes as well as discovery of new materials like graphene recently [5], with claimed mass sensing abilities of zeptogram [6]. These highly sensitive sensors offer immense potential for biosensing in future. Various approaches have been used to measure mass with micro/nano devices, with resonator based techniques being one of the most frequently used ones. In this paper, we review the approaches to mass sensing using MEMS resonators along with various challenges being faced. Section II presents the analysis of using MEMS resonators as mass sensors. Section III describes various options available to a designer while designing such systems. Section IV explores three prominent challenges as well as opportunities with reduction in feature sizes of these resonators. Finally, section V provides the conclusion of the chapter.

II. Mass Sensing using resonators

To appreciate this measurement modality, let us consider a resonating mechanical structure. Physically, this could take any form including mechanical beams, free at one end or clamped at both ends or comb type structures. It could also have any sensing and actual mechanism including electrostatic, piezoelectric, thermal or magnetic. A lumped model for any such device can be expressed through the second order differential equation

$$m\ddot{x} + B\dot{x} + K_s = F \tag{1}$$

where m is the mass of the resonator, B is a damping factor which depends on the medium and K_s is the spring constant of the resonator. On application of a sinusoidal force with frequency ω and amplitude F_0, the response of the resonator can be obtained to be

$$x(t) = X(w)\cos{(wt - \phi)} \tag{2}$$

where the amplitude, $X(\omega)$, and the phase difference ϕ are [7]

$$\begin{aligned} X(w) &= \frac{F/m}{\left[(K_s/m - w^2)^2 + (\omega B/m)^2\right]} \\ \phi &= \tan^{-1}\frac{wB/m}{K_s/m - w^2} \end{aligned} \quad (3)$$

In absence of damping, the resonance frequency of this system can be simplified to

$$w_0 \approx \sqrt{\frac{k}{m}} \quad (4)$$

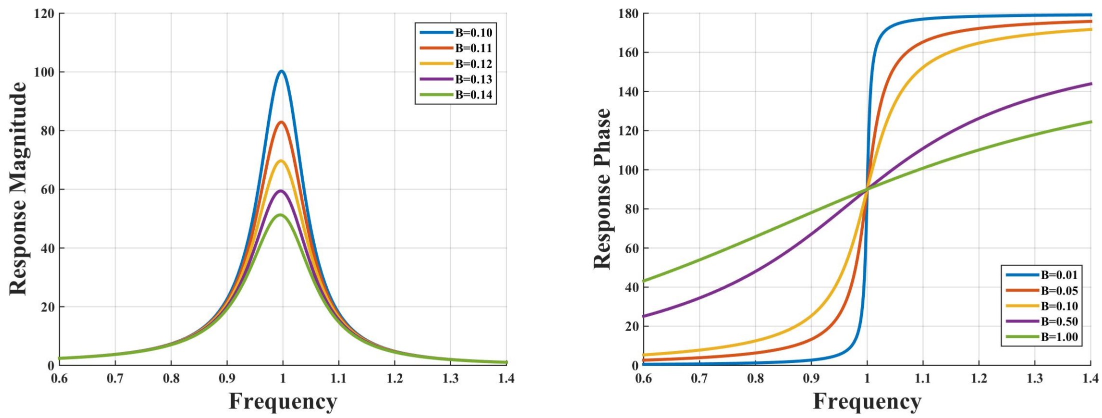

Figure 1: (a) Shifts in resonance frequencies of the system with increase in damping (b) Phase response of the system for different damping

The introduction of damping reduces the resonance frequency as shown in Figure 1, which presents the magnitude response of a normalised resonator ($K_s = 1, m = 1$) with different damping constants. It may be observed that for small changes in the damping, the resonance frequency can be assumed to be constant. In such a resonator, with change in mass of δm, the resonance frequency changes to

$$\begin{aligned} w_0^2 &= \frac{k}{m + \delta m} \\ &\approx w_0^2\left(1 - \delta m/m\right) \end{aligned} \quad (5)$$

Hence, the change in resonance frequency is approximately $w_0(\delta m/m)/2$. This simple equation illustrates the attractiveness of resonators for mass sensing. At one hand, the change in the resonance frequency is directly proportional to the change in mass. This is useful as frequency measurement techniques have been well established and noiseless measurements of sub-hertz resolution are regularly carried. The phase response of the system for varying damping, as shown in Figure 1(b) is very useful here, as the response undergoes a sharp 90^o change at the resonance frequency. This significantly simplifies the instrumentation required, as rather than designing a peak amplitude detector, one can simply use a phase-locked detector and monitor any change in the resonance frequency, and hence any change in the mass of the system.

Second and more importantly, reducing the geometry of the devices would lead to reduction in its mass, m, and therefore would improve the mass resolution of the sensors. With manufacturing dimensions reaching that of nano-meters, it is possible to make mass sensors with the capability of measuring masses of pico and femto-grams levels. It is this reducing resolution, which is attractive for biosensing, as with these resolutions, we are now reaching the mass domains wherein small quantity of mass relevant to biological materials can be measured. With an understanding of the physical foundation, we can now appreciate various physical options we have in making biologically sensitive MEMS resonators.

III. DESIGN CHOICES

The measurement principal described in the previous section provides a number of opportunities for designing mass sensors. These also provide a number of different design choices, some often linked with one another. First, a designer has to select the material from which the resonator will be made. This often also determines the materials which can be measured through the resonating system. In addition, it is possible to functionalise the resonators and hence increase the types of materials which can be measured. Once a material has been determined, once has to decide about the excitation and measurement systems. These could include a number of different modalities including electrostatic, magnetic, thermal or piezoelectric systems. Finally and often related to the excitation system, one has to design the resonator shape. This section provides a review of these potentials without claiming to describe all potential designs, as these will be difficult if not impossible to explain in a single paper.

III.I. Material and Measurand

Most micro/nano resonators utilise resonating structures made of biologically neutral materials. For example, silicon or silicon dioxide is often preferred due to well-established micro/nano fabrication facilities available on account of integrated circuit fabrication. Furthermore, silicon is also very well studied and hence there is a good availability of models in various simulation environments. The other options in a standard micro/nano fabrication process are to use available metal including aluminium, copper, silver or gold. Polymers of different types have also been used to make inexpensive resonators. Recently, new materials like graphene have shown potential to make very small resonators thereby further enhancing the resolution of the sensors [5].

However, most of these materials do not react well or react to a very few biochemical substances. This means that by themselves, they cannot act as biosensors. However, suitable functionalization with a reagent can enhance their bio-selectivity. There is a large number of reagents-measurand pair, which can be used to functionalize the micro/nano resonator, a full description of which will take significant space and is beyond the scope of the paper. Nevertheless, functionalization is a significant challenge for most resonator based sensors, including mass sensors. At one hand, the dimension of the resonating structure is reducing to increase the mass sensitivity. This means that the functionalisation area is being reduced. Furthermore, the functionalization step is often not part of the regular micro/nano fabrication. This means that it is carried out separately using a material dependant process. This also means that this extra step often does not scale with the micro/nano fabrication, thereby introducing a challenge in suitable functionalization. A suitable solution to this challenge would be to integrate the functionalisation process with fabrication. However, there has been limited success in this till date.

III.II. Actuation and sensing mechanism

Once all materials have been identified, the next task would be to select a suitable actuation and sensing mechanism. Resonators are passive devices and hence they require application of a force to induce resonance in them. Simultaneously, a mechanism is required to detect the resonance in the system. The choices available to a system designer here are limited, yet require careful consideration depending upon the material selected as well as the nature of the end-product designed. Many a times, the excitation as well as the sensing mechanism could be the same; however, it is also possible to have different mechanisms for actuation and sensing.

Different forces including that of thermal, magnetic, electrostatic and piezoelectric could be used for excitation of the resonators. Thermally excited resonators act by passing a current through the device, which produces heat on account of the inherent electrical resistance of the device [8, 9]. Thermal actuation can provide large actuation forces for low electric voltage. However, the thermal resonators are often slow actuators suitable only for very low frequency applications. Further, due to thermal actuation, the parasitics and the ohmic loss is quite high and the overall quality factor of the resonator reduces with time. Resonators designed from magnetic materials can be magnetically actuated [10]. It eliminates the effects of charging or stiction in small gaps often found in other actuation mechanism [11]. However, it is difficult to miniaturise and often prone to external magnetic and electric forces.

Another technique that has been used to actuate the mass resonators is to use a piezoelectric excitation. As one approach, travelling waves can be developed in a small slab of a piezoelectric film and the changes in mass can be detected by observing its propagation characteristics [12]. As another approach, one can use piezoelectric forces to just excite the sensor and measure through any other means. For example, Kumar and Bhaskaran utilise changes in resistance to measure resonance while Choubey and co-workers have utilised optical means to measure from the sensor [13]. As the resonators move, high speed imaging or vibrometry can be deployed to measure resonance. Measuring in-plane resonance, however, is often very difficult. Furthermore, integration of optical measurement system with the MEMS device is often very challenging. In addition, piezoelectric transduction requires integration of piezoelectric thin film with the micromechanical elements. Such integration usually results in a drastic decrease in the resonator quality factor and could be impractical during the fabrication.

Yet another approach to excite resonators is to use electrostatic forces. These often utilise capacitive devices, wherein the capacitance between two parts of a resonator or between resonator and a fixed measuring surface changes with the movement of device. Often the capacitance change introduced by a single capacitor is not enough to introduce large enough change in signal level. Hence, large parallel structures with a number of a capacitances are often used as shown in Figure 2[14].

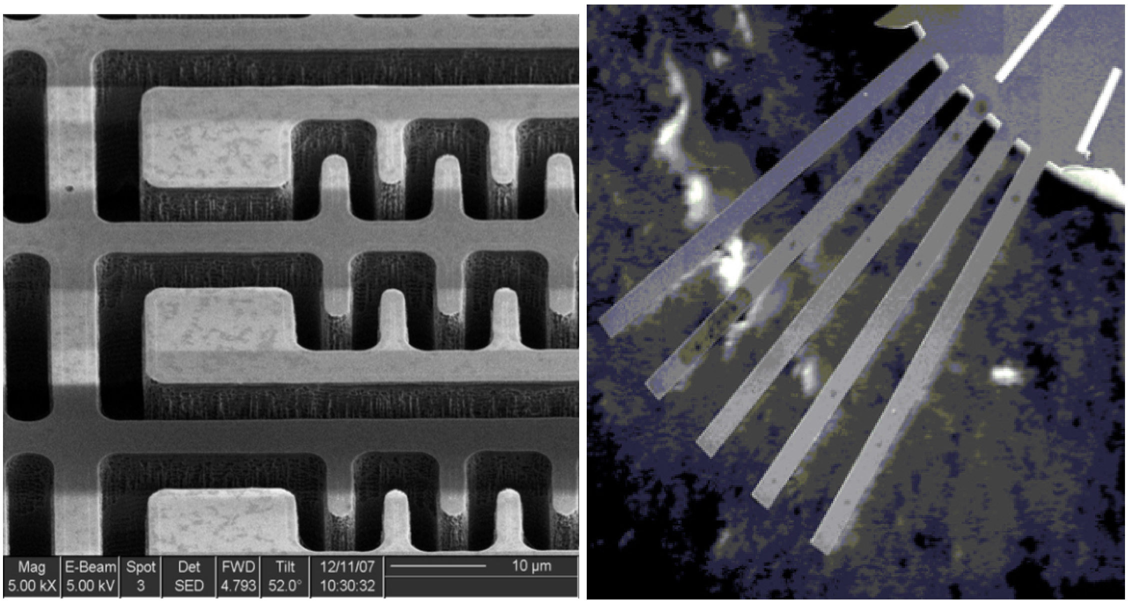

Figure 2: (a) Comb resonators showing parallel capacitances increasing the throughput of the system (b) An array of simple resonators, which move out of plane

III.III. Resonator Shapes

As there are no standard structures in electro-mechanical systems, there is a wide variety in physical shapes, which have been used as resonator structures. A complete review is beyond the scope of this paper. However, we have already seen the use of comb structures. The physical shape of the structure is often determined by the excitation and measurement system, ease of manufacturing, damping, the mode in which measurement is required as well as often the intellectual property of previous designs. The simplest resonating structure would be a simple beam, anchored at one side. Figure 2(b) shows one such array of simple cantilevers wherein the resonant motion is out of plane of the resonators (vertical to the substrate) [13]. These structures generally excite the first mode of resonance. As an alternative, structures which are clamped at both ends [5] or at multiple ends have also been used. Often low damping or better frequency response and high sensitivity is claimed from these structures [15, 16]. In addition, circular structures or structures which utilise rotational resonance have also been used [17].

IV. Design Challenges and opportunities

We have explored various design choices in typical micro/nano resonator based sensors. We will now consider three important design challenges and related opportunities when designing these sensors at the nano-scale.

IV.I. Quality Factor

In all of our discussions till now, we have assumed that the resonators have high quality factors and hence very low damping. This increases the amplitude at resonance, reduces the bandwidth and simplifies the circuitry required to measure the response. To obtain high quality factor, one needs to reduce the different sources of damping in the system. Damping is a collective measure of various dissipation mechanism inside the resonator as well as its surrounding. A number of factors affect the damping in a resonator. These include the material of resonator, its shape, its operation mode and most importantly its environment [18].

The interaction between the structure of the resonator and its surrounding medium is one of the foremost sources of damping, which is primarily due to the viscous damping by the fluid surrounding the resonator. In addition, squeeze-film damping has also been known to affect MEMS resonators [19]. A very simple technique, often employed in a number of experiments with MEMS resonators to reduce the effect of damping, is to operate the device in very low air pressure thereby reducing the viscous damping. While this does indeed reduce the damping, it often fails to imitate the actual operational conditions. In addition, material damping also plays a significant role in the operation of MEMS resonators. This often arises due to thermoeslastic damping as well as internal friction due to crystal defects.

Studies have been reported which aim to either reduce the dissipation mechanism in the resonators or increase the available energy [20]. In addition, a simple electronic technique to improve the quality factor of single resonators is to provide electronic feedback and reduce the damping parameter as [21]

$$m\ddot{x} + B\dot{x} + K_s x = F + B_{FB}\dot{x} \tag{6}$$

In any resonator system, either the displacement, x or the velocity $\dot{x}$ of the resonator is measured. It is hence possible, to provide a parametric excitation using an external amplifier, which provides a gain of B_{FB}. This will effectively reduce the effect of B in the resonator expression and hence increase the quality factor.

However, when designing such systems, one has to ensure that the resultant damping $B - B + FB$ does not become negative, as this would introduce unwanted oscillations in the system and would lead to significant instability. To appreciate the difficulty in designing such feedback system, it is worth exploring a typical normalised system with very low quality factor and hence high damping. To increase the quality factor by three orders of magnitude in a system of normalised damping B of 1, one has to utilise B_{FB} of 0.999 to lead to resultant damping of 0.001. However, an error due to noise or otherwise of more than 0.1% in the feedback path would lead to instability in the system. Hence, the feedback network has to be carefully designed.

With biological mass measuring often utilised in liquid medium with unknown priori damping, quality factor control becomes even more challenging. The feedback network, hence has to be designed with an automatic gain control mechanism. Furthermore, liquid media also introduce second order nonlinearities on account of the viscosity as surface tension in the system. This further complicates the design of the feedback mechanism. Nevertheless, an electronic feedback can be a very simple mechanism to increase the quality factor of most resonating biosensors.

IV.II. NONLINEARITY

Our discussion till now has been limited to linear sensors however as the size of individual resonators reduces and the force applied does not reduce in the same proportion, these sensors start showing increasing nonlinearity. This poses significant challenge all the sensor design as practically most design principles as well as the related signal conditioning circuits are often for linear sensors. The first non linearity to be observed in mechanical resonators is often the Duffing nonlinearity as per the following expression [22, 23].

$$m\ddot{x} + B\dot{x} + K_s x + K_d x^3 = F \tag{7}$$

Where, K_d can be negative or positive depending upon the design of the resonators. Figure 3 depicts the effect of Duffing type damping on the frequency response of a resonator.

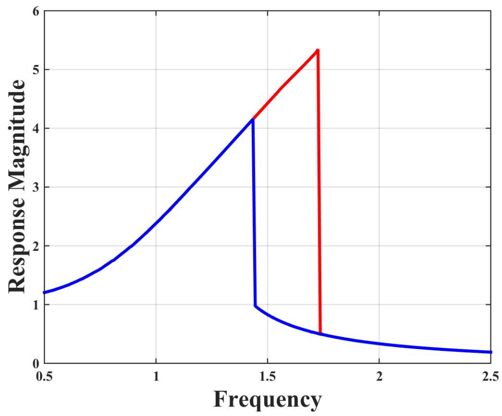

Figure 3: Effect of Duffing nonlinearity on resonator performance. The red line shows the forward sweep, while the blue line shows the reverse sweep of frequency in a Duffing resonator

Two important factors are worth noting in the response of the system. One, unlike the smooth response of a resonator, the resonator's response shows sharp jumps at very small change in the excitation frequency. Second, the frequency response shows a hysteresis and the frequencies at which the magnitude response jumps depends upon whether the excitation is increasing or decreasing. Hence, the techniques used for linear resonators like monitoring the resonance frequency alone are not sufficient, once the resonators start being affected by nonlinearity.

In addition to the nonlinearity in the spring constant, some systems have also reported nonlinearity in the damping parameter of a resonator. Once again, the first nonlinearity to be observed in damping is the third-order nonlinearity, often modelled using the Van-der-Pol system [24, 25]

$$m\ddot{x} + B(1 + \nu x^2)\dot{x} + K_s x = F \tag{8}$$

The typical design approach with any systems showing nonlinearity is to ignore the nonlinearity and design resonators, which will be utilised at smaller applied forces, to ensure linear response. However, the linear region of response available in nano electromechanical resonators is shrinking as the dimension of individual resonators is being reduced. Hence, this increasing nonlinearity is introducing a significant challenge for designing low-dimensional resonators. Nevertheless, it also provides an opportunity as the nonlinearity can provide different and novel sensing paradigms. A simple approach to do so would be to operate the Duffing resonator at a point just around the frequency its magnitude response jumps. With a very small change in the mass, there will be a significant change in the response of the system. This will hence, increase the sensitivity of the resonator significantly. However, due to inherent noise in the system, it is often challenging to ensure the operation of resonators at this particular frequency.

As the resonators size reduces, the effective nonlinearity observed will increase even further. This will lead to introduction of even more complex terms in transfer function of the resonators. Complete description of these nonlinearities is beyond the scope of the paper; however, it is worth noting that though the increasing nonlinearity will lead to difficulties in designing simple linear systems, it has the potential of introducing a number of new sensing modalities, which may lead to innovating sensory solutions.

IV.III. MULTI-RESONATOR SYSTEMS

Our discussion has been limited to single resonators till now. Furthermore, the stated aim has been to make them as small as possible to increase the mass sensitivity. This means that that in modern micro- electromechanical sensors, it is possible to design more than one resonator on the same trip. However, this is generally avoided, as this may lead to parasitic coupling between the sensors and hence reduced sensitivity.

Nevertheless, this could provide two different potential approaches for improved sensing [1, 13, 26]. A simple approach could be to just make a large number of smaller resonators and add their output together. It is worth noting that that in any resonator based sensor, a substance is detected when it is absorbed on the surface of the sensor. However, the size of the absorbing material is smaller than that of resonator. This also means that the total surface of the resonator is not used to record the reagent. This suggests that rather than making one large resonator, it may be beneficial to make several small resonators and connect their outputs together. To further appreciate this system with a typical example, let us consider, a system of n mechanical resonators wherein the resonance frequency of each resonator is 20 KHz. The resultant expression of the system would be

$$nm\ddot{x} + nB\dot{x} + nK_s x = Stimulus \tag{9}$$

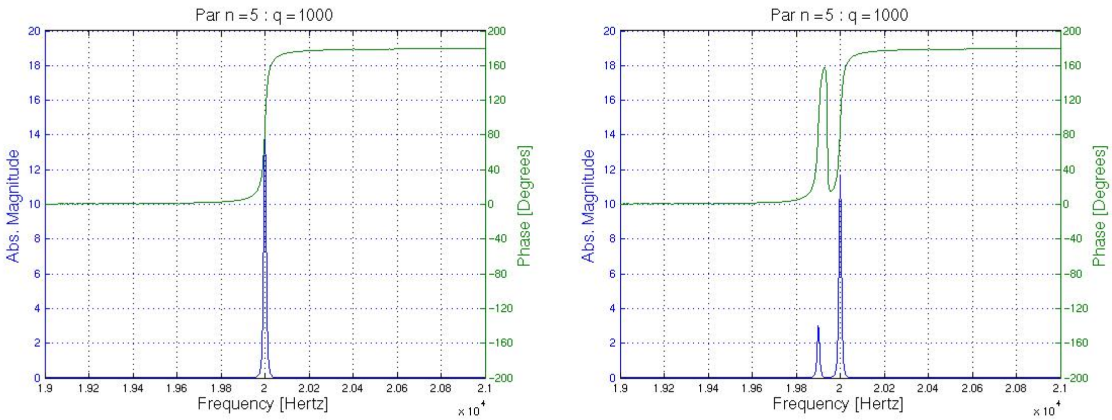

Figure 4: Response of a system of 5 identical resonators, each with a central frequency of 20KHz, when their responses are added together and when one of them changes its mass by 1%

The collective behaviour of the system can be shown by the response curve of Figure 4(a), wherein the response of all resonators (5 in this case) have been added together. When any one of the smaller resonator changes its mass, its resonance frequency will change by a factor of n compared to that of a single large resonator. The effect of this can be observed in Figure 4(b), wherein one of the resonator has changed its mass by 1%. A smaller peak due to this resonator can be observed. The system can be measured by either monitoring the collective behaviour or emergence of new resonant peaks.

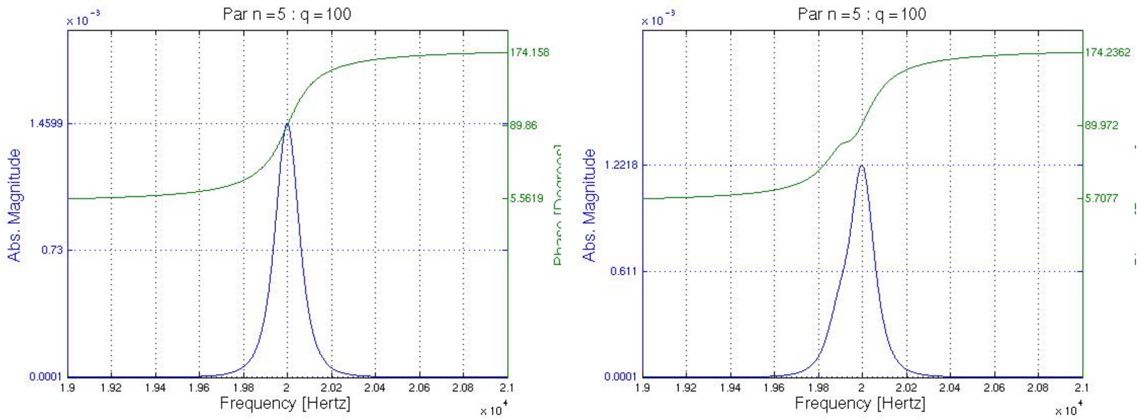

Figure 5: Response of a system of 5 identical resonators, each with a central frequency of 20KHz and high damping, when their responses are added together and when one of them changes its mass by 1%

Herein, we have assumed a high quality factor system; however, such a small change may be difficult to observe in systems with low quality factor as can be observed in Figure 5. Nevertheless, the system can still be used with lower resolution as shown in Figure 6, wherein the same system is simulated with a change in resonance frequency of 2%

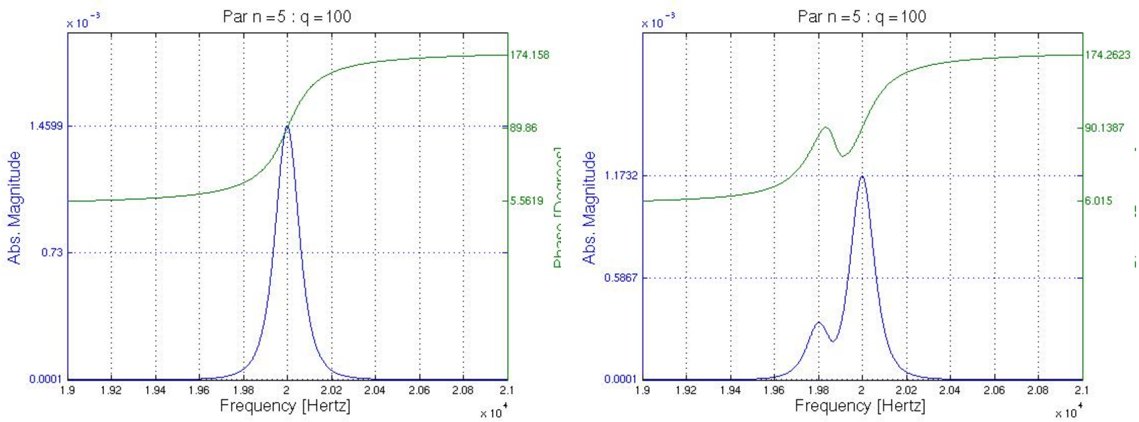

Figure 6: Response of a system of 5 identical resonators, each with a central frequency of 20KHz and high damping, when their responses are added together and when one of them changes its mass by 2%

IV.IV. COUPLED SYSTEMS

The aforementioned technique to add the response of individual resonators in a large system requires each resonator to be identical and hence are prone to process variations. Furthermore, they can also be affected by parasitic coupling between mechanical resonators due to substrate or even the excitation system. As a solution to this problem, one can purposefully couple the resonators. This would lead to a collective behaviour with several resonance peaks, the position of each of which will be determined by all resonators in the system. Such a system can be modelled by

$$
\begin{aligned}
m\ddot{x_1} + B\dot{x_1} + K_s x_1 + K_{cpl}(x_1 - x_2) &= Stimulus \\
m\ddot{x_2} + B\dot{x_2} + K_s x_2 + K_{cpl}(x_2 - x_1) + K_{cpl}(x_2 - x_3) &= 0 \\
m\ddot{x_2} + B\dot{x_2} + K_s x_2 + K_{cpl}(x_2 - x_1) + K_{cpl}(x_2 - x_3) &= 0 \\
\ldots & \\
m\ddot{x_i} + B\dot{x_i} + K_s x_i + K_{cpl}(x_i - x_{i-1}) + K_{cpl}(x_i - x_{i+1}) &= 0 \\
\ldots & \\
m\ddot{x_{n-1}} + B\dot{x_{n-1}} + K_s x_{n-1} + K_{cpl}(x_{n-1} - x_{n-2}) + K_{cpl}(x_{n-1} - x_n) &= 0 \\
m\ddot{x_n} + B\dot{x_n} + K_s x_n + K_{cpl}(x_n - x_{n-1}) &= 0
\end{aligned}
$$

In a matrix form, the system can be written as

$$
[M]\ddot{X} + [B]\dot{X} + [K_s]X = Stimulus \tag{10}
$$

The collective behaviour of such a system will have n resonance peaks where n is the number of resonators. These can then be measured from the response of any one of the resonators. To further understand the system, let us again consider a system with 5 coupled resonators, each with resonance frequency of 20 KHz. With a coupling constant of 10% of the spring constant of individual resonators, the collective eigenfrequencies of the system will be at 23074, 22267, 21227, 20347 and 20000 KHz. Figure 7 shows the collective behaviour of the system as measured from the response of each of the resonators.

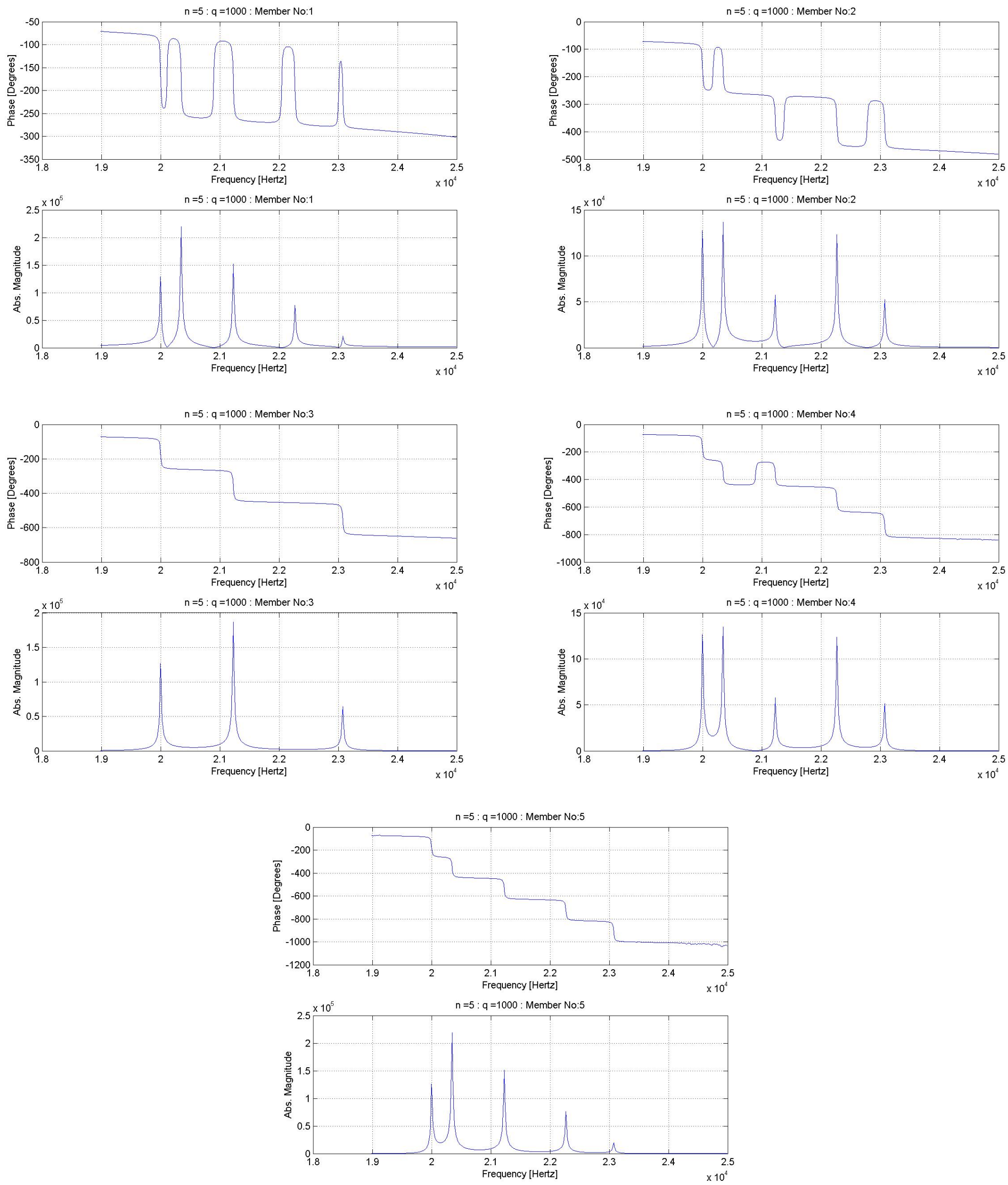

Figure 7: Modal response of all members of an array of resonators, each with a resonant frequency of 20KHz, coupled through a spring constant which is 10 times weaker than individual springs

Let us again introduce a change of 1 % change in mass of a resonator. The effect on the change of the collective response of the system now depends on which resonator has changed mass as shown in Table 1. The first row in the table denotes the modal frequency and the subsequent rows show the change in that particular frequency. In this system, observing the third or second mode is sufficient to determine which mass has changed if we can resolve up to 20 Hz. However, there is a symmetry and hence we can only faithfully record changed in one half of the array.

Natural Mode Changing Mass	23074	22267	21227	20347	20000
1	3.712	13.02	23.685	31.994	20.768
2	25.143	36.557	3.7098	12.233	19.296
3	39.873	0	38.211	0	18.858
4	25.143	36.557	3.7098	12.233	19.296
5	3.712	13.02	23.685	31.994	20.768

Table 1: Change in the modal frequency with change in a particular mass

Nevertheless, it is very easy to break the symmetry by changing any one of the resonators. For example, Table 2 shows the response of the same system when the symmetry has been broken by doubling the coupling constant of the spring attached to the last member. A properly designed divide and rule strategy should be able to determine the changing mass by maximum 3 measurements and frequency resolution of 15 Hz.

Coupling resonators provides a number of novel opportunities for system design. We have only explored linear arrays of resonators. Introduction of nonlinearity introduces a number of interesting design options. Arrays of linear resonators coupled nonlinearly would lead to Fermi-Pasta-Ulam type of systems which can be utilised in different modes for a number of potential novel sensing solutions. Nonlinear resonators coupled linearly or coupled nonlinearly have a very rick nonlinear behaviour [25]. Nonlinear dynamics is still an evolving field even in pure qualitative domain and hence, it has only found very limited application in MEMS resonator designs. With further understanding of the nonlinearity and coupling, a number of results from the Nonlinear dynamics field can be applied to MEMS resonator designs with enhanced sensing.

Natural Mode Changing Mass	23099	22329	21286	20369	20000
1	1.3143	10.609	23.842	34.803	22.611
2	10.502	44.392	10.939	9.9675	21.139
3	25.702	11.138	38.003	1.2277	20.871
4	39.218	11.726	1.2769	22.948	21.7
5	21.622	22.363	21.419	20.602	10.937

Table 2: Change in the modal frequency with change in a particular mass. The coupling constant attached to the last member has been doubled

V. Conclusion

Micro/nano resonators are increasingly being used for mass sensing, with particular importance in biosensing. In this paper, we have reviewed various design choices available to build and use these. As there are no standard shapes, sizes or actuation mechanism in the MEMS devices, a large number of mass sensors have been proposed; however, it is this diversity, which often leads to their poor ability to attract market popularity. We have also reviewed three principal design challenges when designing resonators at nano-scale. These include the low quality factor, increasing nonlinearity and increasing coupling between devices. However, these provide unique opportunities to utilise these higher order effects for enhanced sensing applications. Further research is required to understand the effect of coupling and nonlinearity to make sensors with enhanced sensitivity and fully utilise the potential of nano-sensors.

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