Modeling and Simulating of Mechanically Coupled MEMS Resonators using COMSOL Multiphysics for Potential Gas Sensors

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Abstract: In this project, COMSOL Multiphysics® and SolidWorks® are employed to model and simulate a pair of mechanically coupled MEMS resonators with a mass differential between the two, simulating the mass of absorbed gas on one, with the other acting as a reference. This project focuses on two coupled resonators: one with a 0.52µm thick added gold layer and one with no added mass. As expected the two coupled devices resonated at two distinct resonant frequencies. Using both the "Frequency Sweep" and "Eigen Frequency" module in COMSOL Multiphysics® the effect of changing the density of the added mass was simulated as well as compared to the results of the fabricated device.

Keywords: MEMS Resonator, Thermally Actuated, COMSOL Multiphysics

Introduction

In this project, COMSOL Multiphysics®[1] and SolidWorks®[5] are employed to model and simulate a pair of mechanically coupled MEMS resonators with a mass differential between the two, simulating the mass of absorbed gas on one, with the other acting as a reference. Figure 1 shows the structure. Each of the coupled resonators consists of three main components: a shuttle mass with a gas absorbing layer, springs tethering the shuttle to a substrate yet allowing it to vibrate preferentially in the in-plane or "y-direction", and electrode fingers attached to the shuttle mass to electrically detect the vibration with a similar comb structure fixed on the substrate. The two resonators are driven in the in-plane or y-direction by two shared thermal drivers, which are mechanically coupled through long stiff beams, which also serve as a mechanical coupling between the two resonators.

The structure given in Figure 1 was actually a one-to-one replica of a fabricated device using the "SOI-MUMPs" process[2] with a 25µm thick Silicon MEMS layer with a 0.52µm thick gold mass (gold colored patch in the figure) resting on one of the paired resonators. The resonant frequencies of these mostly-symmetrical resonators can be altered by changing the density of the material placed on the loaded side. The intention is to have the resonant frequency of the loaded side decrease as the mass increases, without affecting the resonant frequency of the un-loaded reference resonator.

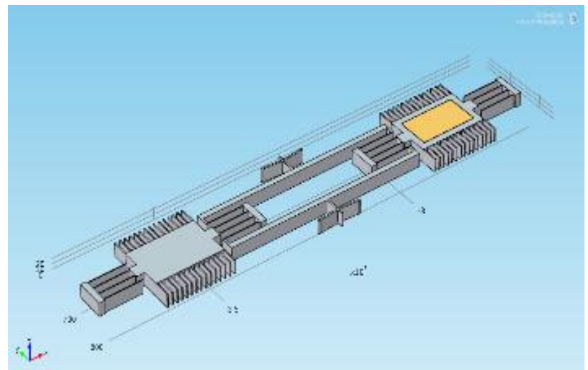

Figure 1a. Mechanically Coupled Resonators with Different Shuttle Masses

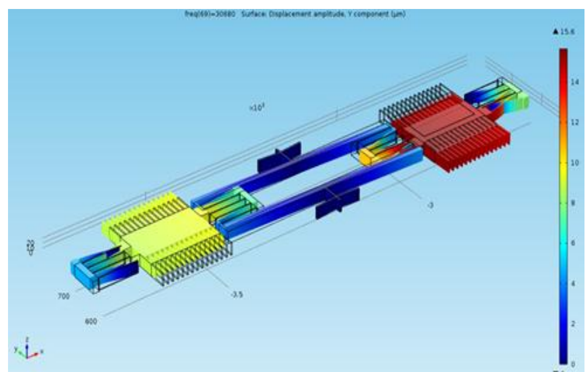

Figure 1b. Mechanically Coupled Resonators Displacement Graph at Loaded Side's Resonant Frequency (30680Hz)

Although electro-thermal-mechanical multi-physics simulations facilitated by COMSOL Multiphysics® were performed initially in both static and time domain analyses, due to excessive computational resources and simulation times required, most of the frequency analysis results presented here were obtained by vibrating the thermal driver at its boundaries mechanically, effectively mimicking a system driven by electro-thermal expansion in the thermal drivers.

Theory / Experimental Set-up

Due to the complexity and expense of fabricating MEMS devices, COMSOL Multiphysics® was a critical part of this project. COMSOL Multiphysics® allowed us to evaluate the performance of the device with a variety of loading masses, providing detailed information about the resonators' response under varying frequency inputs. The software facilitated the simulation of this structure for a variety of masses.

The 3D resonator structure was created in SolidWorks® and imported into COMSOL Multiphysics®. In simulation, the structure was fixed by the four outer corners of the springs, and a prescribed displacement was exerted at the tethers attached to the mechanical coupling beams. During a frequency response study, COMSOL Multiphysics® automatically stepped the frequency of the forced displacement applied from the thermal driver over a range of frequencies of interest, removing the need to manually increment the frequency and pick response to each.

To simplify the process of simulating a varying absorbed gas mass, the gold structure on the resonator shown in Figure 1 was simulated at different densities by placing a "Parameter Sweep" in the frequency sweep study. This was done by creating a variable, which was then multiplied by the density. That variable was changed during simulation using the "Parameter Sweep" option. Using the "Parameter sweep" option with a high resolution sweep resulted in a large simulation file, making saving this file unreasonable. Instead, the results were exported into Excel under the "Data sets" option in "Results".

The frequency sweep simulations for complex structures may take several hours, and the resonant frequency may not be originally known. To speed up the process, the Eigen frequency simulation was used to ascertain the location of the resonance, and use it to setup the frequency sweep range to avoid unnecessary computation away from the actual resonance frequencies.

The Eigen frequency study significantly reduced the simulation time from several hours to a few minutes. The results produced by COMSOL Multiphysics® were determined to be an invaluable asset for testing and understanding modes of resonance and the operation of the actual device.

Governing Equations / Numerical Model / Simulation / Methods / Use of Simulation Apps

The actual structure is driven by thermal expansion, induced by the V-shaped N-type doped silicon beam, shown in figure 3, to push the tip in the Y-direction. This expansion is induced by Joule heating from externally applied AC voltage at its terminals. Such thermal drivers have been tested extensively and modeled in our previous COMSOL Multiphysics® work[3,4] and simulations. Our results showed that these thermal drivers can achieve 0.1μm to 0.6μm displacement magnitudes at the tip while not exceeding the safe operating range of Silicon MEMS device, limited at 360°C, the Silicon- Gold eutectic point.

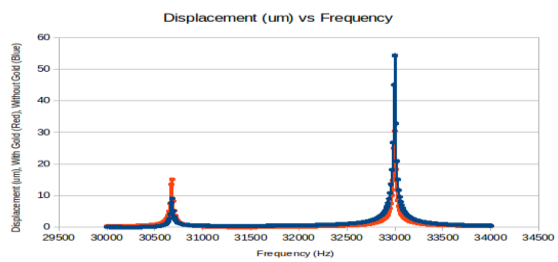

Figure 2. Mechanically Coupled Resonators' Frequency Response (Frequency vs displacement)

To simplify the simulation, the simulated device was driven using a "Prescribed Displacement," however, the actual device was driven by thermal expansion. COMSOL Multiphysics® was also used to simulate an AC current applied to the thermal drivers to determine how much displacement to expect from them. These results were then used in the "Prescribed Displacement" simulation for the peak value. The "Prescribed Displacement" used in all subsequent simulations was 0.1μm.

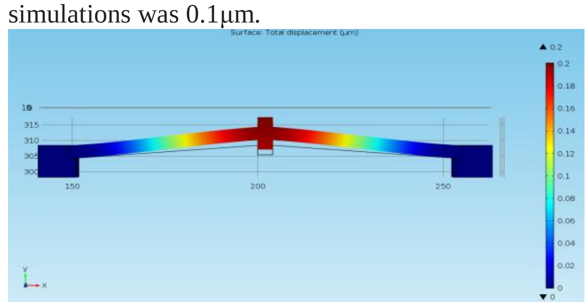

Figure 3. Displacement Graph of Thermal Driver Due to Heat Expansion (Showing max displacement of 0.2μm)

The structure in this study has interweaving "fingers" on both the structure and the substrate. These "fingers" act as electrodes, producing a capacitance between them. While the device is resonating, the area (A) of overlap of these electrodes changes and produces a varying capacitance.

$$C = \frac{A\varepsilon}{d}$$

This change in capacitance, in turn, induces a current.

$$I(t) = C\frac{dV}{dt}$$

This current can be measured using a current to voltage converter circuit. In our experimental determination of the resonant frequencies we used optical microscope to view the motion of the resonator and vary the frequency of AC voltage applied to the thermal driver. We determined the resonant frequency and amplitude from the blurring of the image in the y-direction. Figures 4 through 6 display in- and off-resonance photos captured.

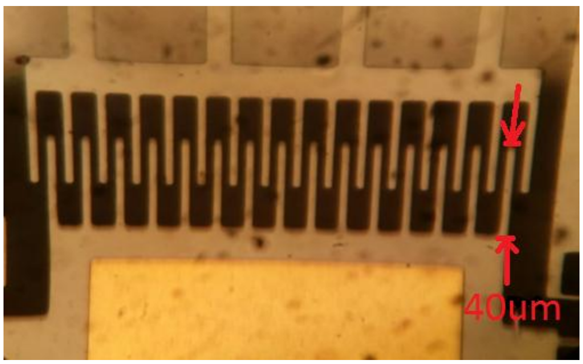

Figure 4. Fabricated Device Showing Interweaving "fingers"

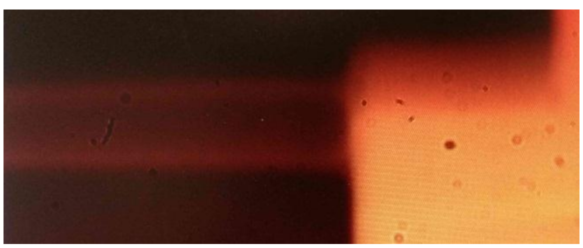

Figure 5. Fabricated Device at Resonance (31.964 kHz)

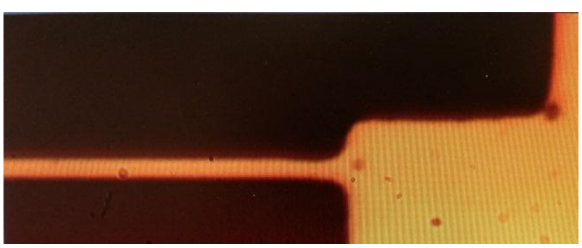

Figure 6. Fabricated Device off Resonance

Experimental Results / Simulation Results / Discussion

The simulations showed two resonant frequencies for this resonator. The first for the gold loaded side was 30.69 kHz, and the second for the unloaded side was 32.93 kHz. The simulation showed that the two resonators resonated at each other's resonant frequencies as well as their own. However, the total displacement of the resonators at the opposite resonator's resonant frequency showed half as much displacement as the other side. Since both resonators resonate at both frequencies, the device needed to be probed only at one point to detect both of the resonant frequencies. This observation clearly seen in the simulations helps in simplifying oscillator design with such resonators as well as reducing the number of wire bonding and pads needed which create parasitic capacitance. COMSOL Multiphysics® simulations proved to be an effective way to make these observations and benefit from them. However, at the beginning the simulation's default setting produced misleading results in the form of a dip to zero when the devices were driven at resonance (see the red curve in Figure 7.). It was later discovered that the COMSOL Multiphysics® default "total displacement" is not the absolute magnitude but the real part of the total displacement phasor. Since near the peak of resonance, the resonators undergo a 90° phase shift as shown in Figure 8, the real part is automatically forced to become zero on the frequency response plot whereas in reality the magnitude actually should go through its maximum. Figure 7 displays the true magnitude, that is, the absolute magnitude of the total displacement phasor in y-direction which is labeled as "solid.uAmpY" and plotted in blue for comparison with the misleading default displacement of COMSOL Multiphysics® (red).

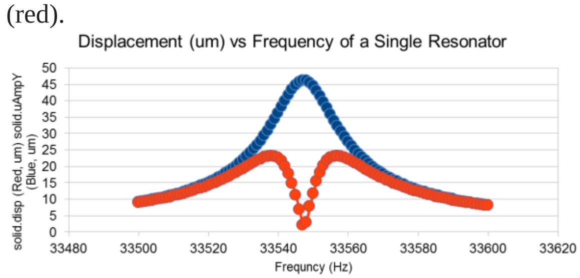

Figure 7. Uncoupled (Single) Resonator's Frequency Response (Displacement versus Frequency)

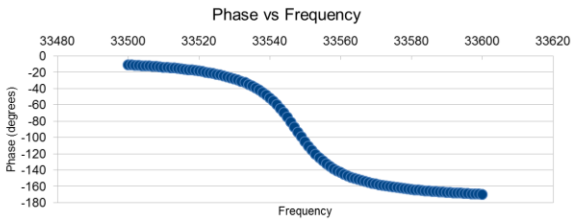

Figure 8. Uncoupled Resonator Frequency Response (Frequency vs. Phase)

Fine frequency sweep data takes a significant period of time to generate and creates extremely large data files.

Eigen frequency simulations were also performed in COMSOL Multiphysics® and their results were compared with the peaks produced with the frequency sweep results. These results were used to test the possible applicability of them for use in simplifying the simulation and reducing computation time. The Eigen frequency simulations produced similar results to the swept frequency simulations as seen in Table 1, which covers a density parameter range of 0.2 to 2.2 (i.e., 20% through 220% density of Gold). Table 1 gives the data obtained from both and compares them. The results were also compared with the experimental measurements as given in Table 2. All three agree very closely at the 100% density for which actual fabricated device measurements exists. However, when the density of the loaded side was small, i.e., in the zero to 0.2 (i.e. 20%) of Gold density, the Eigen frequency simulations deviate significantly from reality and should not be employed.

PD	LS-Sweep	LS-Eigen	Diff	ULS-Sweep	ULS-Eigen	Diff
0	33450	31393	2057	33450	33448	2
0.2	31230	31269	39	33310	33328	18
0.4	31110	31134	24	33210	33225	15
0.6	30965	30989	24	33120	33137	17
0.8	30815	30836	21	33045	33061	16
1	30690	30676	14	32925	32997	72
1.2	30495	30512	17	32925	32943	18
1.4	30330	30344	14	32885	32896	11
1.6	30155	30174	19	32840	32856	16
1.8	29980	30002	22	32800	32821	21
2	29815	29830	15	32750	32791	41
2.2	29635	29658	23	32750	32765	15

Table 1. Differences between Eigen Frequency Results and Frequency Sweep Results as Density Factor is varied from zero to 2.2 (i.e. 220%) of Gold.

Resonant Frequency	Actual Device	Frequency Sweep - Simulated	Eigen Frequency - Simulated
With Gold	29,650Hz	30,690 Hz	30,676 Hz
W/O Gold	31,964 Hz	32,925 Hz	32,997 Hz

Table 2. Resonance Frequency results compared, (1) Measured on fabricated resonators, (2) Frequency sweep Simulation, (3) Eigen value calculation

Conclusions

COMSOL Multiphysics® was utilized in simulating a series of mechanically-coupled resonators. The simulation showed that the two mechanically-coupled resonators resonated at two different frequencies, both at their own and also at their partner's resonance frequency which makes it possible to employ only one probe to detect both of the resonant frequencies from one.

The frequency sweep simulations done in COMSOL Multiphysics® produced very accurate and close results, as compared with measurement results on fabricated mechanically-coupled MEMS resonators of the same dimensions. However, these simulations often took days to complete, and the default probe output produced misleading zero displacements at the resonance peaks. The latter was resolved by replacing the default displacement parameter in COMSOL Multiphysics® with a realistic displacement parameter "solid.uAmpY".

Direct Eigen frequency simulations available in COMSOL Multiphysics® were shown to be a viable alternative to the long and expensive frequency sweep simulations. Eigen frequency simulations are much faster and equally accurate, as long as the mass loading density values remained above 20% in Gold but failed to be accurate below 20%. The frequency sweep is the only viable method to get accurate results at low density parameters below 0.2 (i.e. 20% density of Gold).

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