Impact of Geometry on Thermoelastic Dissipation in Micromechanical Resonant Beams

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Abstract

Thermoelastic dissipation (TED) is analyzed for complex geometries of micromechanical resonators, demonstrating the impact of resonator design (*i.e.* slots machined into flexural beams) on TED-limited quality factor. Clarence Zener first described TED for simple beams in 1937. This work extends beyond simple beams into arbitrary geometries, verifying simulations that completely capture the coupled physics that occur. Novel geometries of slots engineered at specific locations within the flexural resonator beams are utilized. These slots drastically affect the thermal-mechanical coupling and have an impact on the quality factor, providing resonators with quality factors higher than those predicted by simple Zener theory. The ideal location for maximum impact of slots is determined to be in regions of high strain. We have demonstrated the ability to predict and control the quality factor of micromechanical resonators limited by thermoelastic dissipation. This enables tuning of the quality factor by structure design without the need to scale its size, thus allowing for enhanced design optimization.

Introduction

Silicon micromechanical resonators are being considered for frequency reference applications because of their potential as high frequency, high quality factor, Q, resonators in a very small volume [1]. The fundamental behavior of these silicon resonators must be well understood in order to make silicon resonators a viable option for replacement of existing frequency reference technologies. The Q is important because it affects parameters that are critical in frequency reference applications (*e.g.* motional, resistance, phase noise). Quality factor in this case is a measure of the amount of mechanical energy the resonator dissipates. The ways in which the resonator can dissipate energy include air damping, clamping loss through the anchors, surface losses, material losses, and thermoelastic dissipation (TED), many of which are still not well understood. This work focuses on design techniques to improve and control Q of resonators limited by TED, which is the energy loss due to the relaxation of mechanically induced temperature gradients (Figure 1), as well as the simulation and experimental verification of resonant beams with TED-limited Q.

Background and Theory

Zener initially formalized the theory of thermoelastic dissipation in 1937 (he called it internal friction)[2, 3] for the case of a vibrating reed, which is a similar structure to a resonant beam currently used at the microscale. Many reformulations of the problem have occurred since [4-7], including investigations of ring-shaped resonators [8] and extraction of the flexural component of arbitrary mechanical modes to determine the effect of classic thermoelastic damping on a resonant structure [9].

Zener derived a relationship to provide the maximum possible TED-limited Q for a simple beam. Other loss mechanisms could cause additional dissipation, and thereby cause the Q to be lower than the value predicted by Zener, but the Q could not be any greater than the TED imposed limit. He began by defining the dominant thermal time constant, which comes from the thermal eigenmode solutions of the system,

$$\tau = \left(\frac{b}{\pi}\right)^2 \frac{c_p \rho}{\kappa} \tag{1}$$

where τ is the time constant at which the temperature gradient decays in the fundamental eigenmode, b is the thickness in the direction that the beam flexes, c_p is the specific heat at constant pressure, ρ is the density, and κ is the thermal conductivity. The maximum TED-limited quality factor, Q_{TED}, a resonant beam can attain is dependent on the resonant frequency of the beam,

$$Q_{TED} = \left(\frac{c_p \rho}{E\alpha^2 T_0}\right) \frac{1+(\omega\tau)^2}{\omega\tau} \tag{2}$$

where E is the Young's Modulus, T_0 is the equilibrium temperature of the beam, α is the coefficient of thermal expansion, and ω is the angular frequency of mechanical resonance.

The Zener theory was derived explicitly for the case of a simple beam, as this kept the problem tractable with the tools available at the time. The Zener theory contains the valid approximation for simple beams that only one thermal mode is significantly

coupled to the mechanical mode. An exact expression for the Q of TED in simple beams was subsequently derived [5]. The Zener theory works well for simple beams and has been experimentally verified at the microscale [10-13]. However, in order to treat more complex structures, it is necessary to use the more general theory derived by Zener that includes multiple thermal modes, as opposed to the more commonly cited derivation for a simple beam with a single, dominant thermal mode. The work in this paper gives experimental results that do not agree with predictions made by the simple Zener theory, showing that the more general theory is required. Resonant beams that have openings, or slots, in the beams disrupt the heat flow across the beam, causing multiple thermal modes to interact significantly with the mechanical mode.

Other Energy Loss Mechanisms

A significant difficulty in quantifying the different energy loss mechanisms that limit quality factor in micromechanical resonators is the isolation of one specific energy loss mechanism. All loss mechanisms contribute to the quality factor as shown by equation 3,

$$\frac{1}{Q_{total}} = \sum \frac{1}{Q_{individual}} \tag{3}$$

where Q_{total} is the overall Q observed in measurement and $Q_{individual}$ is the Q from each of the loss mechanisms, such as air damping, surface loss, material losses, anchor damping, and TED. This interrelated nature has kept many of the energy losses from being well

understood. Therefore, in order to isolate one energy loss mechanism, efforts must be made to minimize the impact of all the others.

A tuning fork architecture was used to minimize clamping loss. Clamping loss in micromechanical resonators is an area that has been receiving an increasing amount of attention [14-18], but it is still not fully understood. The tuning fork architecture should place a node at each anchor, because the beams are actuated 180° out-of-phase. The fact that the Q varied significantly while the tuning fork anchor architecture was constant for all the resonators is an indicator that it did not have a significant influence on Q. The clamped-clamped architecture was used to increase the resonant frequency of the devices over the single-clamped architecture. Air damping, common Q-limiting mechanism, is often mitigated with hermetic vacuum packaging. The resonators in this study were fabricated in a wafer-scale vacuum encapsulation at a pressure of < 0.003 mBar [19]. Recent work elsewhere has confirmed that vacuum encapsulation can lead to excellent stability in micromechanical resonators [20]. Demonstration that the encapsulation provides an adequate vacuum is given in the results section.

Intrinsic material losses and surface dissipation losses are two other energy loss mechanisms that are often mentioned. Material losses are defined here as losses inherent in the material structure, affected by the material properties and frequency but not by the resonator geometry. Bulk mode silicon resonators have been reported at 12 MHz with a Q of 180,000 [21]. Since the resonators in this paper were in the same frequency range and made of the same material but had lower quality factors than the cited work, intrinsic material damping is not likely to be dominant. Surface dissipation losses, which are thought to be caused by the chemical states at the resonator surface, become more

prominent as any of the resonator dimensions are scaled toward the nanometer regime [11, 22-24]. Since all the dimensions of our resonators are in the micrometer regime and our packaging provides a chemically stable environment, it is unlikely that surface dissipation mechanisms play a role.

Design

For silicon resonators, a minimum occurs in the TED limited Q (~10,000) at about 1 MHz for flexural beams with a thickness of 12 μm. A specific addition to the geometry, slots cut into the beams, was added in an effort to improve the quality factor of beams. The slots act to disrupt the heat flow across the beam, thereby altering the process of thermoelastic dissipation.

If heat-disrupting slots are to be used in an attempt to alter the TED-limited Q, the optimal location of the slots must be determined. Resonant beams were designed with two slots in each beam, shown in Figure 2. The slot location is varied along the beam to determine the impact of slot location on TED-limited Q.

Once the slot locations that maximally impact Q were determined by experiments and simulation, as described below, another set of tuning forks was designed. Tuning forks without slots were designed to confirm the classical Zener theory at the microscale, as well as tuning forks with four slots on each beam, to confirm that complex geometries need a more advanced treatment to predict the TED limited Q. It was necessary to fabricate resonators with a range of frequencies, $f_{resonant}$, while keeping the beam thickness constant. A fixed beam thickness would maintain the same thermal time constant, τ, which is defined by the thickness of the beam. So, a parameterized spread of tuning forks

without slots was fabricated that had a thickness of 12 μm and a length, L, that varied. Since $f_{resonant} \propto \frac{1}{L^2}$, a considerable frequency range was covered, ~150 kHz to ~ 10MHz. The highest frequency of beams was limited by small length-to-thickness ratios that could cause problems with anchor loss and measurement difficulties due to small capacitive area and high stiffness. Additional parameterized spreads of tuning forks were fabricated with slots. In an effort to maintain a similar thermal mode profile, the slots in the beams were scaled with beam length. A set of tuning forks with slots that had length 1/10 of the beam length, as well as a set of tuning forks with slot length 1/6 of the beam length were fabricated. Four slots were used on each beam, as can be seen in Figure 3. Using insight from the moving slot experiment, the slots were placed where they would have the greatest impact, at the ends and center of the beams.

Simulation

The simulation results given below were obtained from a 2-D fully coupled thermal-mechanical finite element eigensolution in FEMLAB. The coupled mechanical and thermal differential equations are solved for a complex eigenvalue, and the TED-limited Q can be extracted from the real and imaginary components of the eigenvalue. Information regarding the methodology of these can be found in [25-27].

Some intuition regarding why slot location is important can be gained from viewing the fully coupled simulation of a regular clamped-clamped beam. As can be seen in Figure 4, the temperature gradient from one side of the beam to the other is not uniform. It is greater near the anchor and center of the beam. This is due to the higher strain gradient at these locations. The high strain gradient causes a temperature gradient, causing heat to flow, which is the energy loss mechanism of TED. This logic implies that

slots near the anchor and center of the beam will have the greatest impact. Results given below were found to confirm this.

Simulations showed a clear relationship between slot location and TED-limited Q. Two slots were placed on each beam a specified distance from each of the anchors, as shown in Figure 2. This distance was varied to test for dependence of TED limited Q on slot location. Geometrical parameters used for the beam and slots of the two slot beams, as well as material parameters for the two and four slot beams, are given in Table 1. The same material parameters were used for single crystal and polycrystalline silicon. Previous measurements have suggested the material parameters were similar for single-crystal silicon and our highly-doped polycrystalline silicon process. In particular, a thermal conductivity of 90 W/m/K is a reasonable value for highly doped single and polycrystalline silicon when compared to values previously reported [28, 29].

Simulating just one of the beams in the tuning fork is done to reduce the number of elements in the simulation and improve convergence. This neglects heat lost in the coupling beams and may overestimate Q. To the extent that the resonating beam dominates thermoelastic losses, this approach predicts the overall trends in Q very well, as our experiments show. The temperature profiles from fully coupled-eigensolutions for several beams in the parametric slot location study are shown in Figure 5.

Experimental Results

Resonators were fabricated inside a single-wafer vacuum encapsulation process [19, 30], Figure 6, which provides a hermetic seal at a pressure < 0.003 mBar. The devices with two slots were made of polycrystalline silicon, while the devices with four slots were made from single-crystal silicon.

The resonators were capacitively actuated and capacitively sensed in-plane across a 1 μm gap, and the measurements were performed with a probe station at the wafer scale. The actuation and sensing were done on the outer electrodes and inner electrode (Figure 2), respectively, and a DC voltage (typically ~10 V) was applied to the resonator beam. A low input-capacitance active probe, GGB industries picoprobe model 34A, was used to sense the output signal. Standard tungsten probe tips were used for the rest of the connections. A typical measurement result is shown in Figure 7.

Resonators with different slot locations were tested and compared to simulation. In the study where slot location was varied, the length of the two slots was fixed at 40 μm, and the beam length was 400 μm. Figure 8 shows that the experimental results confirm the dependence of TED-limited Q on slot location. While the location of slots affected Q by more than 40%, the resonant frequency was changed only 5% by the different slot placements.

Simulations for the second set of tuning forks where *resonant frequency* is varied by changing the *length,* are given in Figure 9. Notice that the addition of slots into the beams allows for beams with quality factors greater than theory would predict for simple beams. In these studies where slot length was varied, the slot location along the beam was kept fixed. These studies used fours slots, with a slot 2 μm from each end of the beam, and two slots separated by 4 μm at the center, as shown in Figure 3.

The resonators were tested and compared to simulation. As shown in Figure 10, the measured Q values follow the trend predicted by the simulations. There is an offset in the data for the resonators with slot length 1/10 of beam length, likely due to an additional energy loss mechanism. Also, the material parameters and process variations

are not perfectly known, which could lead to some shift in the simulation. The shape of the Q dependence on frequency, however, is similar to that predicted by simulations. If another loss mechanism, Q_{other}, which incorporates all loss mechanisms other than TED, is assumed for the 1/10 slot length case, equation 3 can be used to extract the likely Q limitation of TED from the Q_{total} that is experimentally measured. As can be seen in Figure 10d, assuming a relatively large Q_{other} of 100,000, which implies a relatively small energy loss, causes the experiments and simulations to converge.

The addition of slots was shown to increase Q by as much as a factor of four. While this case demonstrated that the introduction of slots could affect the heat flow to improve the Q, it is important to also note that there are regions of the design space where the addition of slots will *decrease* Q, such as the high frequency range of Figure 9. Therefore, it is necessary to carefully consider a proposed design change to guarantee that it will have the desired effect.

For the resonators of Figure 10, the highest Q device was measured in a vacuum chamber after the encapsulation was removed, and the Q was not different from the Q measured in encapsulation. As can be seen in Figure 11, the Q of a 328kHz resonator with 1/6 slot length to beam length ratio in vacuum was 41,000. This is in the same range as the Q measured in the vacuum encapsulation. From the data given in Figure 10, the 328kHz resonator with 1/6 slot length had the lowest resonant frequency and the highest Q. Since the pressure-limited Q would increase as the beam is scaled to shorter lengths, it is reasonable to conclude that none of the parts are limited by air damping.

Coupling of Multiple Thermal Modes for Slotted Beams

There are several subtle points regarding TED in slotted beams that deserve explanation. Most importantly is that the mechanical mode of slotted beams can couple to more than one thermal mode. Zener proved that only one thermal mode is well-coupled (98.6%) to the mechanical mode of a cantilever structure, while the coupling of all other modes is negligible [2]. In fact, the use of the Zener equation for clamped-clamped beams is not technically correct, as the thermal mode that is well coupled to clamped-clamped beams is different than the one that is well coupled to cantilevers. However, the frequency of the dominant thermal mode in the clamped-clamped beam is within a few percent of the frequency of the thermal mode in the cantilever case, so the classic Zener equation is still a fair approximation for clamped-clamped beams.

For beams with slots, multiple thermal modes can have significant coupling to the mechanical mode. The involvement of multiple thermal modes in the thermoelastic dissipation of slotted beams explains three phenomena that may be counterintuitive. First, a frequency shift of the minimum Q between the slotted resonators and the simple beam resonators (no slots) can be seen in Figure 9. This frequency shift is caused by a shifting of the coupling from the initial thermal mode of the simple beam to higher frequency thermal modes in the slotted beams, with multiple thermal modes contributing to the Q. To restate this point, a single thermal mode is fully coupled to the mechanical mode in simple beams, while multiple thermal modes each couple partially to the slotted beams. The original thermal mode is still partially coupled in slotted beams, but other (higher frequency) modes also cause energy dissipation. The frequency of minimum Q differs between the two sets of slotted beams, because the differing slot length ratios alter the thermal modes and their coupling to the mechanical mode. Second, the minimum Q

is different for the beams without slots and beams with slots, Figure 9. This is because the addition of slots causes the initial thermal mode to be less than fully coupled to the mechanical mode. The increased coupling of the higher frequency thermal modes is not enough to overwhelm the reduced coupling to the initial thermal mode, so the Q minimum is increased with the addition of slots. In other words, there is a reduction in energy dissipation for the worst-case frequency for the slotted beams as opposed to the simple beams. The two sets of slotted beams with different slot length ratios have different Q minima, again because the different slot length ratio alters the thermal modes and coupling of these modes. Third, the Q for slotted beams is worse than the Q of simple beams for some frequency regimes. While the *Q minimum* is higher for the slotted beams, the Q is not higher for all frequencies of slotted beams, with the higher frequency slotted beams having a Q that is *worse* than regular beams of the same frequency, Figure 9. This is because the higher frequency slotted beams are partially coupled to higher frequency thermal modes, while the coupling of simple beams is only to the initial thermal mode with negligible coupling to these higher frequency modes, as stated by Zener.

Conclusion

We have performed a comprehensive study, including modeling and experimental verification of thermoelastic dissipation as a Q-limiting phenomenon in micromechanical resonators. Our work highlights the importance of using advanced modeling techniques to optimize structures for high Q. The equation by Zener that is frequently cited lends itself to analytical study of only the simplest case, and cannot be easily used to optimize Q in more complex structures. By applying a fully coupled finite elements simulation,

we demonstrate the predictive capability in our design and optimization process. Leveraging this tool, we designed, fabricated, and tested resonators with a proscribed thermoelastic damping. In particular, we designed slots into flexural beams to drastically alter the coupling of mechanical and thermal eigenmodes. The impact of slot location on the beam was studies, showing that slots at points of high strain had the largest impact on Q. We successfully demonstrated the ability to produce resonant beams with similar dimensions and frequency but with a wide range (up to a factor of four) in quality factor.

Acknowledgement

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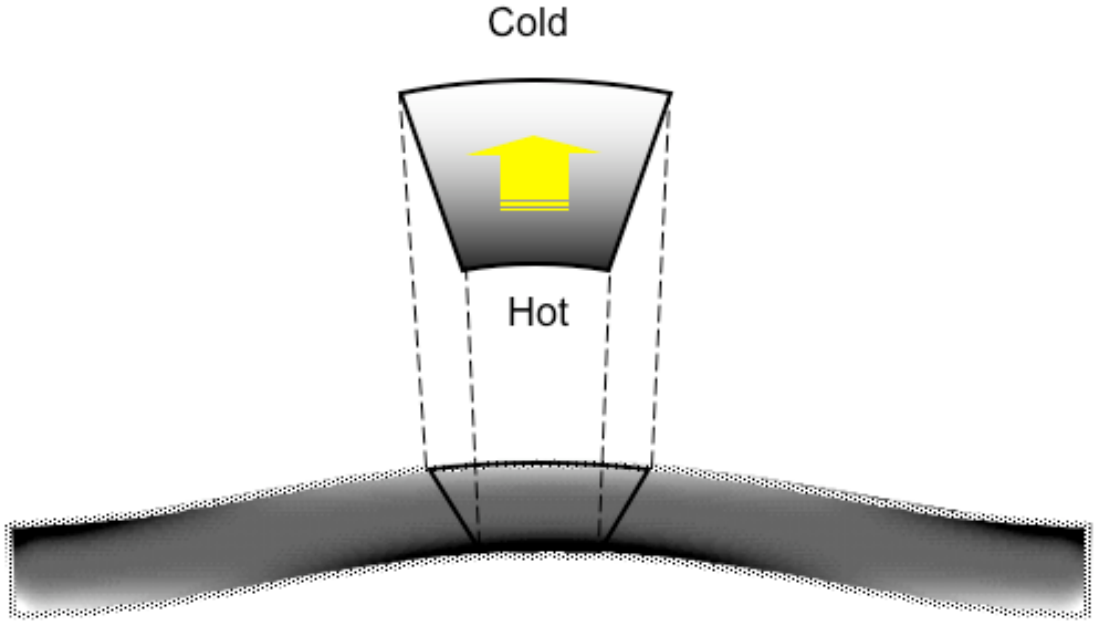


Figure 1. Conceptual drawing of heat flow across a flexed beam, which leads to thermoelastic dissipation.

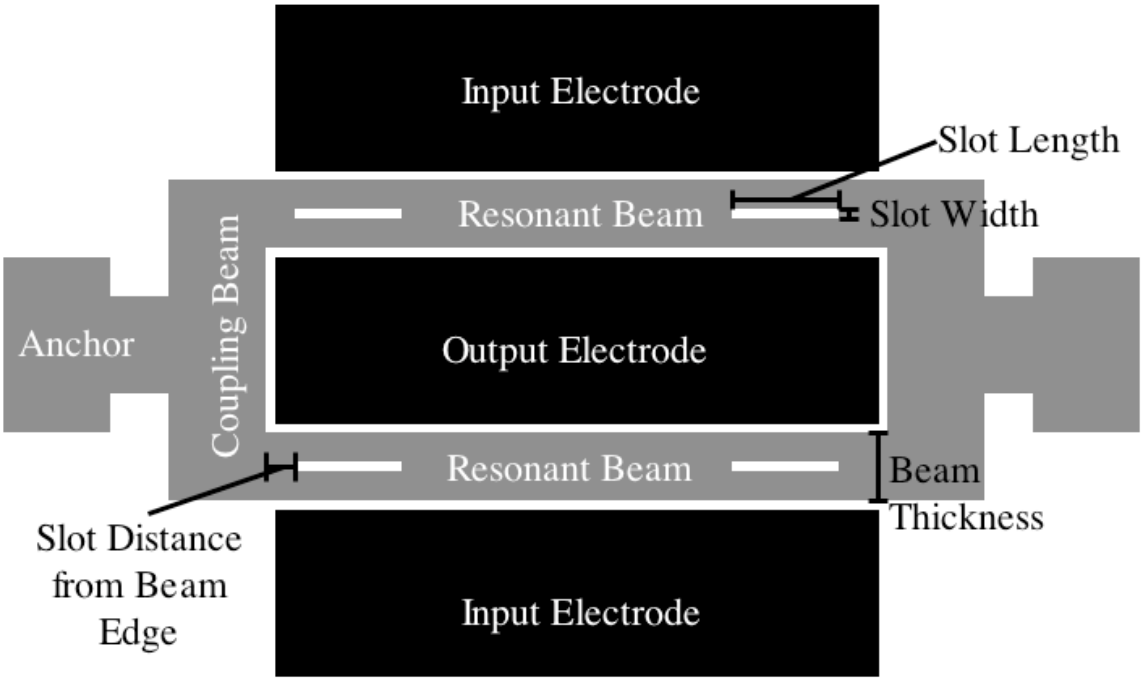


Figure 2. Schematic top view of clamped-clamped resonator. The resonator consists of two beams coupled together at both ends. Each beam has two slots cut into it a certain distance away from the anchor. Slot width is 1 μm, and beam thickness is 12 μm. The tuning fork resonates in-plane.

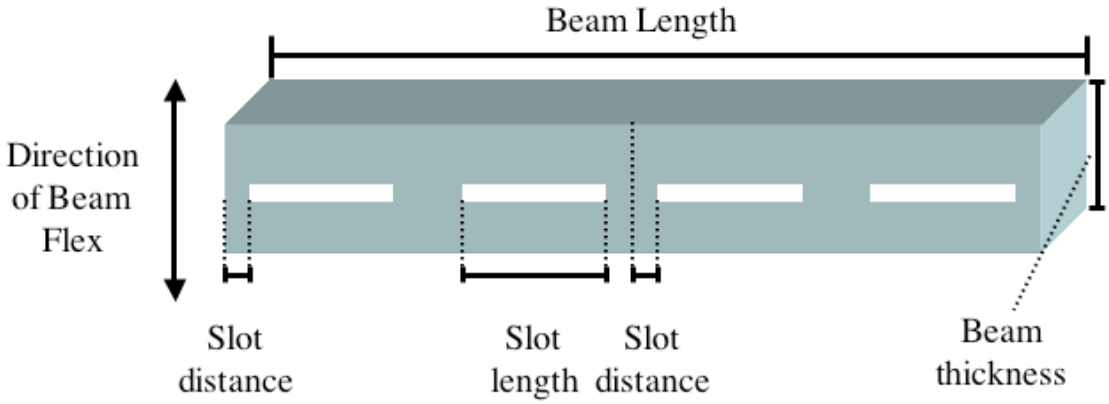


Figure 3. Schematic of slotted beam. Beam length is scaled to achieve a range of resonant frequencies. The ratio of beam length to slot length is fixed. Slot distance and beam thickness are fixed at 2 µm and 12 µm, respectively.

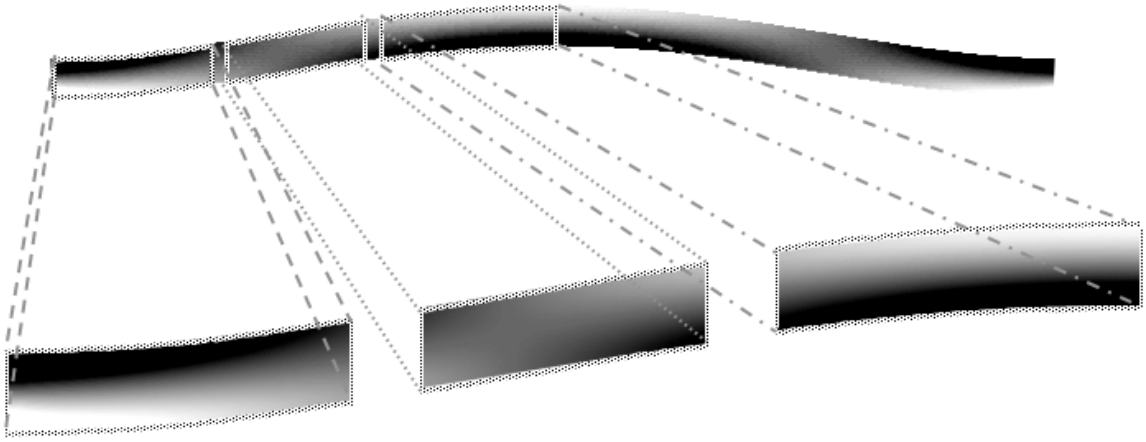


Figure 4. Temperature profile of solution for fully-coupled eigensolution solved with FEMLAB. Note the increased temperature gradient near the end and center of the beam.

Parameter	Value	Units
Slot Length	40	μm
Slot Width	1	μm
Beam Length	400	μm
Beam Thickness	12	μm
Resonant Frequency	~600	kHz
Density, ρ	2330	kg/m^3
Young's Modulus, E	157	GPa
Poisson's ratio, ν	0.3	
Coefficient of Thermal Expansion, α	2.6e-6	1/K
Thermal Conductivity, k	90	W/m/K
Specific Heat, c_p	700	J/kg/K
Temperature, T	300	K

Table 1. Material properties and design information for beams with heat-interrupting slots.

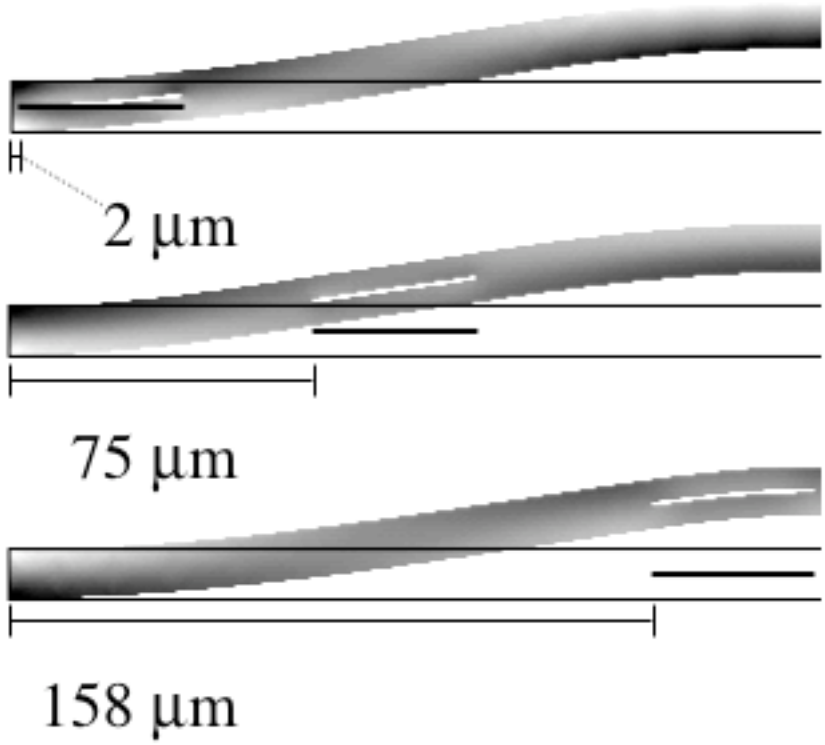


Figure 5. FEMAB fully-coupled solution for 400 µm beam with slots 2 µm, 75 µm, and 158 µm from each end of the beam. Temperature profile is shown on deformed beam. Half of each beam is shown.

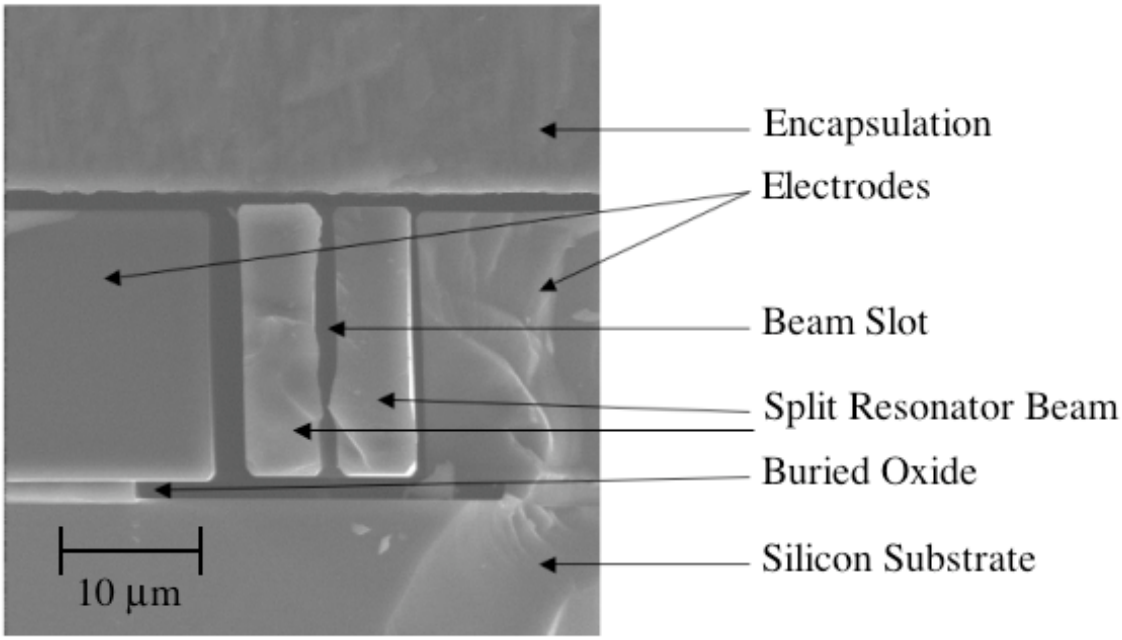


Figure 6. SEM Cross section of encapsulated tuning fork resonator with slot.

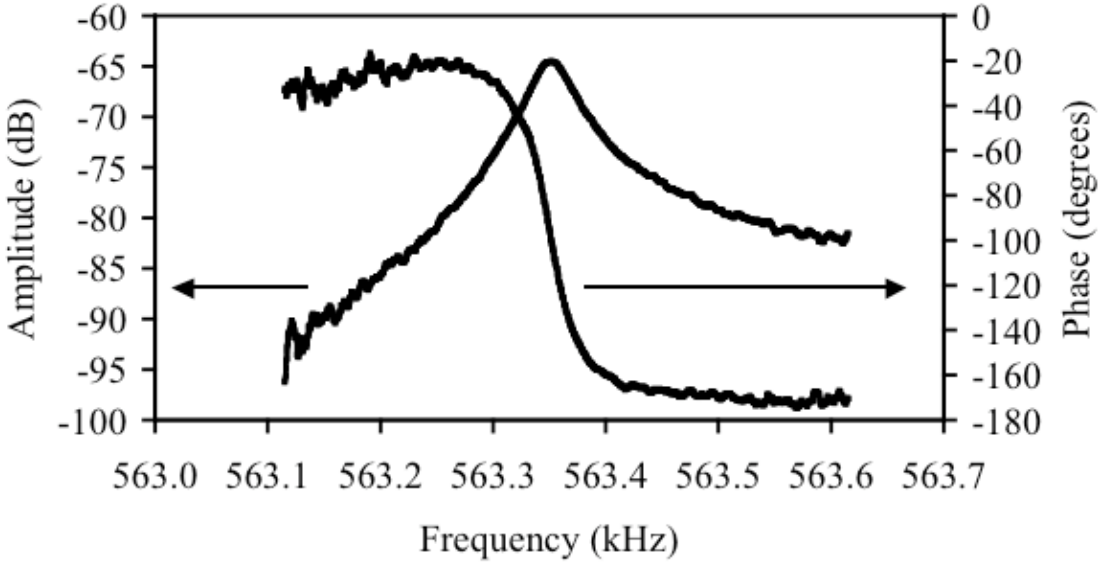


Figure 7. Gain-Phase plot for tuning fork with slots 2 μm from beam edge.

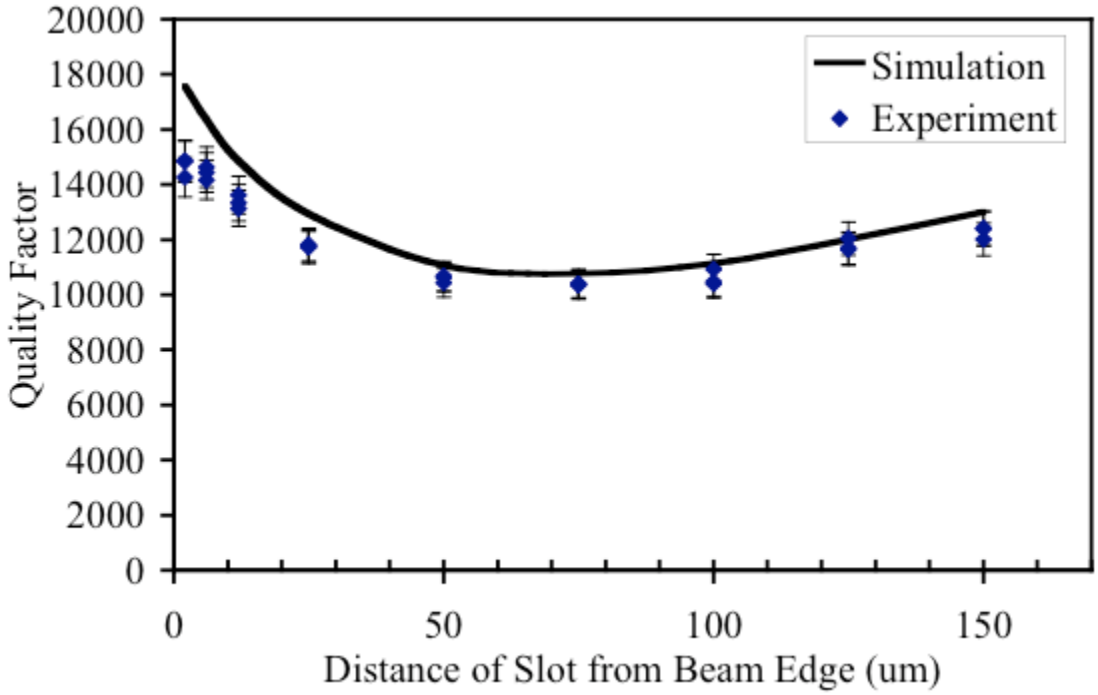


Figure 8. Comparison of simulation to experimental results for resonators with the same geometry, *except* for the location of the heat interrupting slots (desing from Figure 2). Experimental data confirms that the location of slots on resonant beams has an impact on quality factor. Simulations were performed before experiments, and no adjustments were made to the model parameters to fit the simulations to the experiments. At least eight simulation points were used to get the simulation curves of Figure 8, Figure 9, and Figure 10. Simulation points were left off the graph were left off for clarity of the data points.

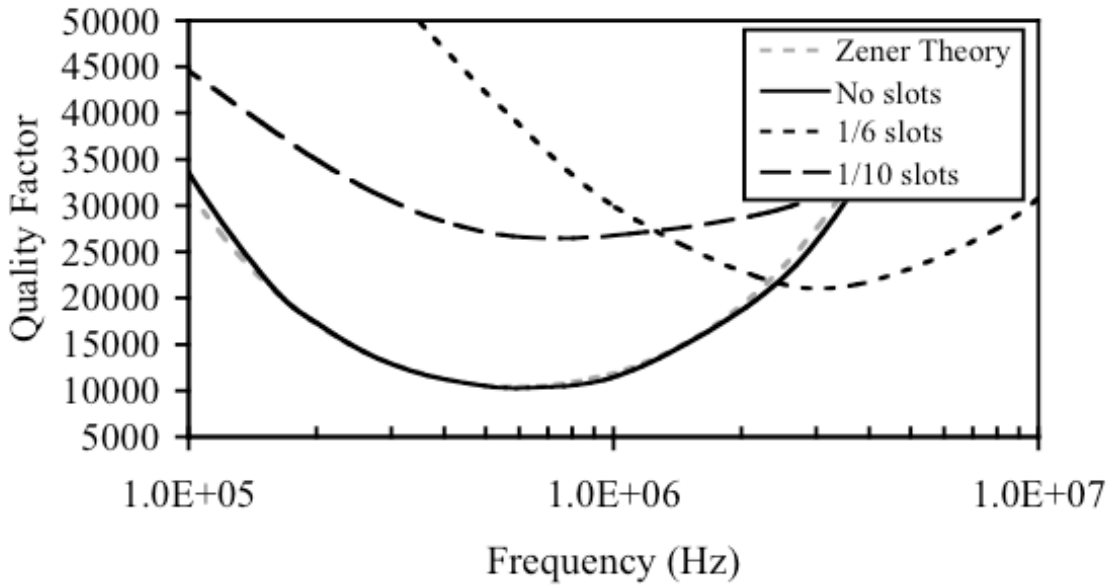
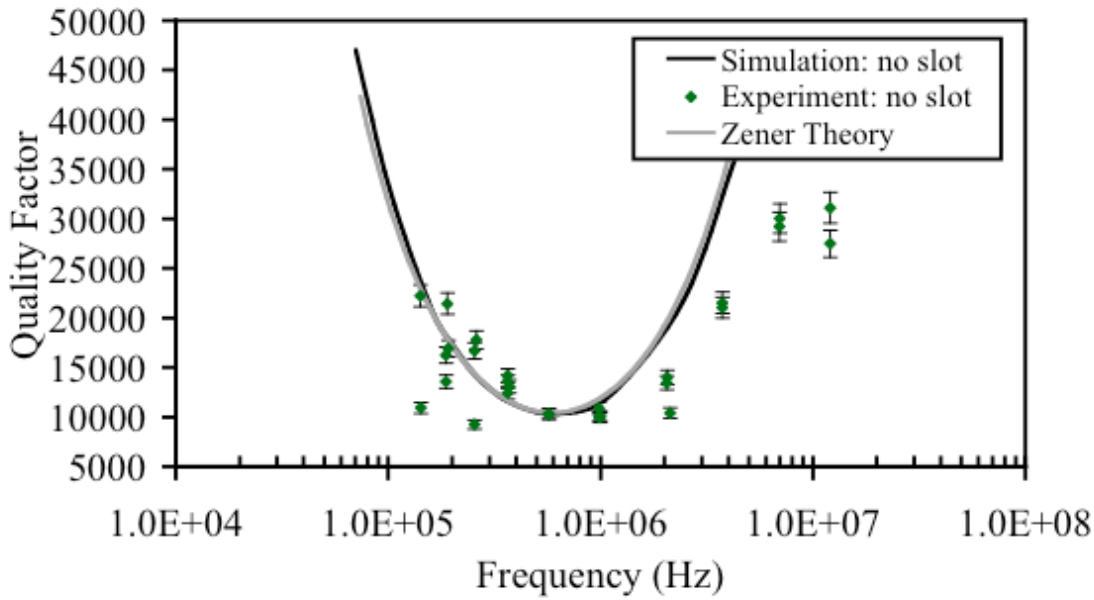
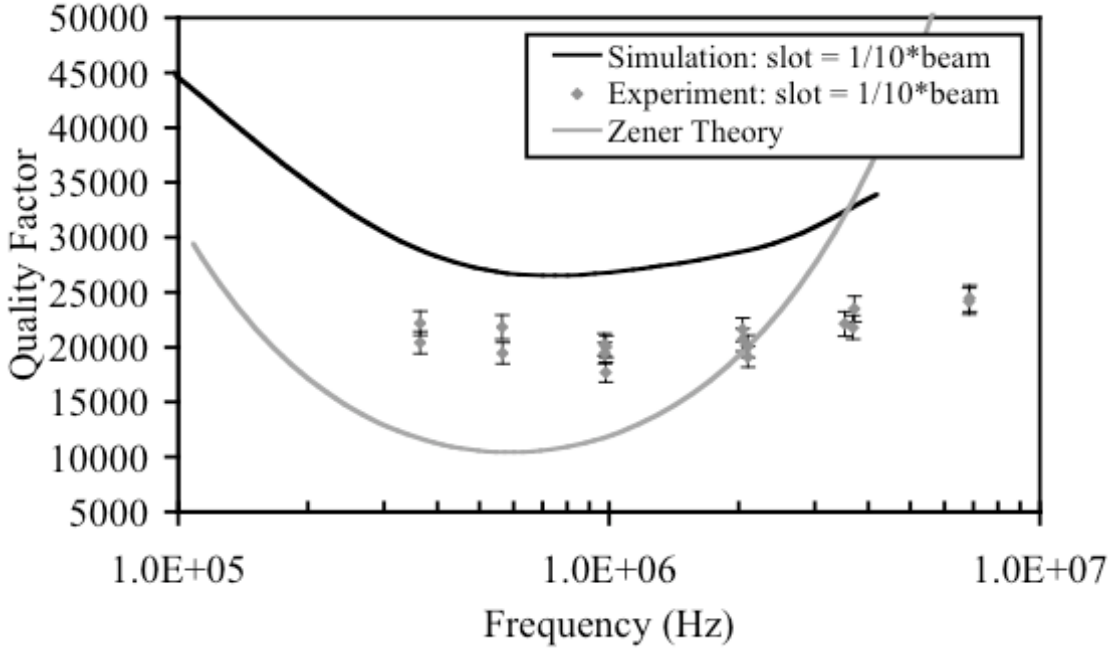


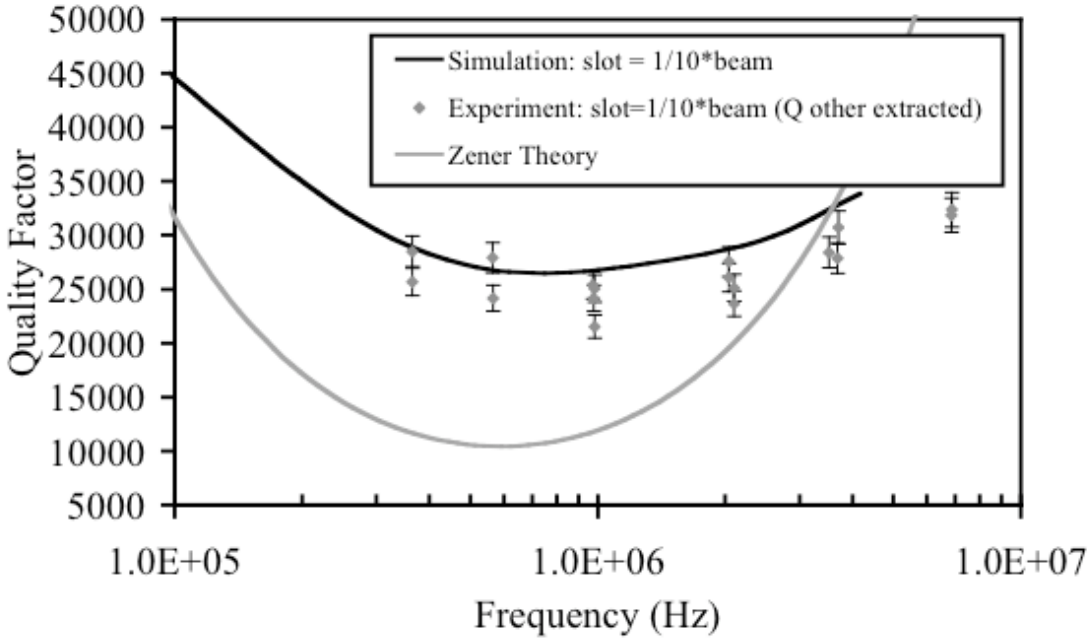
Figure 9. Simulation results for beams with no slots, slot length = 1/6 beam length, and slot length = 1/10 beam length plotted against Zener theory. Simulations for beams with no slots agree with Zener theory to within 7% for all the data shown. Note that the predicted TED-limited quality factor varies greatly for the three types of beams, even though the only difference in geometry between the types of beams is the addition of slots. As can be seen, slotted beams allow for quality factors that would be theoretically unachievable with solid beams.


Simulation: no slot
Experiment: no slot
Zener Theory
Quality Factor
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
1.0E+04
1.0E+05
1.0E+06
1.0E+07
1.0E+08
Frequency (Hz)

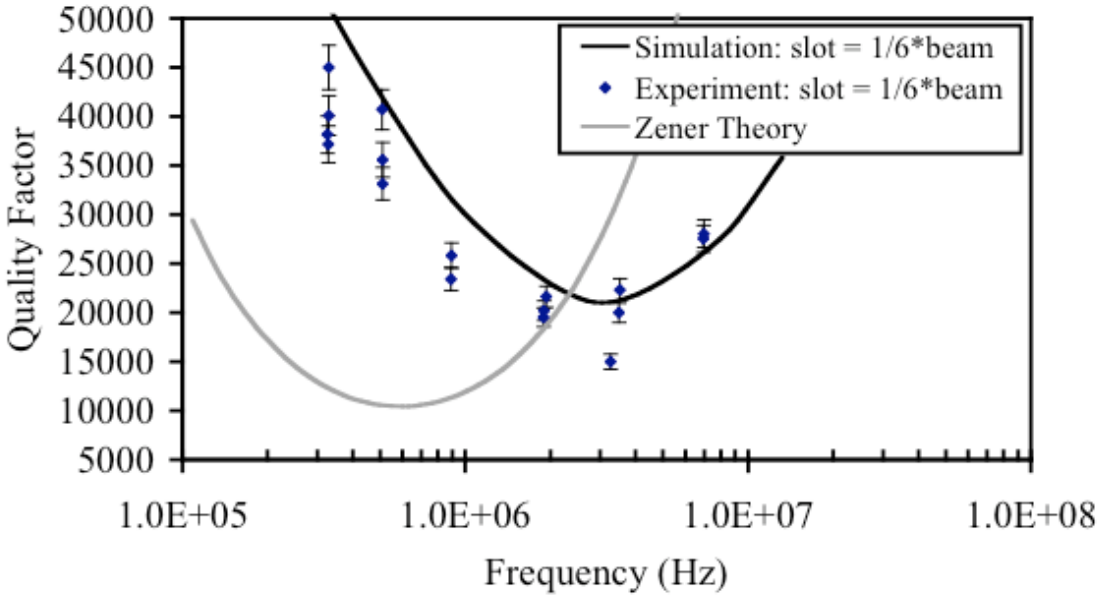
(a)


Simulation: slot = 1/10*beam
Experiment: slot = 1/10*beam
Zener Theory
Quality Factor
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
1.0E+05
1.0E+06
1.0E+07
Frequency (Hz)

(b)



(c)



(d)

Figure 10. Experimental results of beams with four slots, the same width, and varying length compared to finite element simulation and simple Zener theory. (a) Beams without slots. (b) Beams with slots = 1/10*beam length. (c) Beams with slots = 1/10*beam length, where Q_{other} = 100,000 has been removed (d) Beams with slots = 1/6*beam length.

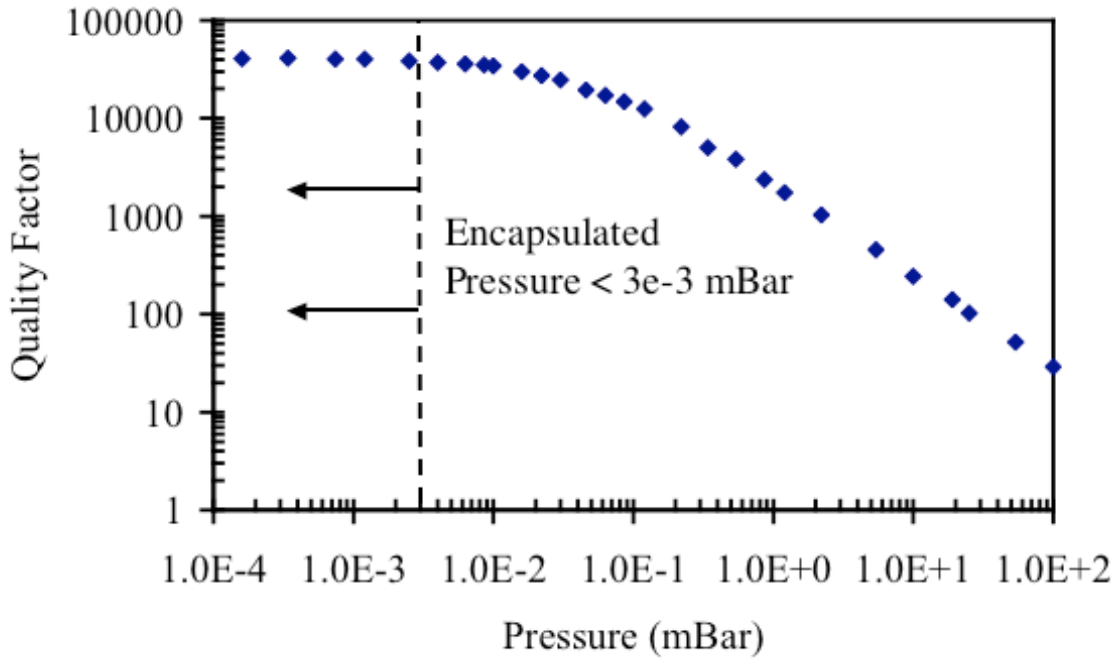


Figure 11. Quality Factor vs. Pressure for 328 kHz resonator (slot length = 1/6 beam length). The Q of the lowest frequency, highest Q part was not pressure limited, indicating that none of the resonators shown above were pressure limited.