Design of a quartz microresonator for infrared sensor applications

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Abstract

A quartz crystal resonator's resonance frequency is sensitive to temperature, and a quartz thermometer can accurately detect temperature changes of microkelvins. Making the resonator in a microscopic scale increases its temperature detectivity as well as enables a large array for an IR sensor. Incoming radiation energy of such an IR sensor needs to be absorbed in the resonator as much as possible, and this requires a different geometry of the electrodes from those of a conventional resonator; e.g., a ring electrode on the IR illumination side and a solid electrode on the other side. The geometry of these electrodes should be optimized in order to obtain a maximum energy trapping, which maximizes the value of Q and minimizes the resonator noise, resulting in maximizing the detectivity. Analytical and numerical solutions of the approximate scalar differential equation of Stevens and Tiersten describing the transverse behavior of essentially thickness modes are obtained for a rectangular resonator with a ring electrode on one side and a solid electrode on the other side. These solutions are used to study the performance of this electrode geometry and a general design is presented.

Introduction

The essential requirement for a good thermal IR sensor includes small thermal mass and good thermal isolation of the sensor element in addition to large temperature sensitivity. Such a configuration of a small isolated device can be easily fabricated by micromachining of a quartz resonator: a high fundamental frequency resonator having etched isolation channels along with the boundary of the resonator except its electrode area. Recall a special cut of a quartz resonator such as a doubly rotated LC (linear coefficient)-cut has been utilized for a thermometer due to its precise resolution in the temperature change. Another crucial requirement is that the device should have a low noise performance. A quartz resonator can provide an extremely low noise source. Combining those properties of a quartz resonator will make a quartz microresonator a candidate for an excellent IR sensor. Application of a quartz resonator to an IR sensor has been reported by several authors [1-3]. Even though their experimental results of the devices couldn't achieve the practical usefulness in the device performance, they could show the potential feasibility of a quartz resonator for the IR sensor application. In addition, the theoretical background and feasibility of microresonator arrays for IR sensor array applications has been presented [4].

Quartz itself is an IR absorbing material in the several bands over 8 μm wavelength range [5]. The IR absorption of quartz resonators has been already explored by J. R. Vig for fast oscillator warm-up using an IR heating [6]. In order to utilize the direct absorption, the surface area of the open quartz, especially acoustically active area, needs to be maximized since the electrode area reflects most of the IR energy. Some trial patterns of ring electrodes [2] and grid electrodes [3] have been employed without optimizing the resonators' performance, and in each case the top and bottom electrode pattern employed the same patterns.

Applying a good reflector on the back side of the quartz while the IR illumination side is open, the IR energy transmitted through the plate is reflected back, resulting in the increase of the IR energy absorption. Recall a shiny metallized surface of the electrode reflects the IR energy. This idea leads to a non-conventional asymmetric electrode structure having a ring electrode on the IR illumination side and a solid electrode on the other side. Simple scaling of conventional solid electrodes to design this asymmetric structure may cause the generation of undesirable inharmonic overtone resonant modes. Such inharmonic overtone modes associated with the resonator structure has been analyzed using the concept of acoustic energy trapping [7]. An optimal design can suppress the inharmonic overtones to achieve the optimal performance represented by high Q factor and low noise.

A proper energy trapping can be achieved by contouring of the acoustically active region of conventional quartz resonators as convex-convex or plano-convex shapes. But, the fabrication of such contouring is not an easy task in the microresonator fabrication where microfabrication technique using photolithography is required to define small dimensions in microscopic scales. Adjust-
ing the geometry of the electrode and thickness of the electrodes on a plano-plano plate would rather be done more easily than contouring. In this paper, such a design is presented to achieve an optimal resonator performance by analyzing the electrodes with the energy trapping concept.

The IR absorption can be improved by applying a uniform IR absorbing coating on either the IR illumination side or the both sides over the entire surface. Since the thickness of the microresonator is expected to be very thin (for example, less than 10 μm), a very thin and light coating is more desirable than a thick and heavy coating like a common gold black in order to reduce the mass loading effect which degrades the Q factor. The acoustic effect caused by such a light coating will decrease the center frequency slightly, but the overall effect is negligibly small.

Fig. 1 shows the schematic of a microresonator. The dimensions and orientations used in this paper are shown in Fig. 2. The plate of AC-cut (31°46' rotated y-cut) is considered here due to its close orientation to AT-cut. Many high frequency AT-cut resonators are being currently manufactured using wet etching techniques in industries. The AC-cut plate has the lowest frequency constant of 1656 KHz mm among rotated y-cut plates, a frequency temperature coefficient of +20 ppm/°C, and the freedom from coupling to face-shear modes, which makes it relatively free from frequency perturbations [8].

The electrode design shown in this paper is performed in terms of the acoustical energy trapping only. The equivalent circuit parameters of the resonator varies as the dimensions of the electrode changes. The simple expressions to calculate the parameters associated with electrode geometry and quartz thickness can be found elsewhere [8], and its calculation is not presented here.

Simple Thickness Solutions

When the displacements and electric potential are functions of only, the so called simple thickness modes are obtained. In general, three cases will be considered: 1.) two free surfaces, open circuit on top and bottom, 2.) two electroded surfaces, short circuit on top and bottom, and 3.) with the top surface free and open circuit, and the bottom surface electroded and shorted. The general solution for case 1.) is given by [9]

\[ u_1 = B_1 \sin \eta_n x_2, \quad \phi = \frac{e_{2kz}}{\varepsilon_{22}} u_k, \quad \eta_n = \frac{n \pi}{2h}, \quad \text{and} \]

\[ \omega_n = \frac{n \pi}{2h} \sqrt{\frac{c(1)}{\rho}}, \quad (1) \]

where \( u_1 \) is the displacement component along \( x_1 \), \( \phi \) is the electric potential, \( \eta_n \) is the wave number along \( x_2 \) for the \( n^{th} \) odd harmonic, and \( \omega_n \) is the corresponding frequency for a plate of thickness \( 2h \). For case 2.) the mechanical displacement, electric potential, wave number and frequency for the \( n^{th} \) odd harmonic are given as [9]

\[ u_1 = B_1 \sin \eta_n x_2, \quad \phi = \frac{e_{2kz}}{\varepsilon_{22}} \left[ u_k - \frac{x_2}{h} u_k(h) \right], \]

\[ \eta_n = \frac{n \pi}{2h} \left[ 1 - \frac{4k_1^2}{n^2 \pi^2} - R \right], \quad \text{and} \]

\[ \omega_n = \frac{n \pi}{2h} \sqrt{\frac{c(1)}{\rho}} \left[ 1 - \frac{4k_1^2}{n^2 \pi^2} - R \right], \quad (2) \]

where \( k_1^2 = \frac{e_{26}^2}{\varepsilon_{22} c(1)} \), and \( R = \frac{2p'h'}{\rho h} \)

represent, respectively, the piezoelectric coupling factor and mass ratio of the electrodes with \( c(1) \) the eigenvalue corresponding to the dominant thickness shear mode, and \( 2h' \) the thickness of the electrode plating on the top and bottom surfaces. When the top surface is free and open circuit, and the bottom surface electroded and shorted as described in case 3.), these quantities are given as

\[ u_1 = B_1 (\sin \eta_n x_2 + \beta_n \cos \eta_n x_2), \]

\[ \phi = \frac{e_{2kz}}{\varepsilon_{22}} [u_k - u_k(-h)], \quad \eta_n = \frac{n \pi}{2h} \left[ 1 - R' \right], \]

\[ \omega_n = \frac{n \pi}{2h} \sqrt{\frac{c(1)}{\rho}} \left[ 1 - R' \right], \quad \beta_n = \frac{n \pi}{2} R', \quad \text{and} \]

\[ R' = \frac{p'h''}{\rho h}, \quad (3) \]

where \( 2h'' \) is the thickness of the electrode plating. In Eq. 3, the quantity \( \beta_n \) represents the relative amplitude of a displacement component, even in \( x_2 \), which is caused by
the mass imbalance on the major surfaces. It should be noted that \( \beta_n \) is of \( O(R') \) which is typically a few percent.

**Asymptotic Solutions For a Strip**

The asymptotic solution for a strip operating in the vicinity of an odd overtone of thickness shear is given by Tiersten’s analysis [9] and is repeated here. For the unelectroded case

\[
\begin{align*}
    u_1 &= \left( B_1 \sin \eta_1 x_2 - r \frac{\xi}{\eta_2} B_2 \sin \eta_2 x_2 \right) \cos \xi x_1, \\
    u_2 &= \left( r \frac{\xi}{\eta_1} B_1 \cos \eta_1 x_2 + B_2 \cos \eta_2 x_2 \right) \sin \xi x_1,
\end{align*}
\]

where \( \eta_1 \) and \( \eta_2 \) are thickness wave numbers and \( \xi \) is the propagation wave number along \( x_1 \). For the electroded case, identical quantities are obtained as

\[
\begin{align*}
    u_1 &= \left( B_1 \sin \eta_1 x_2 - r \frac{\xi}{\eta_2} B_2 \sin \eta_2 x_2 \right) \cos \xi x_1, \\
    u_2 &= \left( r \frac{\xi}{\eta_1} B_1 \cos \eta_1 x_2 + B_2 \cos \eta_2 x_2 \right) \sin \xi x_1.
\end{align*}
\]

Following a procedure which parallels Tiersten’s [9], equivalent expressions for case 3.) are obtained as

\[
\begin{align*}
    u_1 &= \left[ \tilde{B}_1 \left( \sin \tilde{\eta}_1 x_2 + \beta^{(1)} \cos \tilde{\eta}_1 x_2 \right) \
        - r \frac{\tilde{\xi}}{\tilde{\eta}_2} \tilde{B}_2 \left( \sin \tilde{\eta}_2 x_2 - \beta^{(2)} \cos \tilde{\eta}_2 x_2 \right) \right] \cos \tilde{\xi} x_1, \\
    u_2 &= \left[ r \frac{\tilde{\xi}}{\tilde{\eta}_1} \tilde{B}_1 \left( \cos \tilde{\eta}_1 x_2 - \beta^{(1)} \sin \tilde{\eta}_1 x_2 \right) + \tilde{B}_2 \left( \cos \tilde{\eta}_2 x_2 + \beta^{(2)} \sin \tilde{\eta}_2 x_2 \right) \right] \sin \tilde{\xi} x_1,
\end{align*}
\]

where

\[
\beta^{(1)} = \tilde{\eta}_1 h R' \quad \text{and} \quad \beta^{(2)} = \kappa \beta^{(1)} \tag{10}
\]

In obtaining Eqs. 8, 9, and 10, small terms have been neglected, as in [9], except the terms which are first order in \( R \) ratio are retained in the relative amplitude coefficients, i.e. \( \beta^{(1)} \) and \( \beta^{(2)} \). For all three cases,

\[
B_2 = \frac{(-1)^{(n+1)/2} (c_{22} r + c_{12}) \xi}{c_{22} \eta_2 \sin \eta_2 h} B_1, \tag{11}
\]

\[
\eta_2 = \kappa \eta_1 \quad \text{and} \quad \kappa = \sqrt{\frac{\tilde{c}_{66}}{c_{22}}}. \tag{12}
\]

Comparison of the preceding equations shows that to within \( O(R) \), the three solutions are identical, and it can be shown that the asymptotic relations for the small frequency deviation caused by dispersion along the plate directions are also identical to within error of order \( R \).

**Design Procedure**

To simplify the design procedure, an approximate model is used to obtain optimal electrode dimensions. Since the dispersion relations are nearly identical for the three cases examined, it is sufficient to match the cutoff frequencies in the center regions and in the ring region to allow the structure to be viewed as one containing solid electrodes on a flat plate, as shown in Fig. 4. The conditions to be satisfied by center electrodes/quartz for the equivalent flat plate-solid electrode model are given as follows: For case I

\[
h'' = \frac{4 k_1^2 \rho}{n^2 \pi^2} h + 2 h'. \tag{13}
\]

For small piezoelectric coupling, this condition reduces to

\[
h'' \approx 2 h'. \tag{14}
\]

For case II

\[
\dot{h}_1 = \frac{h}{\sqrt{1 - \frac{4 k_1^2}{n^2 \pi^2} - R}}. \tag{15}
\]

For small piezoelectric coupling, this condition reduces to

\[
h_1 \approx \frac{h}{1 - R}. \tag{16}
\]

And for case III,

\[
h_1 = \frac{\left[ 1 - R \right]}{\frac{4 k_1^2}{n^2 \pi^2} \left[ 1 - \frac{1 - R}{\frac{4 k_1^2}{n^2 \pi^2} - R} \right]} h. \tag{17}
\]

and for small piezoelectric coupling.
Development of Finite Element Equations For a Strip

A more detailed analysis for the partially electroded strip can be performed using the finite element method. Solutions obtained from the finite element analysis can be used to compare with the approximate solutions obtained using the assumptions of the previous section. As with the asymptotic analysis, the planar variations of the electric variables are assumed to be negligible, and the same mass loading effects of the thin electrodes are assumed. With these assumptions, the equations of Motion are given as

\[ \ddot{c}_{ijkl} u_{k,i} - \rho \dot{u}_j = 0, \]

where \( \ddot{c}_{ijkl} = c_{ijkl} + \frac{e_{2ij} e_{2k2}}{\varepsilon_{22}} \delta_{2l} \)

are effective elastic constants, with

\[ \phi = \frac{e_{2k2}}{\varepsilon_{22}} \mu_k \]

in region I of Fig. 3, and

\[ \phi = \frac{e_{2k2}}{\varepsilon_{22}} \left[ u_k - \frac{1}{2} \left( u_k^+ - u_k^- \right) \right] \]

in region II. With these forms of the electric potential the stresses are given as

\[ T_{ij} = \ddot{c}_{ijkl} u_{k,i} \]

in region I, and

\[ T_{ij} = \ddot{c}_{ijkl} u_{k,i} - \frac{1}{2h} \frac{e_{2ij} e_{2k2}}{\varepsilon_{22}} \left( u_k^+ - u_k^- \right) \]

in region II. Likewise, the electric displacement is given as

\[ D_2 = 0 \]

in region I, and

\[ D_2 = -\frac{1}{2h} e_{2k2} \left( u_k^+ - u_k^- \right) \]

in region II.

The boundary conditions on the major surfaces in region II are given as

\[ T_{2j} = \mp 2h' \rho' \omega^2 u_j \quad \text{on } \Gamma_e^{+/-}. \]

The development of the finite element equations begins with the variational form of the equations of motion

\[ \int \left[ T_{ij} \delta u_{j,i} - \rho \omega^2 u_j \delta u_j \right] dA = \int_{\Gamma_e} 2h' \rho' \omega^2 u_j \delta u_j d\Gamma \]

The finite element discretization process is applied by interpolating the displacements with a set of shape functions, \( N_p \) as follows:

\[ u_j = N_p \hat{u}_j \]

where \( \hat{u}_j \) are the nodal displacements. In Eq. 22 the superscripts are intended to imply a sum over nodes within an element or an entire mesh, depending upon context. This notation will be employed throughout to save space. The shape functions \( N_p \) may take on several forms and will not be explicitly defined here. The reader is referred to [11] and [12] for these and other omitted finite element definitions. Using the shape functions in Eq. 21 gives

\[ \int \Omega \ddot{c}_{ijkl} \frac{\partial N_p \partial N_q}{\partial x_i \partial x_j} d\Omega - \int_{\Gamma_e} \frac{e_{2ij} e_{2k2}}{\varepsilon_{22}} N_p \frac{\partial N_q}{\partial x_j} d\Gamma + \int_{\Gamma_p} 2h' \rho' \int N_p N_q d\Gamma \delta_{ik} \]

which can be written as

\[ \left[ K_{pq}^{ik} + \bar{K}_{pq}^{ik} \right] \hat{u}_k - \omega^2 \left[ M_{pq}^{ik} + \bar{M}_{pq}^{ik} \right] \hat{u}_k = 0 \]

where

\[ K_{pq}^{ik} = \int \ddot{c}_{ijkl} \frac{\partial N_p}{\partial x_i} \frac{\partial N_q}{\partial x_j} d\Omega \]

is the usual stiffness matrix,

\[ \bar{K}_{pq}^{ik} = -\int_{\Gamma_e} \frac{e_{2ij} e_{2k2}}{\varepsilon_{22}} N_p \frac{\partial N_q}{\partial x_j} d\Gamma + \int_{\Gamma_p} e_{2ij} e_{2k2} N_p \frac{\partial N_q}{\partial x_j} d\Gamma \]

and

\[ M_{pq}^{ik} = \int \frac{e_{2ij} e_{2k2}}{2h} N_p \frac{\partial N_q}{\partial x_j} d\Omega \]

is the usual mass matrix.
is the addition to the stiffness caused by the shorting of the major surfaces in region II,

\[ M_{ik}^p = \rho \int N^p N^q d\Omega \delta_{ik} \]  (33)

is the usual mass matrix, and

\[ \overline{M}_{ik} = 2h'p' \int N^p N^q d\Gamma \delta_{ik} \]  (34)

is the addition to the mass matrix caused by the mass loading of the electrodes on the major surfaces in region II. Eq. 30 represents corrections which can be made to the usual finite element formulation to allow an approximate accounting of the effects of piezoelectricity and electrode plating. It should be noted that the present formulation is very specific to the case of a single pair of perfectly parallel electrodes on surfaces normal to \( x_2 \), and not to a general case of multiple, arbitrarily placed electrodes.

Fig. 5 shows graphically the results of a finite element study performed on an AC-cut quartz strip with an aluminum ring electrode of thickness 1000 \( \mu \)m on the top surface, and a solid electrode on the bottom surface with variable center thickness (case I). The curves which have been plotted represent the distribution of the \( u_1 \) displacement component sampled on the top and bottom surfaces of the plate. The outer most curve (solid line) represents the case when \( 2h'' = 0 \), a ring electrode on top and bottom. It is observed that in this case, the mode strength is diminished in the center region with a distribution which closely follows \( \cosh (\xi x_1) \). The inner most curve represents the case when \( 2h'' = 2000 \) \( \mu \)m which satisfies the condition in Eq. 14. In this case the distribution of the \( u_1 \) displacement component closely matches the behavior of a trapped energy resonator with a solid electrode on top and bottom, in which case the distribution of \( u_1 \) closely follows \( \cos (\xi x_1) \). This resemblance is further illustrated in Fig. 6. This figure shows a comparison of the finite element solution shown in Fig. 5 with \( 2h'' = 2000 \) \( \mu \)m with a solution of Stevens and Tiersten's asymptotic equations [10] for a plate with a solid square electrode of thickness \( 2h' = 1000 \) \( \mu \)m on the top and bottom surfaces. The \( u_1 \) displacement component is seen to match almost identically for the two solutions.

### Design Lengths For Square Electrode Patterns

Table I: \( 2h'_{\text{max}} \) For 1 trapped mode using square electrodes  

<table>
<thead>
<tr>
<th>( h ) (( \mu )m)</th>
<th>( 2h'_{\text{max}}=0.9X10^{-7} )</th>
<th>( 2h'_{\text{max}}=1.0X10^{-7} )</th>
<th>( 2h'_{\text{max}}=1.1X10^{-7} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>13.377443</td>
<td>12.711981</td>
<td>12.136874</td>
</tr>
<tr>
<td>4</td>
<td>37.226933</td>
<td>35.430105</td>
<td>33.870630</td>
</tr>
<tr>
<td>6</td>
<td>67.321794</td>
<td>64.166148</td>
<td>61.416342</td>
</tr>
<tr>
<td>8</td>
<td>102.07846</td>
<td>97.427824</td>
<td>93.359912</td>
</tr>
<tr>
<td>10</td>
<td>140.56134</td>
<td>134.33215</td>
<td>128.86390</td>
</tr>
</tbody>
</table>

When the conditions defined by Eqs. 13 through 18 are met, energy trapping parameters can be calculated for the electrode lengths for the three cases using Stevens and Tiersten's analysis [10], the details of which are not shown here. The reader is referred to [10] for a detailed discussion of trapped energy resonators with rectangular electrodes. Listed in Table I are the maximum electrode lengths for a single trapped mode for square aluminum electrodes on AC-cut quartz. These values are also plotted in Fig. 7.

### Conclusion

The unique metallization structures proposed here are formed by depositing ring electrodes on one or both sides of a flat plate to allow maximum IR absorption in the center region, while achieving good energy trapping, without the use of contouring. To design such structures, a simplified model has been employed which allows the resonator to be approximated as a conventional crystal plate with solid electrodes on top and bottom. This model is valid only when careful proportioning of the center thicknesses of quartz and/or metal is achieved. The accuracy of this model's ability to predict the fundamental thickness shear mode has been verified by comparison with a very accurate finite element solution.

Further analysis is necessary to determine the effects of coupling of the thickness shear mode to various unwanted modes which can perturb the frequency-temperature behavior of the resonator. Coupling with other modes of vibration can cause so called activity dips in the normally smooth frequency-temperature curve for the thickness shear mode, which can potentially effect the performance of a thermal sensor. In addition to this, the thermal and acoustic effects of various IR absorbing coatings needs to be investigated, as well as the steady state and transient thermoelastic behavior of the structure.
References

Fig. 4. Three basic design concepts can be approximately modeled as a flat plate with solid electrodes.

Equivalent Flat Plate With Solid Electrodes

Fig. 5. Finite element solution sampled on top and bottom surfaces for case I.

Fig. 6. Comparison of finite element solution for fundamental thickness shear mode sampled at the top surface for case I with approximate asymptotic solution using equivalent flat plate solid electrode model.

Fig. 7. Maximum electrode lengths as a function of thickness for square aluminum electrodes on AC-cut quartz. Data taken from Table I.