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Abstract In this paper, we investigate free thickness-shear and thickness-twist vibrations of a finite crystal resonator of AT-cut quartz carrying a thin mass layer at the central portion of its top surface operating as a quartz crystal microbalance. The equations of anisotropic elasticity are used with the omission of the small elastic constant c_{56} . An analytical solution is obtained using Fourier series from which the resonant frequencies, mode shapes and vibration confinement by the mass layer are calculated and examined.

1 Introduction

Resonant frequencies of an elastic or piezoelectric body can be affected by many effects like a temperature change, initial stress, surface mass layers, contact with a fluid, etc. Therefore frequency shifts in a vibrating body (resonator) can be used to make various acoustic wave sensors. Piezoelectric crystals are often used so that the operating mode can be directly excited electrically. Otherwise transducers are needed for the excitation and detection of acoustic modes. Specifically, when a thin layer of another material is added to the surface of a resonator, the resonant frequencies of the resonator become lower due to the inertia of the mass layer [1–5]. This effect has been used to make mass sensors for measuring the density and thickness of the layer. These mass sensors are called quartz crystal microbalances (QCMs) and have important applications in monitoring thin film deposition and in chemical and biological sensing [6].

A typical QCM operates with the fundamental thickness-shear (TSh) mode of a quartz plate. Theoretically TSh modes can only exist in unbounded plates without edge effects [7, 8]. In these modes, motions of material particles are parallel to the surfaces of the plate, and particle velocities vary along the plate thickness only, without in-plane variations. These TSh modes are the ideal operating modes of many acoustic wave devices. In reality, however, due to the finite sizes of devices, the crystal plates are finite and pure TSh modes cannot exist because of edge effects. Therefore, in real devices, the operating modes have slow in-plane variations in the plates. These modes are referred to as transversely varying TSh modes [9]. There exist relatively systematic theoretical results for TSh modes with in-plane variation only in the direction parallel to the TSh particle velocity, either from the exact three-dimensional (3D) equations of anisotropic elasticity or piezoelectricity, or the corresponding approximate two-dimensional plate equations [10]. In the case when the in-plane mode variation is in the direction perpendicular to the TSh particle velocity, the corresponding modes are called thickness-twist (TT) modes [11]. For this case reported studies are much fewer, especially from the 3D equations which are what is relevant to the present paper. Propagating waves in unbounded plates with or

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without mass layers were studied in [11–14]. Since crystal devices are made smaller and smaller for device miniaturization, edge effects have become more pronounced and in-plane variations in both of the in-plane directions are equally important. It is our recent general effort to provide new knowledge of TT waves to reach the same level of understanding as the in-plane variation in the other direction.

An important issue in QCM design is the mass layer size when the layer covers the central portion of the crystal plate only. In such a case the inertia of the mass layer affects the so-called energy trapping through which the vibration is confined under the mass layer and decays rapidly outside it. Energy trapping is crucial to device mounting. It is relatively better understood in quartz TSh resonators with a pair of identical electrodes or effectively two mass layers at the plate top and bottom surfaces. For a QCM, there is essentially only one mass layer on one side of the plate which breaks the symmetry about the plate's middle plane. Its effects on energy trapping and other vibration characteristics are relatively less known. In this paper we study energy trapping of TSh and TT modes in a finite-size QCM with a partial mass layer. The equations of anisotropic elasticity are used instead of the approximate plate equations. We want to examine how the resonant frequencies, mode shapes, and energy trapping are affected by the mass layer and its dimension.

2 Governing equations

The equations for anisotropic crystals vary considerably according to crystal symmetry. A particular cut of a crystal plate refers to the orientation of the plate when it is taken out of a bulk crystal. As a consequence crystal plates of different cuts exhibit different anisotropies in coordinates normal and parallel to the plate surfaces. The most widely used AT-cut quartz plate is a special case of rotated Y-cut quartz plates which are effectively monoclinic in the plate coordinate system. Consider an AT-cut quartz plate as shown in Fig. 1. The plate is unbounded in the x_1 direction and does not vary along x_1 . Figure 1 shows a cross section. It carries a thin mass layer at the central portion of the top surface. This structural configuration is typical for QCMs. The mass layer may be due to the selective film often used in QCMs and the measurand attracted to the film or their combination. As long as they are very thin, only their combined inertia matters and their stiffness can be neglected in the lowest-order approximation [2]. Quartz has very weak piezoelectric coupling [15]. For free vibration frequency analysis the small piezoelectric coupling is usually neglected and an elastic analysis is sufficient. For monoclinic crystals, shear-horizontal (SH) or antipplane motions with only one displacement component are allowed by the linear theory of anisotropic elasticity. The corresponding modes are TT modes in general and include TSh and face-shear modes as special cases. SH motions in rotated Y-cut quartz are described by

$$u_1 = u_1(x_2, x_3, t), \quad u_2 = u_3 = 0, \quad (1)$$

where $\mathbf{u}$ is the displacement vector. The nonzero components of the strain tensor S and the stress tensor T are:

$$S_5 = 2S_{31} = u_{1,3}, \quad S_6 = 2S_{21} = u_{1,2}, \quad (2)$$

$$T_{31} = c_{55}u_{1,3} + c_{56}u_{1,2}, \quad T_{21} = c_{56}u_{1,3} + c_{66}u_{1,2}, \quad (3)$$

where c is the elastic stiffness tensor. The relevant equation of motion is

$$T_{21,2} + T_{31,3} = \rho \ddot{u}_1. \quad (4)$$

The equation to be satisfied by u_1 is obtained by substituting (3) into (4), giving

$$c_{66}u_{1,22} + c_{55}u_{1,33} + 2c_{56}u_{1,23} = \rho \ddot{u}_1. \quad (5)$$

For the plate in Fig. 1, the boundary condition at the plate top surface is

$$T_{21} = \begin{cases} -2\rho'h'\ddot{u}_1, & x_2 = h, \quad |x_3| < a, \\ 0, & x_2 = h, \quad a < |x_3| < b, \end{cases} \quad (6)$$

where ρ' and $2h'$ are the density and thickness of the mass layer. In $|x_3| < a$, the boundary condition in (6) represents Newton's second law applied to the mass layer. The plate bottom surface is traction free with

$$T_{21} = 0, \quad x_2 = -h, \quad |x_3| < b. \quad (7)$$

Fig. 1 An AT-cut quartz plate with a partial mass layer

The boundary conditions at the left and right edges are

$$T_{31} = 0, \quad x_3 = \pm b, \quad |x_2| < h. \quad (8)$$

Due to the c_{56} term with mixed derivatives, (5) is not separable and thus presents considerable mathematical challenges. In spite of the importance of the problem, known theoretical results are limited to unbounded plates [11–14]. For the practically more useful case of finite rectangular plates there are little theoretical results. The fact that the mass layer covers only part of the plate surface and the related piecewise boundary condition in (6) make the problem more challenging. Therefore, for quite some time there has been little theoretical progress on this topic. For AT-cut quartz plates, $c_{55} = 68.81 \times 10^9 \text{ N/m}^2$, $c_{56} = 2.53 \times 10^9 \text{ N/m}^2$, and $c_{66} = 29.01 \times 10^9 \text{ N/m}^2$ [15]. c_{56} is very small compared to c_{55} and c_{66} . Therefore, in the rest of this paper, we will make the usual approximation of neglecting the small c_{56} [16]. This approximation has been used in analyzing quartz resonators but not in mass sensors. With this approximation, (5) becomes separable.

3 Fourier series solution

Consider free vibrations. Let

$$u_1(x_2, x_3, t) = u_1(x_2, x_3) \exp(i\omega t). \quad (9)$$

The plate in Fig. 1 is symmetric in x_3 . For resonator and QCM applications, we are interested in modes that are even in x_3 . However, in the x_2 direction, the presence of the mass layer destroys the symmetry about the plate middle plane and hence both odd and even functions of x_2 are needed. Therefore we construct the following solution from separation of variables:

$$u_1 = A_0 \cos(\eta_0 x_2) + B_0 \sin(\eta_0 x_2) + \sum_{m=1}^{\infty} [A_m \cos(\eta_m x_2) + B_m \sin(\eta_m x_2)] \cos \frac{m\pi x_3}{b}, \quad (10)$$

where A_0 , B_0 , A_m and B_m are undetermined constants, and

$$\eta_m^2 = \frac{\rho \omega^2}{c_{66}} - \frac{c_{55}}{c_{66}} \left(\frac{m\pi}{b} \right)^2 = \frac{\pi^2}{4h^2} \left[\frac{\omega^2}{\omega_s^2} - \frac{c_{55}}{c_{66}} \left(m \frac{2h}{b} \right)^2 \right], \quad m = 0, 1, 2, 3, \dots, \quad (11)$$

$$\omega_s = \frac{\pi}{2h} \sqrt{\frac{c_{66}}{\rho}}. \quad (12)$$

Equation (10) satisfies (5) and (8). ω_s is the resonant frequency of the fundamental TSh mode in an unbounded quartz plate without mass layers. Resonators and QCMs operating with TSh modes are usually with large length/thickness ratios, i.e., $b \gg h$. In this case, for an m that is not large, η_m^2 is positive. We are interested in the first few TSh and TT modes with no more than a couple of nodal points along the x_3 direction for which a large m is not needed. In the case when η_m^2 is nonpositive, the construction of the solution in (10) will be different. To apply the boundary conditions at the plate top and bottom, we need

$$T_{21} = c_{66} u_{1,2} = -c_{66} A_0 \eta_0 \sin(\eta_0 x_2) + c_{66} B_0 \eta_0 \cos(\eta_0 x_2) + c_{66} \sum_{m=1}^{\infty} [-A_m \eta_m \sin(\eta_m x_2) + B_m \eta_m \cos(\eta_m x_2)] \cos \frac{m\pi x_3}{b}. \quad (13)$$

Fig. 2 Reference case. $a = 7.5$ mm and $R = 3\%$. Two trapped modes

Substitution of Eqs. (10) and (13) into (6) and (7) gives

$$\begin{aligned}
 & -c_{66}A_0\eta_0 \sin(\eta_0 h) + c_{66}B_0\eta_0 \cos(\eta_0 h) \\
 & + c_{66} \sum_{m=1}^{\infty} [-A_m\eta_m \sin(\eta_m h) + B_m\eta_m \cos(\eta_m h)] \cos \frac{m\pi x_3}{b} \\
 & = \begin{cases} 2\rho'h'\omega^2[A_0 \cos(\eta_0 h) + B_0 \sin(\eta_0 h)] \\ \quad + 2\rho'h'\omega^2 \sum_{m=1}^{\infty} [A_m \cos(\eta_m h) + B_m \sin(\eta_m h)] \cos \frac{m\pi x_3}{b}, & |x_3| < a, \\ 0, & a < |x_3| < b, \end{cases} \quad (14)
 \end{aligned}$$

$$\begin{aligned}
 & c_{66}A_0\eta_0 \sin(\eta_0 h) + c_{66}B_0\eta_0 \cos(\eta_0 h) \\
 & + c_{66} \sum_{m=1}^{\infty} [A_m\eta_m \sin(\eta_m h) + B_m\eta_m \cos(\eta_m h)] \cos \frac{m\pi x_3}{b} = 0, \quad |x_3| < b. \quad (15)
 \end{aligned}$$

Fig. 3 Effects of a longer mass layer on the distribution of the trapped modes. $a = 11.5$ mm and $R = 3\%$. Two trapped and wider modes

We multiply both sides of (14) by $\cos(n\pi x_3/b)$ ($n = 0, 1, 2, \dots$) and integrate the resulting expression over $(-b, b)$ to obtain

$$\begin{aligned} & \left[-c_{66}A_0\eta_0 \sin(\eta_0 h) + c_{66}B_0\eta_0 \cos(\eta_0 h) \right] 2b \\ &= 2\rho'h'\omega^2 [A_0 \cos(\eta_0 h) + B_0 \sin(\eta_0 h)] 2a \\ &+ 2\rho'h'\omega^2 \sum_{m=1}^{\infty} [A_m \cos(\eta_m h) + B_m \sin(\eta_m h)] \frac{2b}{m\pi} \sin \frac{m\pi a}{b} \Bigg], \quad n = 0, \end{aligned} \quad (16)$$

$$\begin{aligned} & c_{66}[-A_n\eta_n \sin(\eta_n h) + B_n\eta_n \cos(\eta_n h)]b \\ &= 2\rho'h'\omega^2 [A_0 \cos(\eta_0 h) + B_0 \sin(\eta_0 h)] \frac{2b}{n\pi} \sin \frac{n\pi a}{b} \\ &+ 2\rho'h'\omega^2 \sum_{m=1}^{\infty} [A_m \cos(\eta_m h) + B_m \sin(\eta_m h)] C_{nm}, \quad n = 1, 2, 3, \dots, \end{aligned} \quad (17)$$

Fig. 4 Effects of a longer mass layer on the number of trapped modes. $a = 13$ mm and $R = 3\%$. Three trapped modes

Fig. 5 Effects of a shorter mass layer on the number of trapped modes. $a = 6$ mm and $R = 3\%$. One trapped mode

where

$$C_{nm} = \int_{-a}^a \cos \frac{n\pi x_3}{b} \cos \frac{m\pi x_3}{b} dx_3 = C_{mn}, \quad m, n = 1, 2, 3, \dots \quad (18)$$

Similarly, from (15) we obtain

$$c_{66}A_0\eta_0 \sin(\eta_0 h) + c_{66}B_0\eta_0 \cos(\eta_0 h) = 0, \quad (19)$$

$$A_n\eta_n \sin(\eta_n h) + B_n\eta_n \cos(\eta_n h) = 0, \quad n = 1, 2, 3, \dots \quad (20)$$

Equations (16), (17), (19) and (20) are linear homogeneous equations for A_0 , B_0 , A_m and B_m . For nontrivial solutions the determinant of the coefficient matrix has to vanish, which determines the resonant frequencies. The nontrivial solutions of A_0 , B_0 , A_m and B_m determine the corresponding modes. This is a complicated eigenvalue problem because the eigenvalue or the resonant frequency is present in every η_m . To simplify these equations a little we solve (19) and (20) for A_0 and A_m :

$$\begin{aligned} A_0 &= -B_0 \cot(\eta_0 h), \quad n = 0, \\ A_n &= -B_n \cot(\eta_n h), \quad n = 1, 2, 3, \dots \end{aligned} \quad (21)$$

Substitution of Eqs. (21) into (16) and (17) results in the following linear equations for B_0 and B_m :

$$\begin{aligned} &\left[c_{66} \cos(\eta_0 h) \eta_0 b + \rho' h' \omega^2 \frac{\cos(2\eta_0 h)}{\sin(\eta_0 h)} a \right] B_0 \\ &= \sum_{m=1}^{\infty} -B_m \rho' h' \omega^2 \frac{\cos(2\eta_m h)}{\sin(\eta_m h)} \frac{b}{m\pi} \sin \frac{m\pi a}{b}, \quad n = 0, \end{aligned} \quad (22)$$

$$\begin{aligned} &2B_0 \rho' h' \omega^2 \frac{\cos(2\eta_0 h)}{\sin(\eta_0 h)} \frac{b}{n\pi} \sin \frac{n\pi a}{b} \\ &+ \sum_{m=1}^{\infty} \left[c_{66} \cos(\eta_m h) \eta_m b \delta_{nm} + \rho' h' \omega^2 \frac{\cos(2\eta_m h)}{\sin(\eta_m h)} C_{nm} \right] B_m = 0, \quad n = 1, 2, 3, \dots \end{aligned} \quad (23)$$

Fig. 6 Effects of a thicker mass layer on the number of trapped modes. $a = 11.5$ mm and $R = 4\%$. Three trapped modes

4 Numerical results and discussions

For quartz, $\rho = 2649 \text{ kg/m}^3$ [15]. We also introduce another frequency

$$\bar{\omega}_s = \omega_s(1 - R), \quad R = \frac{\rho' h'}{\rho h}. \quad (24)$$

$\bar{\omega}_s$ is the resonant frequency of the fundamental TSh mode in an unbounded quartz plate fully covered by a mass layer at the plate top surface. R is the mass ratio between the layer and the crystal plate. The resonant frequencies of the modes we are interested in are within $\bar{\omega}_s < \omega < \omega_s$. In this narrow frequency range we have trapped modes useful in devices. We fix the plate thickness $2h = 1 \text{ mm}$ and the plate length $b = 20 \text{ mm}$.

We begin with the case when the film length $a = 7.5 \text{ mm}$ and the mass ratio $R = 3\%$. This will be used as a reference case for later comparisons. In this case two resonant frequencies are found within $\bar{\omega}_s < \omega < \omega_s$. When using 9 and 10 terms in the series, the two frequencies are always found to be $\omega_1/\omega_s = 0.974089$ and $\omega_2/\omega_s = 0.996126$. Numerical tests show that A_0, B_0, A_n and B_n are very sensitive to the frequencies. Six significant figures are used to ensure sufficient accuracy of the frequencies. In this case the corresponding modes also converge very well, without noticeable differences. Therefore all calculations below are based on

Fig. 7 Effects of a thinner mass layer on the number of trapped modes. $a = 7.5 \text{ mm}$ and $R = 2\%$. One trapped mode

Fig. 8 Effects of the mass layer on the displacement distributions at the plate top and bottom surfaces. $a = 7.5 \text{ mm}$ and $R = 10\%$

calculations using 10 terms in the series. In this case η_m^2 is positive. 12 or more terms will make η_m^2 negative. The two modes corresponding to the two frequencies are shown in Fig. 2 which is not drawn to scale. The vibration in Fig. 2 is large in the central region and small near the plate edges. In other words the vibration is mainly under the mass layer and decays outside the layer. This is the so-called energy trapping of TSh and TT modes. The first mode has no nodal points along the x_3 direction and is the mode of interest and useful in applications. It is a transversely varying TSh mode. The second mode has two nodal points along the x_3 direction and is a TT mode.

If we keep $R = 3\%$ and increase the mass layer length to $a = 11.5$ mm, there are still two resonant frequencies within $\bar{\omega}_s < \omega < \omega_s$: $\omega_1/\omega_s = 0.972518$ and $\omega_2/\omega_s = 0.984604$. They are slightly lower than in the previous case because of the longer mass layer and more inertia. The corresponding modes are shown in Fig. 3. They are similar to those in Fig. 2 but have wider distributions because of the longer mass layer.

If we still keep $R = 3\%$ and increase the mass layer length further to $a = 13$ mm, then three resonant frequencies appear within $\bar{\omega}_s < \omega < \omega_s$: $\omega_1/\omega_s = 0.972221$, $\omega_2/\omega_s = 0.982111$ and $\omega_3/\omega_s = 0.998867$. The first two are slightly lower than the previous case as expected. The corresponding modes are shown in Fig. 4. The first two modes are similar to those in Figs. 2 and 3. The third mode is a TT mode with four nodal points along the x_3 direction.

On the other hand, if we keep $R = 3\%$ and reduce the mass layer length to $a = 6$ mm, there exists one frequency only within $\bar{\omega}_s < \omega < \omega_s$ with $\omega_1/\omega_s = 0.975346$, slightly higher than the case of $R = 3\%$ and $a = 7.5$ mm. The corresponding mode is shown in Fig. 5. This mode has no nodal points along the x_3 direction.

In the following we examine the effect of the mass ratio R . Consider the case when $a = 11.5$ mm and $R = 4\%$. This case differs from the case in Fig. 3 by a one per cent increase of R . This causes an increase of the number of modes from two to three (see Fig. 6) with $\omega_1/\omega_s = 0.963331$, $\omega_2/\omega_s = 0.975928$ and $\omega_3/\omega_s = 0.997799$. The first two frequencies are slightly lower than in the case of $a = 11.5$ mm and $R = 3\%$.

Next consider the case when $a = 7.5$ mm and $R = 2\%$. This case differs from the case in Fig. 2 by a one percent decrease of R . This causes a drop of the number of modes from two to one (see Fig. 7) with $\omega_1/\omega_s = 0.983295$, which is slightly higher than the first mode when $a = 7.5$ mm and $R = 3\%$.

To show the effects of R on displacement distributions graphically we exaggerate the mass ratio a little and consider the case with $a = 7.5$ mm and $R = 10\%$. There are three trapped modes: $\omega_1/\omega_s = 0.914855$, $\omega_2/\omega_s = 0.942886$ and $\omega_3/\omega_s = 0.992584$. For the first mode, Fig. 8 shows the displacement distributions at the plate top $x_2 = h$ and bottom $x_2 = -h$. The modes are exactly even in x_3 but are not exactly odd in x_2 due to the mass layer. At the plate bottom there is no mass layer and the vibration amplitude is slightly larger than that at the top.

Also in the case with $a = 7.5$ mm, for two values of $R = 3$ and 10% , we plot the displacement distributions at the plate middle cross section $x_3 = 0$ in Fig. 9. The figure shows that, because of the mass layer and the related loss of symmetry about $x_2 = 0$, the nodal point along the plate thickness deviates slightly from the plate middle plane toward the plate top where the mass layer is attached. The deviation is larger for a larger R .

Fig. 9 Effects of mass layer thickness on the displacement distribution at the plate middle cross section $x_3 = 0$. $a = 7.5$ mm

5 Conclusion

A partial mass layer on one side of a QCM can lead to energy trapping of TSh and TT modes. The trapped modes are sensitive to the mass layer inertia and dimension. Typically there exist a few trapped modes near the fundamental TSh frequency. A longer and thicker mass layer tends to trap more modes and lower resonant frequencies. A longer mass layer also widens the vibration distribution. The modes are no longer exactly anti-symmetric about the plate middle plane. The plate top with the mass layer has slightly smaller displacement amplitude than the plate bottom. The nodal point of the displacement distribution along the plate thickness of the TSh mode moves toward the mass layer slightly.

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