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Effects of a Mass Layer With Gradually Varying Thickness on a Quartz Crystal Microbalance

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Effects of a Mass Layer With Gradually Varying Thickness on a Quartz Crystal Microbalance

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Abstract—We study the effects of the nonuniform thickness of a thin mass layer on a quartz crystal microbalance. A theoretical analysis is performed on thickness-shear vibration of an AT-cut quartz plate with a nonuniform mass layer. Mindlin's two-dimensional equation for thickness-shear vibration of a quartz plate is used. Free vibration frequencies and modes are obtained. The effects of the mass layer nonuniformity are examined. It is shown that resonant frequencies and energy trapping of thickness-shear modes are sensitive to mass layer nonuniformity.

Index Terms—Mass sensor, plate, resonator, thickness shear.

I. INTRODUCTION

QUARTZ CRYSTAL RESONATORS (QCRs) operating with plate thickness-shear (TSh) modes have been used for monitoring thin-film deposition and mass sensing based on the inertial effect of the thin film or mass layer on the resonant frequencies of the QCR, and are called quartz crystal microbalances (QCMs) for these applications. The effects of a thin film on a QCR are multifold, including the mass density, elastic constants (stiffness), and thickness, etc., of the thin film. In the simplest description (the well-known Sauerbrey equation), the inertia of a thin film lowers the resonant frequencies of a QCR [1], [2]. This effect alone can be used to measure the product of the thin-film mass density and thickness. Researchers also developed more sophisticated one-dimensional models based on pure TSh modes depending on the plate thickness coordinate only, showing both the inertial and stiffness effects of the mass layer [3], [4]. These thickness-mode models are valid for uniform films on unbounded plates only, without in-plane variations or boundary effects. Behaviors of real devices are more complicated for several reasons and can deviate, sometimes considerably, from the results predicted by thickness-mode models. For example, due to the so-called energy-trapping phenomenon, the TSh vibration is not uniform and is mainly under the mass layer and decays exponentially away from the mass layer edge. The in-plane variations of the
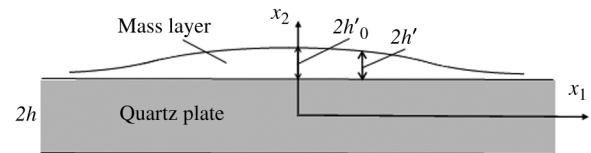
Fig. 1. A quartz plate with a nonuniform mass layer.

TSh modes also cause deviation from the Sauerbrey equation. There have been a few attempts considering the in-plane variations of TSh modes [5]–[7], but overall theoretical results are few and scattered.

Recently, it has been pointed out that the mass layer on a QCM is sometimes nonuniform and little is known about its implications [8]. This is what the present paper is concerned with. While there have been a few published results on nonuniform mass layers or nonuniform electrodes on QCRs either for mass sensing [9], [10] or for energy trapping in resonator applications [11]–[14], these analyses are all for strip resonators with modes and mass layer (or electrode) thickness variations depending on one in-plane coordinate only. For an accurate understanding of the effects of nonuniform mass layers, a more sophisticated analysis with the mass layer thickness and mode variation depending on both of the in-plane coordinates is necessary. In our previous paper [15], a mass layer with a piecewise constant thickness on a QCR was analyzed. The results of [15] showed that the variation of the mass layer thickness has significant effects on the frequencies and mode shapes of the QCR, and further study is necessary. In this paper, we study the case of a mass layer with a continuously varying thickness on a QCR, which is a more realistic situation than the stepped thickness variation considered in [15]. A theoretical analysis is performed using Mindlin's two-dimensional (2D) plate equation [16] for TSh vibrations of a quartz plate.

II. GOVERNING EQUATIONS

Consider an AT-cut quartz plate, as shown in Fig. 1. The plate has a uniform thickness $2h$ and a mass density ρ. There is a thin mass layer with a varying thickness on the top of the crystal plate. The density of the mass layer is ρ'. Its varying thickness is $2h'$. The mass layer is assumed to be very thin. Only its inertia will be considered. Its stiffness will be neglected [1], [2]. Quartz is a material with very weak piezoelectric couplings. For a frequency analysis, we will neglect the small couplings as usual. In general, TSh vibration may be coupled to flexural motion. This coupling depends on the plate dimensions and is strong only for certain aspect (length/thickness) ratios of the plate [16]. For thin plates it is less likely to happen. For our purpose, it is sufficient to assume that the coupling to flexure has been avoided through

design. Therefore, we consider TSh vibration with one displacement component $u_1(x_1, x_2, x_3, t)$ only.

Pure TSh modes are functions of the plate thickness coordinate x_2 and time t. The fundamental TSh mode is used most often in devices. It has a sinusoidal variation along the plate thickness with one nodal (zero) point at the plate middle plane. Higher order TSh modes have more nodal points along the plate thickness. For a plate with a nonuniform mass layer, these modes also have slow in-plane variations. In this paper we focus on the fundamental TSh mode.

Exact analysis of TSh modes with in-plane variations in anisotropic crystal plates using the three-dimensional equations of elasticity is mathematically very challenging and in most cases impossible. Mindlin proposed [16] to use simple and known variations along the plate thickness to approximate the modes and then obtain two-dimensional plate equations governing the in-plane variations of the modes. The small error due to the approximation can be minimized or removed using a correction factor. Mindlin's approach turned out to be very successful and many researchers followed. Specifically, for the most useful fundamental TSh mode we are considering, Mindlin used a linear variation to approximate the sinusoidal variation of the TSh displacement along the plate thickness, i.e.,

$$u_1(x_1, x_2, x_3, t) \cong x_2\psi_1(x_1, x_3, t), \quad u_2 \cong 0, \quad u_3 \cong 0 \quad (1)$$

where $\psi_1(x_1, x_3, t)$ is a slowly varying function of the in-plane coordinates x_1 and x_3. $x_2\psi_1$ has one nodal point along the plate thickness when $x_2 = 0$ which is the plate middle plane. In (1), the variation along the plate thickness is already known. What is needed to determine u_1 is a two-dimensional plate equation governing the dependence of ψ_1 on x_1 and x_3. Such an equation is obtained by multiplying the corresponding three-dimensional equation of anisotropic elasticity by x_2 and integrating it through the plate thickness (moment operation) [16]. When a crystal plate carries a mass layer, the inertial effect of the mass layer can be brought into the plate equation using the traction boundary conditions at the plate top and/or bottom surface(s) and Newton's second law governing the motion of the mass layer [17], [18]. For the specific case of a quartz plate carrying a mass layer in free TSh vibration, the governing equation for ψ_1 is [17], [18]

$$\gamma_{11}\frac{\partial^2\psi_1}{\partial x_1^2} + \gamma_{55}\frac{\partial^2\psi_1}{\partial x_3^2} - 3h^{-2}\kappa^2 c_{66}\psi_1 + (1+3R)\rho\omega^2\psi_1 = 0 \quad (2)$$

where ω is the free vibration frequency which is to be determined and

$$\kappa^2 = \frac{\pi^2}{12}(1+R), \quad R = \frac{\rho'h'}{\rho h}, \quad (3)$$

$$\gamma_{11} = \frac{s_{33}}{s_{11}s_{33} - s_{13}^2}, \quad \gamma_{55} = \frac{1}{s_{55}}. \quad (4)$$

s_{pq} are the usual elastic compliances. For AT-cut quartz, $\gamma_{11} = 79.27$, $\gamma_{55} = 49.90 \times 10^9$ N/m^2. R is the mass ratio between the mass layer and the crystal plate which is very small. We are

interested in first-order effects of R on resonant frequencies. κ is the shear correction factor introduced by Mindlin. With the correction factor, the inaccuracy of resonant frequencies predicted by (2) is higher order infinitesimals of R. For small R, (2) can be approximately rewritten as

$$\gamma_{11}\frac{\partial^2\psi_1}{\partial x_1^2} + \gamma_{55}\frac{\partial^2\psi_1}{\partial x_3^2} + \left[\rho\omega^2 - \rho\omega_\infty^2(1-2R)\right]\psi_1 = 0 \quad (5)$$

where

$$\omega_\infty^2 = \frac{\pi^2 c_{66}}{4h^2\rho}. \quad (6)$$

ω_∞ is the frequency of the fundamental TSh mode of the crystal plate when the mass layer is not present. The difference between (2) and (5) is of the order of $(\omega^2 - \omega_\infty^2)R$, which is a higher order infinitesimal because $\omega^2 - \omega_\infty^2$ is of the order of R and R is very small. We consider the case when the mass layer thickness is varying according to

$$2h' = 2h_0'\left[1 - f_1(x_1) - f_3(x_3)\right] \quad (7)$$

where $2h_0'$ is the mass layer center thickness, f_1 and f_3 are slowly growing functions so that the mass layer is thick in the center and thin away from the center. Therefore, (7) can physically describe a nonuniform mass layer. The specific choice of the thickness variation in (7) is also for the mathematical convenience below so that the problem is solvable. Corresponding to (7), from (3)$_2$, we have

$$R = R_0\left[1 - f_1(x_1) - f_3(x_3)\right] \quad (8)$$

where

$$R_0 = \frac{\rho'h_0'}{\rho h}. \quad (9)$$

Substitution of (8) into (5) gives

$$\gamma_{11}\frac{\partial^2\psi_1}{\partial x_1^2} + \gamma_{55}\frac{\partial^2\psi_1}{\partial x_3^2} +$$
$$\left[\rho\omega^2 - \rho\omega_0^2 - \rho\omega_\infty^2 2R_0(f_1 + f_3)\right]\psi_1 = 0 \quad (10)$$

where we have denoted

$$\omega_0^2 = \omega_\infty^2(1 - 2R_0). \quad (11)$$

ω_0 is the frequency of the fundamental TSh mode of a crystal plate with a mass layer of a uniform thickness $2h_0'$. We are interested in the so-called energy-trapped modes with the frequency ω within

$$\omega_0 < \omega < \omega_\infty. \quad (12)$$

These modes are large near the plate center and decay rapidly away from the center.

III. FREE VIBRATION SOLUTION

As a partial differential equation, (10) is separable. Let
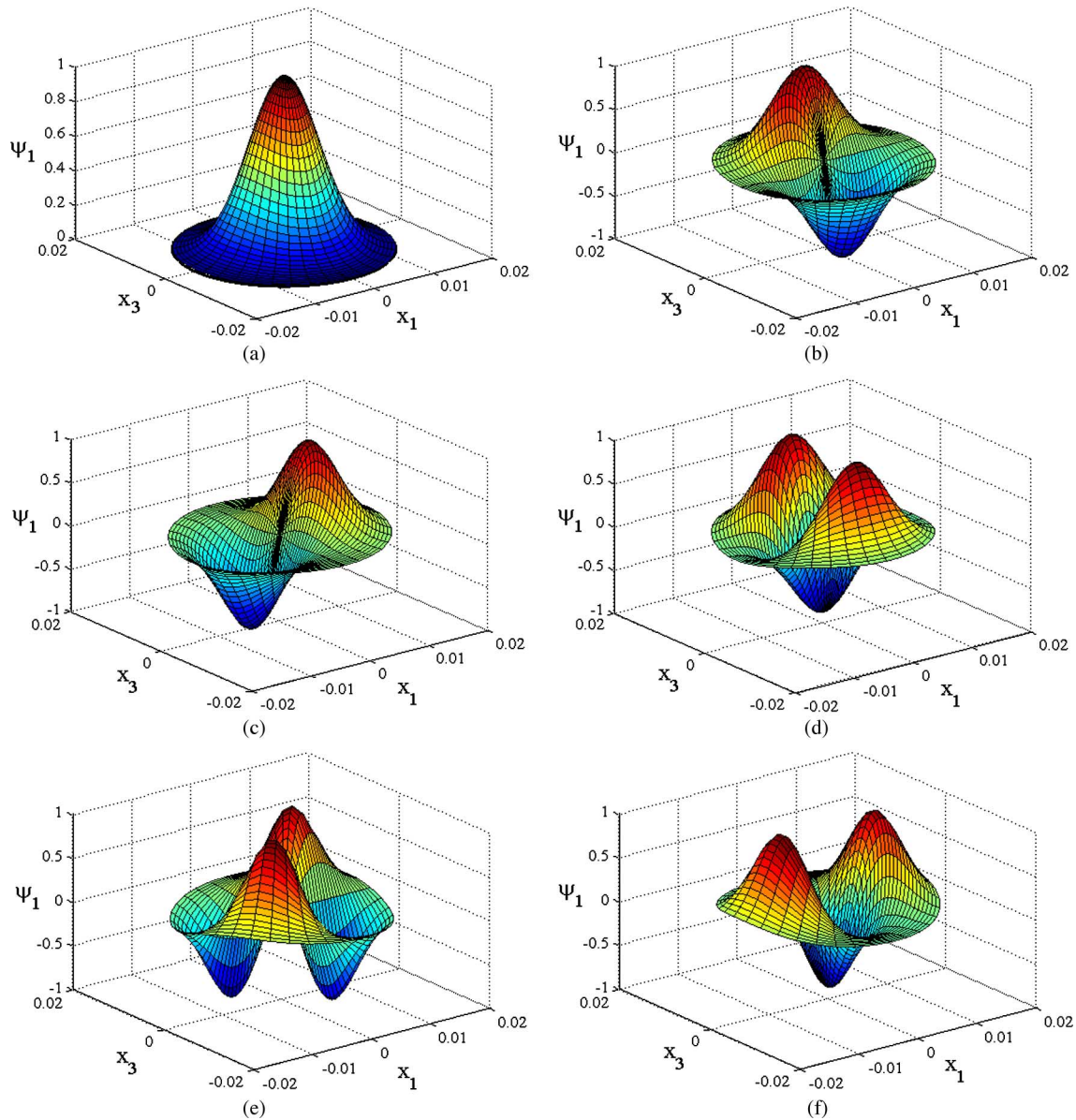
$$\psi_1(x_1, x_3) = F_1(x_1)F_3(x_3). \quad (13)$$

Fig. 2. Distribution of the TSh displacement of the first six trapped modes in the order of increasing frequency. (a) $(n_1, n_3) = (0, 0)$. (b) $(n_1, n_3) = (0, 1)$. (c) $(n_1, n_3) = (1, 0)$. (d) $(n_1, n_3) = (0, 2)$. (e) $(n_1, n_3) = (1, 1)$. (f) $(n_1, n_3) = (2, 0)$.

Then, using the standard method of separation of variables, from (10) we can obtain

$$\gamma_{11} F_{1,11} + \rho \omega_1^2 F_1 - \rho \omega_\infty^2 2 R_0 f_1(x_1) F_1 = 0$$
$$\gamma_{55} F_{3,33} + \rho \omega_3^2 F_3 - \rho \omega_\infty^2 2 R_0 f_3(x_3) F_3 = 0 \qquad (14)$$

where the separation constants ω_1 and ω_3 must satisfy the following equation from (10) which gives the resonant frequencies once ω_1 and ω_3 are determined

$$\omega^2 = \omega_0^2 + \omega_1^2 + \omega_3^2. \qquad (15)$$

To be specific, we consider the case when

$$f_1(x_1) = \beta_1 x_1^2, \quad f_3(x_3) = \beta_3 x_3^2. \qquad (16)$$

Correspondingly

$$\gamma_{11} F_{1,11} + \rho \omega_1^2 F_1 - \rho \omega_\infty^2 2 R_0 \beta_1 x_1^2 F_1 = 0$$
$$\gamma_{55} F_{3,33} + \rho \omega_3^2 F_3 - \rho \omega_\infty^2 2 R_0 \beta_3 x_3^3 F_3 = 0. \qquad (17)$$

Equations similar to (17) were also encountered in the study of contoured resonators with varying thicknesses [19]–[22]. Eq. (17) is mathematically analogous to Schrodinger's equation for a quantum mechanical harmonic oscillator [23]. The two equations in (17) have the same structure. Consider $(17)_1$ first. Introduce the following change of variable:

$$x_1 = A_1 \xi_1. \qquad (18)$$

Then, it can be verified that when

$$A_1 = \left(\frac{\gamma_{11}}{2 \rho \omega_\infty^2 R_0 \beta_1} \right)^{1/4} \qquad (19)$$
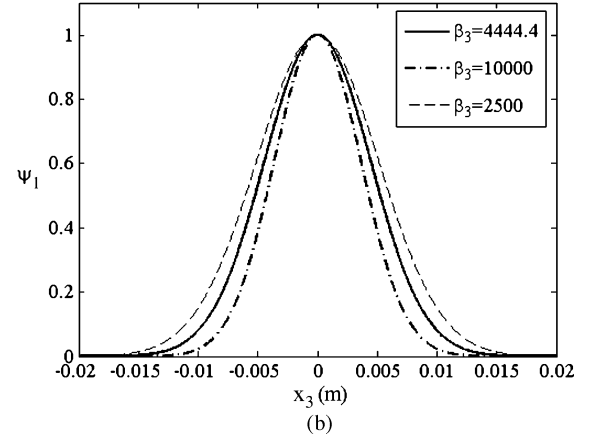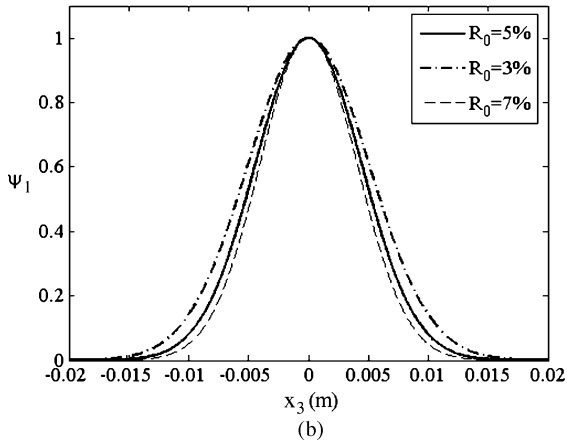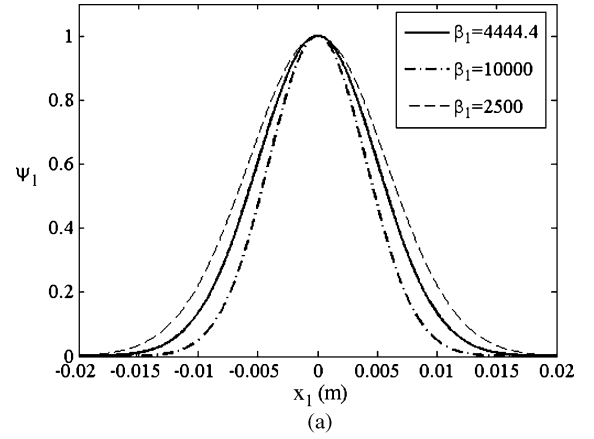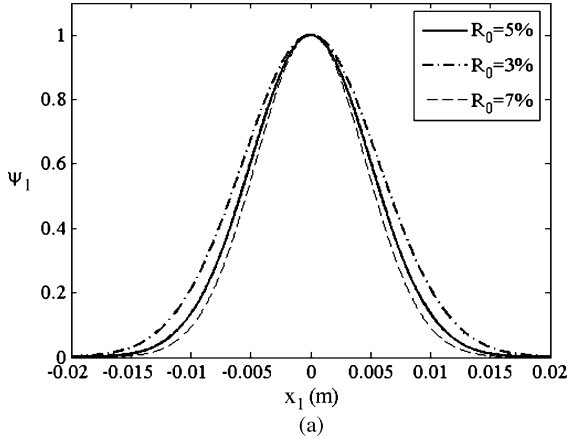
Fig. 3. Effects of R_0 on the first mode, $\beta = 4444.4$ m^{-2}. $f_{(0,0)} = 1\,617\,327$, $1\,586\,981$, and $1\,555\,305$ Hz when $R_0 = 3\%$, 5%, and 7%. (a) x_1 dependence. (b) x_3 dependence.

Fig. 4. Effects of β on the first mode, $R_0 = 5\%$. $f_{(0,0)} = 1\,582\,685$, $1\,586\,981$, and $1\,595\,538$ Hz when $\beta = 2500, 4444.4$, and $10\,000$ m^{-2}. (a) x_1 dependence. (b) x_3 dependence.

$(17)_1$ is transformed into

$$\frac{d^2 F_1(\xi_1)}{d\xi_1^2} + \left(\lambda_1 - \xi_1^2\right) F_1(\xi_1) = 0 \qquad (20)$$

where

$$\lambda_1 = \rho \omega_1^2 \frac{A_1^2}{\gamma_{11}} \quad \text{or} \quad \omega_1^2 = \frac{\gamma_{11}}{\rho A_1^2} \lambda_1. \qquad (21)$$

(20) is the well-known Weber's equation [21], [22]. Let

$$F_1(\xi_1) = \exp\left(-\xi_1^2/2\right) H(\xi_1). \qquad (22)$$

Eq. (20) becomes

$$\frac{d^2 H}{d\xi_1^2} - 2\xi_1 \frac{dH}{d\xi_1} + (\lambda_1 - 1)H = 0. \qquad (23)$$

For odd integers of λ, the solution of (23) are the Hermite polynomials of different orders, i.e., [23]

$$\lambda_1 = 2n_1 + 1, \quad H(\xi_1) = H_{n_1}(\xi_1), \quad n_1 = 0, 1, 2, 3 \cdots \qquad (24)$$

where [23], [24]

$$
\begin{aligned}
H_0 &= 1 \\
H_1 &= 2\xi_1 \\
H_2 &= 4\xi_1^2 - 2 \\
H_3 &= 8\xi_1^3 - 12\xi_1 \\
&\cdots.
\end{aligned}
\qquad (25)
$$

Eq. $(17)_2$ can be treated similarly. Substituting (11), (9), (6), $(21)_2$, and a similar equation from $(17)_2$ into (15) gives the resonant frequencies as

$$\omega^2 = \omega_\infty^2 (1 - 2R_0) + \frac{\gamma_{11}}{\rho A_1^2}(2n_1 + 1) + \frac{\gamma_{55}}{\rho A_3^2}(2n_3 + 1). \quad (26)$$

IV. NUMERICAL RESULTS

As a numerical example, consider an AT-cut quartz resonator with $2h = 1$ mm, and $R_0 = 5\%$. In real applications R_0 is usually less than 1%. An exaggerated value of R_0 is chosen to show its numerical effects more clearly. In this case the TSh mode without a film has a frequency of $f_\infty = \omega_\infty/(2\pi) = 1\,654\,638$ Hz. The frequency when the plate is with a uniform mass layer of $R_0 = 5\%$ is $f_0 = \omega_0/(2\pi) = 1\,569\,727$ Hz. $\beta_1 = \beta_3 = \beta = 4444.4$ m^{-2} is used. For this value of β, the film thickness decreases to zero when its radius is 15 mm, a practically reasonable size. Calculations show that in this case the operating mode of $(n_1, n_3) = (0, 0)$ in fact essentially decays to zero before it reaches the film boundary and thus does not really feel the film boundary.

Fig. 2 shows the first six modes in the interval of (f_0, f_∞) in the order of increasing frequency. $(n_1, n_3) = (0, 0), (0, 1), (1, 0), (0, 2), (1, 1)$, and $(2, 0)$. $f_{(0,0)} = 1\,586\,981$, $f_{(0,1)} = 1\,602\,093$, $f_{(1,0)} = 1\,606\,004$, $f_{(0,2)} = 1\,617\,063$, $f_{(1,1)} = 1\,620\,938$, $f_{(2,0)} = 1\,624\,804$ Hz. The displacements of all these modes are

essentially under the film. This is called energy trapping in TSh resonators. The modes are with different numbers of nodal lines in the x_1 and/or x_3 directions. Roughly, higher order modes have higher frequencies.

Figs. 3 and 4 show the effects of R_0 and β on the most useful mode in devices with $(n_1, n_3) = (0, 0)$. Considering the in-plane material anisotropy of the plate, both the mode variations along the x_1 and/or x_3 directions are shown separately. It is seen that when R_0 becomes larger or the film becomes thicker, the frequencies become lower and the modes are pushed toward the center (Fig. 3). When β becomes larger, i.e., the film thickness variation is more rapid or the film becomes smaller, the frequencies become higher and modes are also pushed toward the center (Fig. 4).

V. CONCLUSION

When a thin mass layer is included into Mindlin's 2D plate equation for TSh modes of a quartz plate, the resulting equation is mathematically analogous to Schrodinger's equation for a particle in a potential field. Specifically, when the film thickness varies quadratically, the plate equation is the same as that of a quantum harmonic oscillator. There exist trapped modes whose motion is mainly under the film. When the film becomes thicker or smaller, the modes are pushed toward the center. In addition to resonant frequencies, impedance is another important property of a resonator-based sensor which needs to be obtained from an electrically forced vibration analysis and is beyond the model in this paper.

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