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The application of second-order approximation of Taylor series in thickness shear vibration analysis of quartz crystal microbalances

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ABSTRACT

The inertia force caused by an additional mass layer is usually adopted to simulate the effective mechanical boundary condition in a quartz crystal microbalance (QCM), which may yield incorrect results when the upper layer becomes relative thicker. Thus, a detail analysis of the thickness shear vibration in a QCM for detecting the characteristics of the upper isotropic layer is proceeded based on a second-order approximation of Taylor series. The result calculated by this method has a higher accuracy than that of inertial-force approximation. According to these outcomes, the free and forced vibration has been illustrated, as well as transient effects during the switching on/off processes or under a sudden fluctuation of the driving-voltage amplitude or frequency. It has been revealed by numerical simulation that the additional mass layer has a great influence on the mechanical performance of QCM, including the resonance frequency, amplitudes of displacement and admittance, response time of the transient processes, and so on. These findings can prove effective guidance for physical phenomenon explanations and experimental measurement in mass sensor devices.

1. Introduction

Owning to its advantage of high sensitivity and distinguishability, the quartz crystal microbalance (QCM) has been regarded as very convenient to detect physical property changes of thin layers at its surfaces, which has been widely used in many regions, such as physics, biology, chemistry and medicine [1]. By changing the quality of the material under test into frequency signal, QCM can be applied to measure the properties of affiliated layer [2]. Sometimes, the resonance frequency can be reached gigahertz, with its thickness typically in the range of some micro-meters. Hence, it is easy to measure mass densities of the attached layer down to a level of 1 $\mu g/cm^2$ [3,4].

The frequency of oscillation, which is partially dependent on the thickness of the mass layer, is the basic performance index of the QCM. During the past decades, the effect of some mechanical characteristics on resonance frequency of QCM have been extensively investigated, including visco-elasticity [1], inhomogeneity of mass layer [5], imperfection of connected interface [6], electrical admittance [7], and so on. Among these explorations mentioned above, an inertia force caused by the thin layer is usually applied for the description of mechanical boundary condition at the upper surface of the crystal plate [5,8,9], which replaces a detailed analysis of mechanical and electrical coupling. Based on this simplification, Sauerbrey's equation provides a simple computational formula about resonance frequency, which is proportional to the mass of the film attached [1]. However, it has been pointed that this kind of simplification may yield incorrect results especially when the upper layer becomes relative thicker [10]. Both the mass and stiffness effects must be considered during the analysis. Hence, the present paper will introduce a second-order approximation of Taylor series, which will be more accurate than the previous inertial-force approximation.

On the other hand, owning to the piezoelectricity of AT-cut crystal plate, an alternative voltage applied on its two surfaces is usually used to excite a particular vibration mode. Another phenomenon, transient effect [11,12], is inevitable during the excitation process of QCM. For instance, the initial switching-on from rest, followed by a sudden switching-off caused by the interruption of incident current, fluctuations in the driving voltage or the frequency, and thermal and mechanical shocks, and so forth. They can disturb resonator operation evidently. There have been a few attempts to study the transient effect on the thickness-shear vibration in quartz crystal resonators [13–15]. However, the theoretical model mentioned above is simplified as a single infinite piezoelectric plate. To the best of our knowledge, little work has been

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performed so far to discuss the transient effect in the composite layered structures, which contains at least two different materials. However, this is significant for the design of high-quality electronic devices.

Synthesis above, a systematic investigation, including resonance frequency solving, forced vibration analysis, and some transient responses, on the thickness shear vibration performance of QCM is carried out in present contribution by using of a second-order approximation of Taylor series. The dispersion equation has been obtained from linear elastic theory, which can be reduced to a few known elastic or quasi-static piezoelectric solutions. Based on this equation, the effect of affiliated mass layer on some property indices of thickness shear mode, such as resonance frequency, displacement distribution, admittance amplitude, and transient response time, has been revealed numerically. Finally, some conclusions are given.

2. Thickness-shear vibration analysis

QCM is inexpensive owning to its simple configuration. For our purpose it is sufficient to consider an AT-cut quartz plate having a thickness of $2h$ and a mass density ρ in Fig. 1. Meanwhile, an additional mass layer with its thickness and mass density being $2h'$ and ρ' respectively is perfectly bonded on its upper surface. The origin of coordinates is set on the middle plane of the AT-cut quartz plate without loss of generality. Meanwhile, the alternating voltage $\pm V\exp(i\omega t)$ which are respectively imposed on the upper and bottom surfaces of the crystal plate, i.e., $x_2 = \pm h$, are used to excite the thickness shear vibration. Here, ω is the circular frequency, t stands for time, and $i^2 = -1$. Generally speaking, the thickness shear vibration may be coupled to flexure and face shear motions, and this kind of coupling depends on the plate dimensions [16]. It has been revealed that at certain length/thickness ratio, thickness shear vibration can be excited independently [16]. Hereby, the displacement vector $\boldsymbol{u}$ and electric potential φ in the AT-cut crystal plate can be described by

$$u_1 = u_1(x_2, t), \quad u_2 = u_3 = 0, \quad \varphi = \varphi(x_2, t). \tag{1}$$

By virtue of constitutive and geometric relations, dynamic equations and Maxwell's law, the governing equations corresponding to u_1 and φ are

$$\begin{cases} c_{66}\frac{\partial^2 u_1}{\partial x_2^2} + e_{26}\frac{\partial^2 \varphi}{\partial x_2^2} = \rho\frac{\partial^2 u_1}{\partial t^2}, \\ e_{26}\frac{\partial^2 u_1}{\partial x_2^2} - \varepsilon_{22}\frac{\partial^2 \varphi}{\partial x_2^2} = 0. \end{cases} \tag{2}$$

where c_{66}, e_{26}, ε_{22} are the elastic and piezoelectric coefficients and dielectric permittivity, respectively. The thickness shear vibration solution in the AT-cut quartz plate can also be expressed as [4,6,10]

$$\begin{cases} u_1 = [A_1\cos(\xi x_2) + A_2\sin(\xi x_2)]\exp(i\omega t), \\ \varphi = \left\{\frac{e_{26}}{\varepsilon_{22}}[A_1\cos(\xi x_2) + A_2\sin(\xi x_2)] + (A_3 x_2 + A_4)\right\}\exp(i\omega t). \end{cases} \tag{3}$$

in which A_1, A_2, A_3, and A_4 are undetermined coefficients, and $\xi = \frac{\omega}{\sqrt{\bar{c}_{66}/\rho}}$ is the wave number with the relative piezoelectric stiffness $\bar{c}_{66} = c_{66} + \frac{e_{26}^2}{\varepsilon_{22}}$. Hence, the corresponding stress and electric displacement components are:

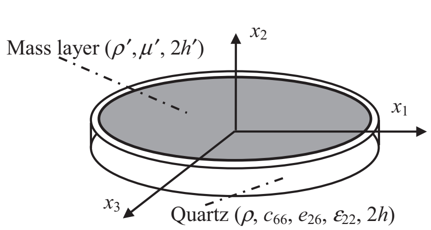

Fig. 1. A quartz crystal microbalance with an additional mass layer on its surface.

$$\begin{cases} T_{12} = \{\bar{c}_{66}\xi[-A_1\sin(\xi x_2) + A_2\cos(\xi x_2)] + e_{26}A_3\}\exp(i\omega t), \\ D_2 = -\varepsilon_{22}A_3\exp(i\omega t). \end{cases} \tag{4}$$

Once the thickness shear mode is excited, the mass layer will vibrates following the plate's motion with its displacement components being

$$u_1' = u_1'(x_2, t), \quad u_2' = u_3' = 0. \tag{5}$$

where $\boldsymbol{u}'$ stands for the displacement vector of the attached mass layer. Based on Eq. (5), the stress component T_{12}' and equilibrium equation can be obtained as:

$$T_{12}' = \mu'\frac{\partial u_1'}{\partial x_2}, \quad \frac{\partial T_{12}'}{\partial x_2} = \rho'\frac{\partial^2 u_1'}{\partial t^2}, \tag{6}$$

with μ' representing elastic coefficient of the mass layer. By using of Eq. (6), we can get the following relation

$$\frac{\partial}{\partial x_2}\boldsymbol{R} = \boldsymbol{M}\boldsymbol{R}. \tag{7}$$

where $\boldsymbol{R} = \begin{bmatrix} u_1' \\ T_{12}' \end{bmatrix}$, and $\boldsymbol{M} = \begin{bmatrix} 0 & \frac{1}{\mu'} \\ \rho'\frac{\partial^2}{\partial t^2} & 0 \end{bmatrix}$. Furthermore,

$$\frac{\partial^n}{\partial x_2^n}\boldsymbol{R} = \boldsymbol{M}^n\boldsymbol{R}, \text{ with } n = 1, 2, 3, \ldots. \tag{8}$$

A quartz crystal microbalance is widely used to measure the characteristics of an additional thin layer upon its surface by calculating the frequency shift. Specifically, the layer is so thin compared with the quartz plate, i.e., let $2h'$ be small, that we can expand the expression of stress T_{12}' at $x_2 = (h + 2h')$ into Taylor series at $x_2 = h$ [8,17]:

$$T_{12}'(h + 2h') = T_{12}'(h) + 2h'\frac{\partial}{\partial x_2}T_{12}'(h) + \frac{(2h')^2}{2!}\frac{\partial^2}{\partial x_2^2}T_{12}'(h) + \frac{(2h')^3}{3!}\frac{\partial^3}{\partial x_2^3}T_{12}'(h) + \ldots \tag{9}$$

In present contribution, we only consider the second-order approximation of Taylor series for simplification. Owning to the fact that the top surface of mass layer is traction free, i.e., $T_{12}'(h + 2h') = 0$, substituting Eq. (9) into Eq. (8) yields

$$\left[1 - 2(\xi' h')^2\right]T_{12}'(h) - 2h'\rho'\omega^2 u_1'(h) = 0. \tag{10}$$

where $\xi' = \frac{\omega}{\sqrt{\mu'/\rho'}}$ is the wave number of the layer. If we only consider the first-order approximation in Eq. (9), i.e., the terms containing h'^2 should be zero, Eq. (10) can be degenerated as

$$T_{12}'(h) = 2h'\rho'\omega^2 u_1'(h). \tag{11}$$

which is the boundary condition that is usually used in previous research [1,9], i.e., only considering the inertial force caused by the mass layer. In this paper, we will discuss the performance of QCM based on the second-order approximation described by Eq. (10) that is more accurate than those previous works.

The other boundary conditions at $x_2 = \pm h$ requires

$$T_{12}(-h) = 0, \quad \varphi(-h) = -V. \tag{12}$$

$$T_{12}(h) = T_{12}'(h), \quad u_1(h) = u_1'(h), \quad \varphi(h) = V. \tag{13}$$

Substituting the displacement and stress expressions, i.e., Eqs. (3) and (4), into the above boundary conditions, i.e., Eqs. (10), (12) and (13), yields four linear homogeneous algebraic equations for coefficients A_1, A_2, A_3, and A_4:

$$\bar{c}_{66}\xi[A_1\sin(\xi h) + A_2\cos(\xi h)] + e_{26}A_3 = 0, \tag{14a}$$