FEM simulation and frequency shift calculation of a quartz crystal resonator adhered with soft micro-particulates considering contact deformation

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Abstract. Recently some researchers studied the frequency characteristics of a quartz crystal resonator (QCR) adhered with micro-particles to measure their physical and geometric parameters. Many researchers regard the particles as rigid spheres or consider the elasticity but ignore the contact deformation and contact area of the particles. In fact, the adhesion and vibration of soft particles are coupled together and the interaction is strong and complicated. In this paper, we separately simulated the adhesion and vibration of the particles using finite element method with ANSYS software. Through transmission line model of the QCR, we get the frequency shift induced by surface particles. We found larger, softer and heavier particles produce greater contact deformation and load impedance which cause greater frequency shift (negative). The obtained results can be applied into characterization of size and elastic modulus of micro-particulates.

1. Introduction

The thickness shear mode (TSM) [1] quartz crystal resonator (QCR) are traditionally used as a film thickness monitor in deposition [2]. Nowadays, in the practical application of QCR, particulate matters become a common class of adsorbent or test object, such as dust, colloid, micro/nano-particles, bacteria and so on. Particles adhering to a QCR are perturbed around their equilibrium positions via thickness-shear vibrations at the crystal’s fundamental frequency and overtones. From the frequency of QCR, people can characterize particle size [3,4], bond stiffness [5,6], adsorption and deformation [7], and surface/interface interactions [8]. For a typical non-layered material of particulate matter, the traditional Sauerbrey equation [9] and viscoelastic film model [10,11] is clearly not applicable. It is very difficult to calculate the frequency shift caused by these particulate matter because the particles and QCR are coupled together to form a composite resonator [12].

Many researchers regard the particles as rigid spheres and apply the spring-particle model [12] or Kelvin-Voigt model [5,13] or roll-friction model [14] to study the coupling between particles and QCR. Some scholars [15,16] consider the elasticity of the particles, but ignore the influence of contact deformation and contact radius on particle vibration. In this article, we consider that soft particles slowly adhere to the QCR surface under gravity and then oscillate with the QCR. We will study the effects of contact deformation on coupled vibration and frequency shift of the QCR adhered with soft micro-particulates as shown in Figure 1.
Figure 1. (a) Sketch of a QCR adhered with particles, (b) schematic diagram of the thickness shear vibration of the loaded QCR driven by alternating voltage.

2. Transmission line model of the loaded QCR

The most comprehensive model for representing the response of a coated QCR is the transmission line model, one of which is the equivalent circuit shown in Figure 2 [17]. The impedance of a loaded QCR in fundamental thickness shear modes is written as follows [18]:

$$
Z = \frac{1}{i\omega C_0} \left[ 1 - \frac{K^2}{\varepsilon_q h_q} \frac{2 \tan \left( \frac{\xi_q h_q}{2} / \omega \right)}{1 - i \left( Z_L / Z_q \right) \cot \left( \frac{\xi_q h_q}{2} / \omega \right)} \right],
$$

where

$$
i = \sqrt{-1}, \quad \omega = 2\pi f, \quad C_0 = \varepsilon_{22} A / h_q, \quad K^2 = \frac{e_{26}^2}{c_q \varepsilon_{22}},
$$

$$
\xi_q = \omega \sqrt{\rho_q / c_q}, \quad Z_q = \sqrt{\rho_q c_q}, \quad c_q = c_{66} + \frac{e_{26}^2}{\varepsilon_{22}} + i\omega \eta_q,
$$

and $f$ is the resonance frequency, $C_0$ the static capacitance, $K$ the electromechanical coupling factor, $Z_q$ the quartz characteristic impedance, $Z_L$ the acoustic load impedance, $h_q$ the thickness, $A_e$ the effective electrode area, $e_{26}$ the piezoelectric constant, $\rho_q$ the mass density, $c_{66}$ the shear modulus, $\varepsilon_{22}$ the permittivity and $\eta_q$ the viscosity of the QCR. The real part of electrical admittance, $Y(=1/Z)$, is called the electric conductance. It is a function of driving frequency and can be determined by means of a network analyzer for impedance analysis. Compare the conductance curves for loaded and unloaded cases, we obtain the resonance frequency (see Figure 2).

Figure 2. (a) Representation of the transmission line model for a loaded QCR, (b) Electric conductance spectrum.
3. FEM simulation of the contact and vibration of the particles

We assume the geometric size, physical properties and vibration states of each particle are all the same. In fact, the adhesion and vibration of the particles are coupled together and the analysis is very complicated. For simplicity, we assume that particles very slowly adhere to QCR when it’s power off, and then the particles shake under the drive of QCR which oscillates in thickness shear modes. First, we use FEM with ANSYS software to simulate the adhesion of a particle under gravity, which is simplified into a static contact problem. The $x$-axis and $y$-axis are the vibration direction and height direction of the particle, respectively, as shown in Figure 1(b), and $z$-axis is perpendicular to $xy$ plane (not shown in the figure). Since the model and load are both symmetric about the $y$-axis, we establish an axisymmetric model as shown in Figure 3(a) for analysis. The 2-D, 8-node, quadrilateral, axisymmetric element called PLANE183 is chosen as structural solid element. A contact pair is created for contact analysis. The surface of the particle is set as node-to-surface contact elements called CONTA175, as shown by the point M in Figure 3(b). The upper surface of the QCR is defined as a 2-D rigid target surface called TARGE169, as shown by the segment I-J in Figure 3(b). The contour of deformation in Figure 3(c) shows contact deformation caused by gravity is so small that the particle remains almost spherical shape except for the narrow and flat contact area of the bottom.

We use harmonic response analysis with ANSYS software to simulate the vibration of particles and assume the contact area doesn’t change during the vibration. The 3-D, 10-node, tetrahedral element called SOLID187 as shown in Figure 4(a) is chosen for structural dynamic analysis. Taking into account the symmetry of the entire model with respect to the $xy$ plane as shown in Figure 4(a), we take half model to simulate. The contour of $x$-directional displacement in Figure 4(b) shows most part of the particle only moved a little bit, except for the bottom part near the upper surface of QCR. This is because on the one hand, the surface amplitude of QCR is very small (usually several tens of nanometers [19]), on the other hand, the particle is too soft to be driven easily in our simulation examples.

We denote the shear force at the bottom of particle as $F_s$ (calculated by ANSYS), area-averaged shear stress at the upper surface of QCR as $\tau_{yx}$, surface displacement of QCR as $u_0$. For harmonic response analysis, the time-harmonic factor is set to $\exp(i\omega t)$. Calculation of FEM shows the phase of $F_s$ is 180°. Since the direction of $\tau_{yx}$ is opposite to $F_s$, we know that $\tau_{yx}$ has the same phase as $u_0$. Thus, the load impedance $Z_L$, i.e., area-averaged ratio of shear stress and velocity at the upper surface of QCR, is given by

$$Z_L = -\left\langle \frac{\tau_{yx}}{v_0} \right\rangle = -\frac{N_p F_s}{i\omega u_0 A_y},$$

(3)
where, \( N_p \) is the number of particles, \( v_0 = \ddot{u}_0 \dot{\xi} = \omega_0 u_0 \), the velocity of QCR’s upper surface, and \( A \), the effective electrode area. The result of the FEM shows that \( F_s \) is proportional to \( u_0 \) under the assumption of linear elasticity, hence, \( F_s / u_0 \) has eliminated the influence of surface amplitude of QCR.

![Figure 4](image-url)  
**Figure 4.** (a) 3-D mesh of the particle (1/2 model) for structural dynamics analysis, (b) contour of x-directional displacement.

4. Numerical example and results discussion

For a numerical example, we consider an AT-cut quartz crystal resonator with the following parameters [20,21]:

\[
c_{q6} = 29.47 \times 10^6 \text{N} \cdot \text{m}^{-2}, \quad c_{26} = 9.657 \times 10^{-12} \text{C} \cdot \text{m}^{-2}, \quad c_{23} = 39.82 \times 10^{-12} \text{C} \cdot \text{V}^{-1} \cdot \text{m}^{-1},
\]

\[
\rho_q = 2651 \text{kg} \cdot \text{m}^{-3}, \quad \eta_q = 0.04 \text{N} \cdot \text{m}^{-2} \cdot \text{s}, \quad h_j = 0.1661 \times 10^{-3} \text{m}, \quad A_j = 2.827 \times 10^{-5} \text{m}^2.
\]

We set the surface amplitude of QCR, \( u_0=100\text{nm} \). Radius of the surface electrode is 3\( \text{mm} \) [21] and the area of the inscribed square is about \( 4 \times 4 = 16 \text{ mm}^2 \). We place a particle in each \( 1 \times 1 \text{ mm}^2 \) grid, so that there are \( 4 \times 4 = 16 \) particles in total. The particles are assumed to be an isotropic linear elastic material with Poisson’s ratio \( \mu=0.45 \).

![Figure 5](image-url)  
**Figure 5.** Contact radius v.s. radius of particles.
In Figure 5, we plot the contact radius of different particles calculated by FEM simulation and Hertz contact theory [22] respectively. From Figure 5 we can see that the contact radius is much smaller than the particle radius and the larger the size of the particles, the larger the contact radius. The contact radius of soft and heavy particle is larger than hard and light one. The results of FEM are very close to those predicted by Hertz contact theory, but slightly smaller. This is because we consider the gravity of the particle rather than applying a concentrated force on the top of it in Hertz contact model.

![Figure 6. Impedance spectrum curves.](image)

![Figure 7. Conductance spectrum for three kinds of particles with same radius.](image)

We plot the impedance spectrum curves for three different kinds of particles with $R=0.25\text{mm}$ in Figure 6, from which we find the impedance amplitude, $iZ_L$, of soft and heavy particles is larger than hard and light one. Although the shear stiffness of the soft particles is smaller than hard particles, the larger contact radius make the total shear force exceed the hard particles.

Figure 7 shows the conductance spectrum curves for three different kinds of particles with $R=0.25\text{mm}$. We can clearly see $f_A<f_B<f_C=9969.0145\text{kHz}$ and the frequency shift is much smaller than the fundamental frequency of QCR (i.e. $\Delta f << f_0$). In this case, a simple relation called small-load approximation [23] holds, $\Delta f/f_0 = \text{Re}[iZ_L/(\pi Z_q)]$. Generally speaking, the viscosity of the QCR is very small and negligible, so $Z_q$ can be regarded as a real constant (see Eq. 2). From the formula above, we can deduce that $\Delta f \propto (iZ_L)$, i.e., the larger impedance amplitude, the greater the frequency shift. Since $iZ_L$ is negative (see Figure 6), the frequency shift is negative too. As has been mentioned in Section 3 that $\tau_y$ has the same phase as $\mu_0$ in our simulation examples, so QCR seems to be dragged forward by the particles which means the inertia of the system increases, and then the resonance frequency drops.

![Figure 8. Frequency shift v.s. radius of particles.](image)
Finally, we plot the frequency shift v.s. radius curves for three different particles in Figure 8. It show that heavy and soft particles produce greater frequency shift (negative) and as the size of the particles increases, the resonance frequency becomes lower and lower.

5. Conclusions
The contact radius of the particles is affected by size, density, elastic modulus and stiffness. The contact radius also affects the vibration of the particles, which in turn affects impedance and frequency shift. The obtained results are helpful to precisely characterize the size and elastic modulus of micro-particulates and also to guide the development of QCR based bio-chemical sensors.

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