A simple equation predicting the amplitude of motion of quartz crystal resonators

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The amplitude of motion of quartz crystal resonators, u_0, has been calculated on the basis of the transmission line model by Mason [*Piezoelectric Crystals and Their Applications to Ultrasonics* (Van Nostrand, Princeton, 1948)]. It is predicted to be $u_0 = 4/(\pi n)^2\, Q d_{26} U_{el,0}$, where n is the overtone order, Q is the quality factor, d_{26} is the piezoelectric strain coefficient, and $U_{el,0}$ is the amplitude of the driving voltage. This simple result is in good agreement with previous numerical calculations, with an experimental value from the literature, and with our own experimental checks. As a side result, an equation is provided which allows to estimate the active area of the crystal from the product of the motional resistance R_1 and the Q factor. *© 2006 American Institute of Physics*. [DOI: 10.1063/1.2359138]

INTRODUCTION

Quartz crystal resonators are well-known tools to determine the thicknesses of films deposited on their surface.[1] Other types of acoustic coupling between the crystal and its environment have also been investigated.[2,3] Generally speaking, the amplitude of motion is unessential in these investigations as long as it is small enough to ensure linear stress-strain relations. As far as the crystal itself is concerned, one checks for nonlinearity by determining the "drive-level dependence."[4] At high amplitudes of oscillation, the resonance frequency slightly increases, the main reason being a small anharmonicity in the elastic constants of the crystal. As long as linear stress-strain relations hold (both inside the crystal and in the adjacent sample), the amplitude of motion drops out of the equations predicting frequency shift. The frequency shift only depends on the *ratio* between the stress and the speed at the crystal surface, and the amplitude may therefore be safely ignored.[5] The theoretical literature follows this line of reasoning in the sense that the emphasis is on the frequency of resonance, as opposed to the actual value of the amplitude at resonance.[6]

However, the amplitude of motion is indeed of substantial interest to researches that combine the quartz crystal microbalance (QCM) with atomic force microscopy (AFM) or with experiments probing interfacial mechanical behavior. The amplitude of motion is often comparable to the resolution of the AFM. If this is the case, the motion of the crystal perturbs the imaging process. Also, nonlinear behavior is ubiquitous in contact mechanics experiments (probing friction and adhesion), due to the inherent nonlinear nature of the interfacial friction.[7] For example, the onset of sliding usually occurs at some critical level of lateral force. The determination of the lateral force exerted by the crystal onto the tip of an AFM (or some other object touching it) requires knowledge of the amplitude of motion.

The literature contains a few experimental and numerical studies on the amplitude of oscillation. Martin and Hager have argued that the amplitude should be of the order of $d_{26} Q U_{el,0}$, where $d_{26} = 3.1$ pm/V is the piezoelectric strain coefficient, Q is the quality factor of the resonance, and $U_{el,0}$ is the amplitude of the electrical excitation.[8] Herts *et al.* have described a procedure to measure the oscillation amplitude by optical means.[9] This paper does not contain a comparison to theory. Kanazawa has provided an algorithm simulating the behavior of loaded quartz crystals[10] based on Tiersten's theory of piezoelectric plates.[6] The amplitude of motion is contained in this calculation, but the calculation relies on a numerical solution of a set of implicit equations. There is no explicit algebraic expression for the amplitude. Kanazawa finds a value of $u_0/(Q U_{el,0}) = 1.3$ pm/V, where u_0 is the amplitude. This calculation confirms the conjecture by Martin and Hager. More specifically, Kanazawa states that $u_0 = 0.41 d_{26} Q U_{el,0}$, where the numerical prefactor is nontrivial. Ballato has also reported on a numerical calculation of the amplitude.[11] Borovski *et al.* have experimentally determined the amplitude of oscillation by imaging the surface of a running crystal with a scanning tunneling microscope (STM).[12] Certain patterns appeared elongated after the oscillation had been turned on. The amplitude of oscillation could be inferred from the image distortion. The authors report a value of $u_0/(Q U_{el,0}) = 1.4$ pm/V, which is in fair agreement with Kanazawa's calculation. Full quantitative agreement with theory is not expected because the Tiersten theory assumes a laterally infinite resonator, whereas for real crystals, the oscillation is confined to the center of the crystal by means of energy trapping.[13]

We derive a simple, explicit equation predicting the amplitude of motion based on a transmission line model.[14] In-

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serting values, we arrive at a value of $u_0/(QU_{\mathrm{el},0}) = (1/n^2)1.25$ pm/V, where n is the overtone order. The n^{-2} scaling is numerically confirmed by Kanazawa's calculation.[15] Interestingly, Bruschi *et al.* mentioned as side remark in Ref. 16 that the amplitude of motion should scale as n^{-2}. No argument is provided as to why this should be the case.

DERIVATION OF THE AMPLITUDE FROM THE TRANSMISSION LINE MODEL

The following calculation is based on the electromechanical analogy and on the Mason equivalent circuit[17,6] as depicted in Fig. 1. The electromechanical analogy maps voltages onto forces and currents onto speeds. The following relations hold:[8]

$$I_{\mathrm{el}} = \phi \dot{u},$$

$$U_{\mathrm{el}} = \frac{1}{\phi} F,$$

$$Z_{\mathrm{el}} = \frac{U_{\mathrm{el}}}{I_{\mathrm{el}}} = \frac{1}{\phi^2}\frac{F}{\dot{u}} = \frac{1}{\phi^2} Z_m, \tag{1}$$

$$\phi = \frac{A e_{26}}{d_q},$$

where I_{el} is the electric current, $\dot{u}$ is the lateral speed of motion, U_{el} is the voltage, F is the lateral force, Z_{el} is the electric impedance, Z_m is the mechanical impedance (the force-speed ratio), ϕ links speed and current via the piezoeffect (see below), d_q is the thickness of the crystal, A is the effective area of the crystal (close to the area of the back electrode), and $e_{26} = 9.65 \times 10^{-2}$ C/m^2 is the piezoelectric stress coefficient. Figure 1(a) shows the Mason circuit with open acoustic ports to the left and right. $Z_q = 8.8$ kg m^{-2} s^{-1} is the acoustic impedance of AT-cut quartz, $2h_q = d_q$ is the thickness of the crystal, k_q is the wave number of shear sound, C_0 is the "parallel" electrical capacitance across the electrodes, and the (unessential) element $Z_k = \phi^2/(i\omega C_0)$ accounts for piezoelectric stiffening. Z_k is neglected in the following. Figure 1 indicates how the speed of lateral movement at the crystal surfaces corresponds to a "current" through the respective port. The piezoeffect is depicted as a transformer, where the parameter ϕ—speaking in electric terms—is the ratio of the number of loops on both sides of the transformer. In Fig. 1(b), both faces of the crystal have been short circuited. They are assumed to be stress-free. In application, the crystal is usually loaded on the front (for instance, with a film or a liquid). However, the load usually is small compared to the other circuit elements. A small load is a prerequisite for reliable operation of the QCM. For the purpose of this calculation, we may neglect the load altogether. The load, of course, indirectly affects the amplitude in case it decreases the Q factor [see Eq. (9) below]. A decrease of amplitude brought about by a load-induced decrease of the Q factor is captured by the calculation below. Since there are no open ports in the second circuit, the impedance Z_m across the left-hand side of the transformer can be calculated by application of the Kirchhoff laws to the circuit elements as shown in Fig. 1(c). The current through the left-hand side of the transformer is the ratio of the "voltage" (ϕU_{el}) and the impedance Z_m. This current is twice the speed at the crystal surface $\dot{u}$.

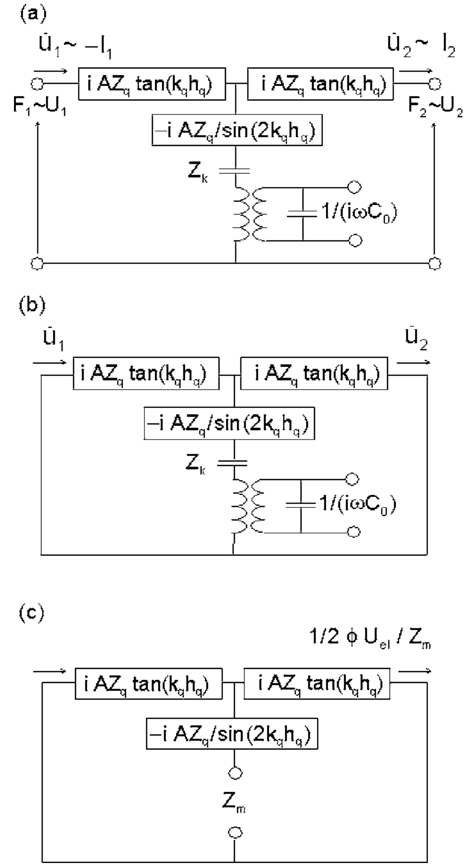

FIG. 1. The Mason equivalent circuit. (a) Open mechanical ports to the right and the left (corresponding to arbitrary stress-speed ratios at the front and back surfaces). (b) The Mason circuit with short-circuited (load-free) surfaces. (c) The mechanical impedance Z_m of the device is the impedance across the left side of the transformer as calculated by application of the Kirchhoff rules to the circuit elements. The lateral speed at the front surface is equal to one-half of the current across the left side of the transformer, which, in turn, is equal to the ratio of the voltage ϕU_{el} and the impedance Z_m.

A resonance is given by the condition that the electrical impedance of the crystal is zero. For real frequencies the impedance can never vanish completely because of viscous losses. For the first part of the calculation, we use complex resonance frequencies, $f_r^* = f_r + i\Gamma$, where f_r is the usual resonance frequency and Γ is the half bandwidth at half maximum.[5] The resonance condition then is $Z_{\mathrm{el}}(f_r^*) = 0$. On resonance, the impedance of the acoustic branch Z_m [consisting of all circuit elements connected to the left-hand side of the transformer, see Fig. 1(c)] is small. Since the element $(i\omega C_0)^{-1}$ is much larger than Z_m (on resonance) and in parallel to the acoustic branch, we may neglect this element as well. Therefore, the resonance condition is equivalent to $Z_m(f_r^*) = 0$. Clearly, we need to calculate the impedance of the acoustic branch Z_m. Applying the Kirchhoff rules to the elements shown in Fig. 1(c) we find[18]

$$Z_m = \frac{-iAZ_q}{\sin(2k_q h_q)} + \frac{1}{2} iAZ_q \tan(k_q h_q) = -\frac{1}{2} iAZ_q \cot(k_q h_q), \tag{2}$$

where the relation $-2/\sin(2x)+\tan(x)=-\cot(x)$ has been used. On resonance $Z_q \cot(k_q h_q)$ vanishes. Note that k_q is a complex number ($k_q=k_q'-ik_q''$) due to internal friction. Requiring that Z_m vanishes on resonance, we find

$$k_q h_q = \frac{2\pi f_r^*}{c_q} h_q = \frac{n\pi}{2}, \quad n=1,3,5,\ldots\ , \tag{3}$$

where c_q is the complex speed of sound and n is the overtone order. For the resonance frequency, we find

$$\begin{aligned} f_r^* &= f_r + i\Gamma \\ &= n\frac{c_q' + ic_q''}{4h_q} = n\frac{\sqrt{G_q' + iG_q''}}{\sqrt{\rho_q} 2d_q} \\ &= f_r\sqrt{1 + i\frac{G_q''}{G_q'}} = f_r\left(1 + i\frac{\tan\delta}{2}\right), \end{aligned} \tag{4}$$

where G_q is the complex shear modulus of the crystal, ρ_q is its density, and $\tan\delta=G_q''/G_q'$ is the loss tangent. The relation $c_q=(G_q/\rho_q)^{1/2}$ was used. Note that the approximation $(G_q'+iG_q'')^{1/2}\approx G_q'^{1/2}(1+i/2G_q''/G_q')$ requires $G_q''\ll G_q'$, which is certainly fulfilled for quartz crystals. The quality factor of the resonance, Q, is given by

$$Q = \frac{f_r}{2\Gamma} = \frac{1}{\tan\delta}. \tag{5}$$

We now calculate the mechanical impedance Z_m on resonance for real frequencies of excitation. For real frequencies, k_q'' is nonzero. Using Eq. (2) in conjunction with $Z_q=Z_q'+iZ_q''=Z_q'(1+ik_q''/k_q')$ and also separating $\cot(k_q h_q)$ into its real and imaginary parts, we find

$$\begin{aligned} Z_m &= -\frac{1}{2} iAZ_q \cot(k_q h_q) \\ &= -\frac{1}{2} iAZ_q'\left(1 + i\frac{k_q''}{k_q'}\right)\left[-\frac{\sin(2k_q' h_q)}{\cos(2k_q' h_q) - \cosh(2k_q'' h_q)}\right. \\ &\quad \left. - i\frac{\sinh(2k_q'' h_q)}{\cos(2k_q' h_q) - \cosh(2k_q'' h_q)}\right]. \end{aligned} \tag{6}$$

On resonance, we have $k_q' h_q=n\pi/2$, $\sin(2k_q' h_q)=0$, and $\cos(2k_q' h_q)=-1$. Assuming $k_q''\ll k_q'$ (small dissipative losses), we can Taylor expand the right-hand side of Eq. (6), yielding

$$Z_m \approx \frac{1}{2} AZ_q k_q'' h_q = AZ_q \frac{n\pi}{8} \tan\delta, \tag{7}$$

where the relations $h_q=n\pi/(2k_q')$ and $k_q''/k_q'=(G_q''/G_q')^{1/2}\approx(\tan\delta)/2$ have been used.

The mechanical current through the left-hand side of the transformer is given by $\phi U_{el}/Z_m$. Given that the speed at the crystal surface $\dot{u}$ is equal to half of this current, we find

$$\dot{u}_0 = \frac{1}{2}\frac{\phi U_{el,0}}{Z_m} = \frac{1}{2}\frac{\phi U_{el,0}}{AZ_q(n\pi/8)\tan(\delta)} \approx \frac{4}{n\pi Z_q} Q \frac{e_{26}}{d_q} U_{el,0}, \tag{8}$$

where Eqs. (1) and (5) were used for the parameters ϕ and $\tan\delta$, respectively. Finally, we calculate the amplitude u_0 from the speed as

$$\begin{aligned} u_0 &= \frac{1}{\omega}\dot{u}_0 = \frac{1}{2\pi n f_f}\frac{4}{n\pi Z_q}\frac{e_{26}}{d_q} Q U_{el,0} \\ &= \frac{4}{\pi^2}\frac{1}{n^2}\frac{e_{26}}{Z_q c_q} Q U_{el,0} = \frac{4}{\pi^2}\frac{1}{n^2} d_{26} Q U_{el,0}, \end{aligned} \tag{9}$$

where f_f is the frequency of the fundamental. Equation (9) made use of the relations $d_q=c_q/(2f_f)$, $c_q=(G_q/\rho_q)^{1/2}$, $Z_q=(G_q\rho_q)^{1/2}$, and $e_{26}=d_{26}G_q=d_{26}Z_q c_q$. The parameter $d_{26}=3.1\times10^{-12}$ V/m is the piezoelectric strain coefficient. The driving voltage $U_{el,0}$ is often quoted in terms of the electrical power in units of decibel, where 0 dBm corresponds to a power of 1 mW. The conversion is $U_{el,0}[\mathrm{V}]=0.317\times10^{(\mathrm{power[dBm]}/20)}$. Inputting values, we arrive at

$$\frac{a}{QU_{el}} = \frac{4}{\pi^2}\frac{1}{n^2} d_{26} = 1.25\frac{1}{n^2}\frac{\mathrm{pm}}{\mathrm{V}}. \tag{10}$$

Equation (10) is the central outcome of the calculation. The result compares well with the experimental value of 1.4 pm/V, where the latter has been determined from the length of the scratches induced by the STM tip.[12] Kanazawa finds a similar value by numerically solving the full Mason circuit.[10] Note that the derivation assumes laterally infinite resonators; it does not account for energy trapping. Equation (9) is therefore expected to miss a numerical factor of order unity.

CALCULATION OF THE ACTIVE AREA FROM THE *Q* FACTOR AND THE MOTIONAL RESISTANCE R_1

Before continuing with the experimental verification, we briefly mention a side result of the above calculation, which is of considerable practical interest. According to Eqs. (1) and (8), the electrical current through the left-hand side of the transformer in Fig. 1 is given as

$$I_{el,0} = 2\phi\dot{u}_0 = 2\frac{Ae_{26}}{d_q}\frac{4}{n\pi Z_q} Q\frac{e_{26}}{d_q} U_{el,0}, \tag{11}$$

where the factor of 2 enters because the current through the transformer is twice the current at the surfaces. Solving this equation for the effective area A we find

$$\begin{aligned} A &= \frac{I_{el,0}}{U_{el,0}}\frac{n\pi Z_q d_q^2}{8Qe_{26}^2} \\ &= \frac{G_{max}}{Q}\frac{n\pi Z_q}{8G_q^2 d_{26}^2}\frac{c_q^2}{4f_f^2} = \frac{G_{max}}{Q}\frac{n\pi}{32 Z_q d_{26}^2 f_f^2}, \end{aligned} \tag{12}$$

where the relations $d_q=c_q/(2f_f)$, $e_{26}=G_q d_{26}$, and $c_q=(G_q/\rho_q)^{1/2}=G_q/Z_q$ were used. The peak conductance $G_{max}=I_{el,0}/U_{el,0}$ is routinely obtained as one of the fit parameters in impedance analysis. It is the inverse of the motional resistance R_1. Both the peak conductance and the Q factor are

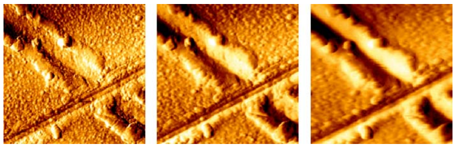

FIG. 2. AFM images of a scratch on the front electrode taken at rest (left), at a drive power of 5 dBm (0.55 V, center), and at a drive power of 15 dBm (1.77 V, right). The image is blurred by the oscillation. The size of the image is about 1 μm.

measures of the sharpness of the resonance. As Eq. (12) shows, the ratio of the two provides the effective area A. The larger the effective area, the more current is drawn on the peak of the resonance. The effective area is a nontrivial quantity because the back electrode confines the amplitude to the center of the crystal via energy trapping and it is *a priori* not clear what—exactly—the amplitude distribution is. The effective area is a measure of the width of this distribution. It can be monitored online in impedance analysis experiments. It turns out that the effective area sometimes varies with the experimental conditions.

EXPERIMENT

Experimental checks on the amplitude of oscillation were performed along the lines of Ref. 12 by imaging a structured surface with an AFM (Fig. 2) and a scanning electron microscope (SEM, Fig. 3). The crystals investigated (149257-1, Maxtek Inc., Santa Fe Springs, CA) had a fundamental frequency of 5 MHz, a diameter of 1 in., and a titanium-gold coating on both sides. The back electrode had the usual key-hole shape, providing energy trapping. As Figs. 2 and 3 show, the images get blurred when the oscillation is turned on. In order to quantify the "blurring" of the images, the edges were enhanced by means of Sobel filtering. Figure 4 summarizes the result of the quantitative analysis. These experiments confirm Eq. (10) to the expected extent, given that energy trapping and the lateral distribution of amplitudes are not contained in the calculation.

CONCLUSIONS

Using the electromechanical analogy we have derived a simple equation for the amplitude of motion of quartz crystal thickness shear resonators. The equation is in agreement with experimental results from our laboratory and from the literature, and also in agreement with a previous numerical calculation.

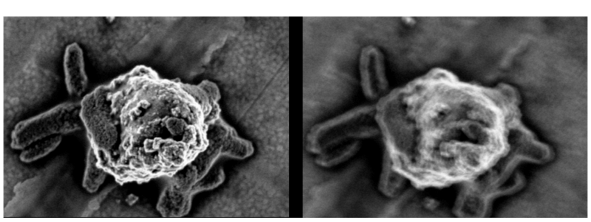

FIG. 3. SEM images of a dust particle taken at rest (left) and at a drive power of 12.5 dBm (1.32 V, right). The size of the image is about 1 μm.

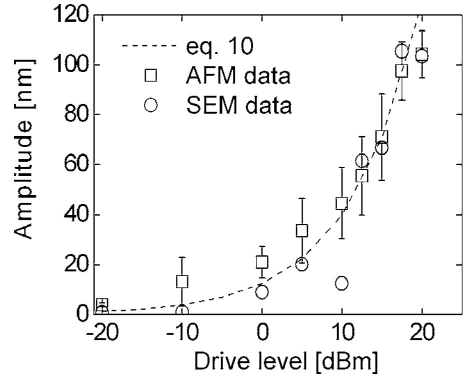

FIG. 4. Comparison of the experimentally determined amplitudes to the prediction of Eq. (10).

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APPENDIX: DERIVATION OF THE AMPLITUDE OF MOTION WITHOUT RECURSION TO EQUIVALENT CIRCUITS

For the sake of completeness, we rederive Eq. (9) from an algebraic relation contained in the literature, not making recursion to an equivalent circuit. We start out from Eq. (36.18) in Ref. 18, which—using our variables—is

$$u_0\left[G_q k_q h_q \cos(k_q h_q) - \frac{e_{26}^{\;2}}{\varepsilon}\sin(k_q h_q)\right] = e_{26}\frac{1}{2}U_{\mathrm{el},0}, \quad \text{(A1)}$$

where ε is the dielectric constant. The second term in brackets deals with piezoelectric stiffening. It slightly shifts the frequency of resonance. We are not concerned with the resonance frequency itself, but with the amplitude at resonance and therefore neglected the term proportional to $\sin(k_q h_q)$. This is equivalent to the neglect of the term Z_k in Fig. 1. Resonances occur when the term in square brackets becomes small. We expand the cosine as $\cos[(k_q' - ik_q'')h_q] = \cos(k_q' h_q)\cosh(k_q'' h_q) + i\sin(k_q' h_q)\sinh(k_q'' h_q)$. At resonance, the real part vanishes, which amounts to $\cos(k_q' h_q) = 0$, $k_q' h_q \approx n\pi/2$, and $\sin(k_q' h_q) = 1$. Assuming small dissipation ($k_q'' \ll k_q'$), we can approximate the imaginary part by $k_q' h_q$, leading to

$$u_0 G_q \frac{n\pi}{2} k_q'' h_q = e_{26}\frac{1}{2}U_{\mathrm{el},0}. \quad \text{(A2)}$$

Further using $k_q'' h_q = (Q/2) k_q' h_q = (Q/2) n\pi/2$ and $e_{26}/G_q = d_{26}$, we find

$$u_0 \frac{n\pi}{2}\frac{n\pi}{4}\frac{1}{Q} = d_{26}\frac{1}{2}U_{\mathrm{el},0}, \quad \text{(A3)}$$

which proves Eq. (9).

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