Equivalent-Circuit Model for the TSM Resonator with a Viscoelastic Layer

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SUMMARY

This paper describes a new equivalent-circuit model for the thickness shear mode resonator with a surface viscoelastic layer operating near film resonance. The electrical impedance of the film is represented by a simple three-element parallel circuit containing a resistor, a capacitor, and an inductor. These elements describe the film's viscous power dissipation, elastic energy storage, and kinetic energy storage, respectively. Resonator response comparisons between this lumped-element model and the general transmission-line model show good agreement over a range of film phase conditions and not just near film resonance.

Keywords: thickness shear mode resonator, QCM, viscoelasticity, equivalent-circuit model

INTRODUCTION

The thickness shear mode (TSM) resonator is an important transduction platform for chemical sensing. A thin viscoelastic layer on the resonator sorbs chemicals from the environment and changes its material properties. In this case, the viscoelastic layer does not always act as a pure mass load according to the Sauerbrey expression [1], but instead one that represents both energy storage and power loss. As the acoustic wave (imparted to the film by the vibrating quartz surface) traverses the layer, it experiences a phase shift, ϕ. If $\phi \ll \pi/2$, the film can be treated as a thin layer loading the surface, exhibiting a monotonic change in energy storage proportional to mass variation. However, as ϕ increases, more power is dissipated in the film. When $\phi = \pi/2$, the film exhibits a resonance and the power dissipation is maximum [2]. At this point, the quartz resonator and the film constitute *coupled resonators*. We describe a new lumped-element equivalent-circuit representation for the viscoelastic layer derived from its behavior near film resonance.

RESONATOR MODEL

The TSM resonator with arbitrary surface load can be represented by a transmission line with complex electrical impedance [3,4]. Near mechanical resonance of the unperturbed quartz crystal, the electrical impedance is reduced to the modified Butterworth-Van Dyke equivalent circuit shown in Fig. 1(a) [5]. The impedance has a static branch (characterized by the resonator capacitance, C_0^*) and a motional branch due to the mechanical vibration of the quartz. The resonator admittance for these two branches is given by

$$Y = j\omega C_0^* + \frac{1}{Z_M} \quad , \qquad (1)$$

where the resonator motional impedance, Z_M, is a linear combination of the contributions from the unperturbed crystal:

$$Z_M^0 = \left(R_1 + \frac{1}{j\omega C_1} + j\omega L_1 \right) \qquad (2)$$

and the surface load, Z_M^L.

Near the quartz crystal resonance, the impedance due to the surface load is given by [6]

$$Z_M^L = \frac{N\pi}{4K^2 \omega_s C_0} \left(\frac{Z_L}{Z_q} \right) = A Z_L \quad , \qquad (3)$$

where N is the resonator harmonic number (odd integers), K^2 is the quartz electromechanical coupling constant, $\omega_s = 2\pi f_s$ is the series resonant frequency, C_0 is the quartz plate capacitance, Z_L is the load surface mechanical impedance, and Z_q is the quartz characteristic impedance. The surface

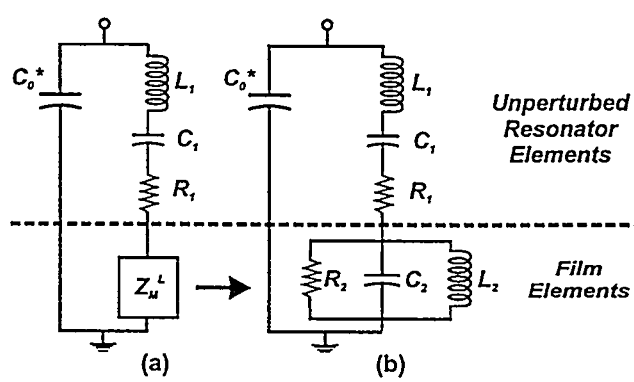

Fig. 1: The equivalent-circuit representation of a TSM resonator with a viscoelastic layer.

DISCLAIMER

mechanical impedance is the ratio of the shear stress imparted by the film to the shear particle velocity at the quartz-film interface. For a finite viscoelastic layer [2]

$$Z_L = \sqrt{\rho G}\tanh(\beta h) \quad , \qquad (4)$$

where ρ is the film density, $G = G' + jG''$ is the film's complex shear modulus (G' is the storage modulus and G'' is the loss modulus), $\beta = j\omega(\rho/G)^{1/2}$ is the shear wave propagation factor, and h is the film thickness. Since Eq. (4) is not readily decomposed into real and imaginary components or other simple elements, previous loaded-resonator models utilized this transmission-line representation of the viscoelastic layer as expressed [7].

Near film resonance, an approximation for the hyperbolic tangent function in Eq. (4) can be implemented [3,8]:

$$\tanh(\beta h) \cong \frac{8\beta h}{(N'\pi)^2 + (2\beta h)^2} \quad , \qquad (5)$$

where N' is the film harmonic number (odd integers). Combining Eqs. (3) through (5) and performing the complex algebra yields

$$Z_M^L \cong \left[\frac{\omega h G''}{2A|G|^2} + j\omega\left(\frac{hG'}{2A|G|^2}\right) + \frac{1}{j\omega}\left(\frac{(N'\pi)^2}{8Ah\rho}\right)\right]^{-1} , \qquad (6)$$

where A is defined in Eq. (3). This expression for the load impedance can be rewritten as

$$Z_M^L = \left(\frac{1}{R_2} + j\omega C_2 + \frac{1}{j\omega L_2}\right)^{-1} , \qquad (7)$$

which is a parallel combination of the film elements as shown in Fig. 1(b). The individual circuit elements are [8]

$$R_2 = \frac{N\pi}{2K^2\omega_s^2 C_0 Z_q}\frac{|G|^2}{hG''} , \qquad (8a)$$

$$C_2 = \frac{2K^2\omega_s C_0 Z_q}{N\pi}\frac{hG'}{|G|^2} , \qquad (8b)$$

and

$$L_2 = \frac{2N}{(N')^2\pi K^2\omega_s C_0 Z_q} h\rho \ . \qquad (8c)$$

R_2 represents *viscous dissipation* in the film, C_2 the *elastic energy storage*, and L_2 the *kinetic energy storage*. Note that L_2 is proportional to $h\rho$, analogous to a mass layer.

MODEL COMPARISONS

A comparison of the TSM resonator responses using both the transmission-line impedance model for the film [Eq. (4)] and the lumped-element impedance model [Eq. (6)] are shown in Fig. 2. Plotted is the shift in series resonant frequency, Δf_s, and the change in resonant resistance, ΔR, for viscoelastic films possessing varying degrees of phase shift. The two quantities Δf_s and ΔR are typically the measurable parameters in a sensor system. As seen in Fig. 2, the TSM resonator system exhibits resonant behavior near $\phi = \pi/2$ due to the film properties. For a low-loss film, where the loss tangent $G''/G' \ll 1$, the lumped-element representation is a good predictor of the response. This occurs over a wide range of phase shifts and not just near film resonance. However, for a lossy film, $G'' \sim G'$, the new model is less accurate, especially for the frequency shift predictions. This deviation arises because the approximation in Eq. (5), upon which the model is constructed, utilizes the entire argument βh, while film resonance depends only on ϕ, the imaginary component of βh. When film loss (the real component of βh) is significant, βh and ϕ diverge.

Response dependence on viscoelastic layer loss can be investigated further by comparing the film resonant frequencies for the two models. For the lumped-element model (LEM), the film resonant frequency occurs when the reactive elements in Eq. (7) cancel. Then using Eqs. (8)

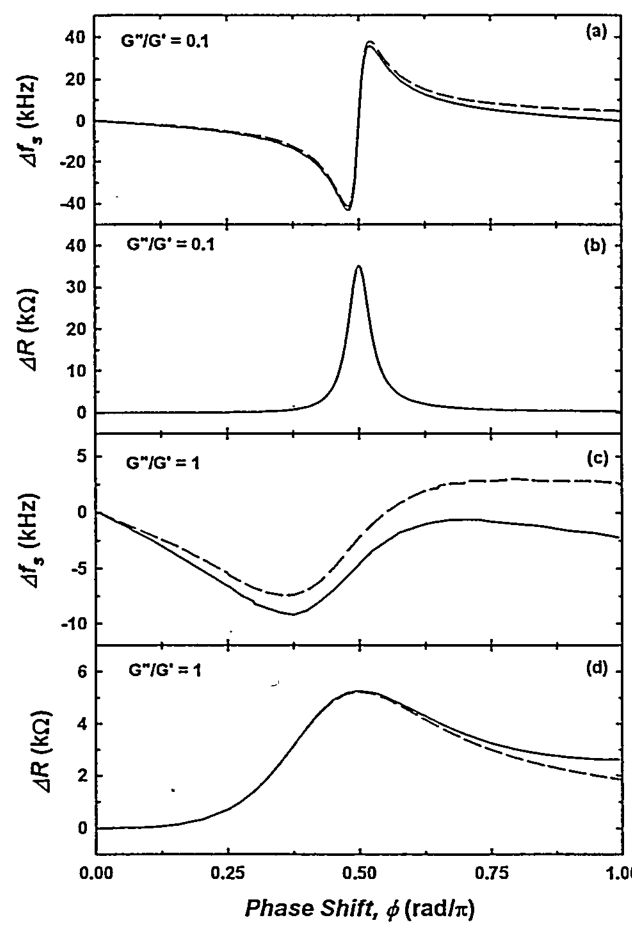

Fig. 2: The shift in series resonant frequency [curves (a) and (c)] and resonant resistance [(b) and (d)] versus acoustic phase shift across a viscoelastic layer computed using the new lumped-element model (dashed curves) and the transmission-line model (solid curves). The two curves in (b) are indistinguishable. For all curves, $G' = 10^7$ dyne cm^{-2}; responses in (a) and (b) are for a low-loss layer, while responses in (c) and (d) are for a lossy layer.

$$\omega_{f,LEM} = \frac{1}{\sqrt{L_2 C_2}} = \frac{N'\pi|G|}{2h\sqrt{\rho G'}} \ . \qquad (9)$$

For the general transmission-line model (TLM), the phase shift across the viscoelastic layer is

$$\phi = \mathrm{Im}(\beta h) = \frac{\omega h}{|G|}\sqrt{\frac{\rho(|G|+G')}{2}} \ . \qquad (10)$$

Film resonance occurs when the phase shift is $N'\pi/2$, which leads to

$$\omega_{f,TLM} = \frac{N'\pi|G|}{2h}\sqrt{\frac{2}{\rho(|G|+G')}} \ . \qquad (11)$$

The ratio of the film resonant frequencies for the two models is then

$$\frac{\omega_{f,LEM}}{\omega_{f,TLM}} = \sqrt{\frac{|G|+G'}{2G'}} = \sqrt{\frac{1+\sqrt{1+(G''/G')^2}}{2}} \ . \qquad (12)$$

Figure 3 is a plot of Eq. (12) illustrating the divergence of the film resonant frequencies between the two models as G''/G' increases. When $G'' = G'$, the difference between the two film resonant frequencies is ~ 10%. This relative difference, however, is much smaller than that observed in Fig. 2(c) for the measurable frequency shift, Δf_s. Model discrepancy for Δf_s at $\phi = \pi/2$ is ~ 50% when $G'' = G'$.

Combining Eqs. (6) and (9) yields an expression for the complex electrical impedance of the lumped-element representation as a function of the film resonant frequency and the film loss tangent:

$$Z_M^L \cong \left[\frac{8A\rho h}{(N'\pi)^2}\frac{\omega_f^2}{\omega}\right]\left[\frac{G''}{G'} + j\left(1+\frac{\omega_f^2}{\omega^2}\right)\right]^{-1} . \qquad (13)$$

It is interesting to compare this impedance to that of the ideal mass layer for acoustically thin films ($\phi \ll \pi/2$):

$$Z_m = j\frac{N\pi}{4K^2\omega_s C_0 Z_q}\omega\rho h \ . \qquad (14)$$

The impedance ratio for the lumped-element model near film resonance is then [8]

$$\left(\frac{Z_M^L}{Z_m}\right)_{LEM} = \frac{8}{(N'\pi)^2}\frac{j(\omega_f/\omega)^2}{(G''/G') + j[1-(\omega_f/\omega)^2]} \ . \qquad (15)$$

A plot of this impedance ratio as a function of (ω/ω_f) is shown in Fig. 4 for the same two values of film loss tangent used in Fig. 2. Also plotted in Fig. 4 is the equivalent impedance ratio for the transmission-line model. That impedance expression is found from Eqs. (3), (4), and (14):

$$\left(\frac{Z_M^L}{Z_m}\right)_{TLM} = \frac{\tanh(\beta h)}{\beta h} \ . \qquad (16)$$

This impedance representation is similar to that derived by Behling, *et al.* [9]. βh as a function of the film resonant frequency and loss tangent can be found using

$$\beta h = j\omega h\sqrt{\frac{\rho}{G}} = \alpha + j\phi \ , \qquad (17)$$

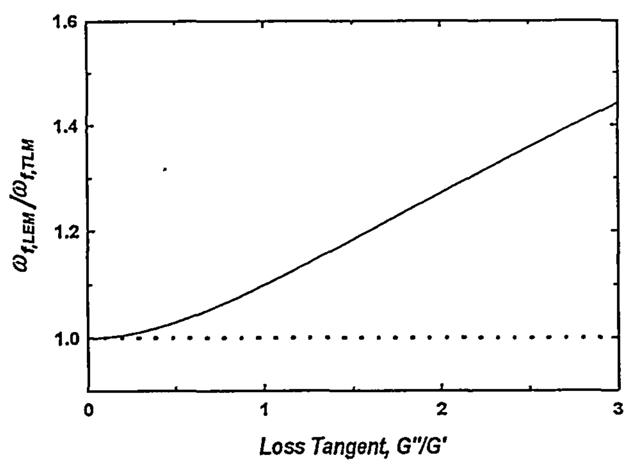

Fig. 3: The computed ratio of film resonant frequencies between the lumped-element model, $\omega_{f,LEM}$, and the transmission-line model, $\omega_{f,TLM}$, as a function of the viscoelastic film loss tangent.

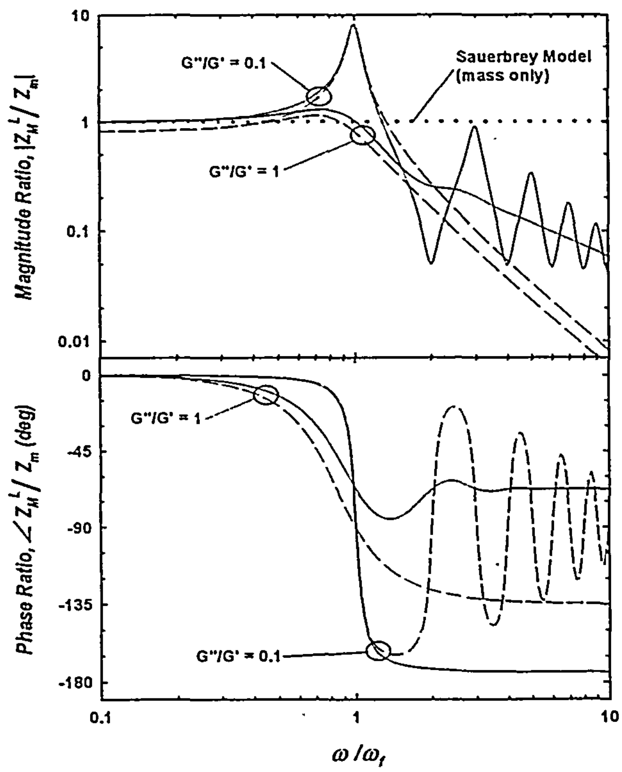

Fig. 4: The magnitude (top) and phase (bottom) of the layer impedance ratio versus the oscillation frequency relative to film resonance. Impedance ratios are shown for the lumped-element model (dashed curves) computed from Eq. (15) and the transmission-line model (solid curves) computed from Eq. (16).

where the film loss, α, is given by

$$\alpha = \mathrm{Re}(\beta h) = \frac{\omega h}{|G|}\sqrt{\frac{\rho\left(|G| - G'\right)}{2}} \quad . \tag{18}$$

Substituting Eqs. (10), (11), and (18) into Eq. (17) provides a final expression for βh:

$$\beta h = \frac{N'\pi}{2}\left(\frac{\omega}{\omega_f}\right)\left(j + \sqrt{\frac{\sqrt{1+(G''/G')^2} - 1}{\sqrt{1+(G''/G')^2} + 1}}\right) . \tag{19}$$

Several features are noted about the plots in Fig. 4. Near film resonance, $\omega = \omega_f$, the impedance magnitude and phase for the two models is in very good agreement when the viscoelastic layer is low loss, $G''/G' = 0.1$. Significant deviations between the models exist for the lossy layer, $G''/G' = 1$, as discussed earlier. Away from film resonance, the equivalent circuit model is not always a good representation of the layer response. For acoustically thin films, $\omega \ll \omega_f$, the impedance magnitude ratio is 0.81, indicating that kinetic energy storage found from L_2 in Eq. (8c) is not exactly that expressed by Sauerbrey in his mass loading model [1]. Note, however, that in the acoustically thin regime, the impedance phase ratios agree well for both values of film loss tangent. At the higher oscillation frequencies, $\omega \gg \omega_f$, large model deviations occur. Some of these differences are due to the harmonic resonances predicted by the transmission-line model and Eq. (16) that are not expressed in Eq. (15) for the lumped-element model with $N' = 1$. Better fits for the response resonance at $3\omega/\omega_f$ would occur if $N' = 3$ were used in Eq. (15); however, model deviations would then occur at all other film resonances.

CONCLUSIONS

The new lumped-element model for a TSM resonator with a viscoelastic layer provides a simple equivalent-circuit representation that is easy to analyze for sensor systems. For low-loss layers, the model shows excellent agreement with the transmission-line representation when operating near film resonance and good agreement for the measurable response parameters for most other layer phase conditions. For lossy viscoelastic layers, however, the lumped-element model can deviate significantly from the transmission-line model. These differences are due to the approximation used near film resonance. In general, this new model provides a suitable mechanism for characterizing many viscoelastic layers and chemical sensing systems. In combination with the Sauerbrey model [1], it expands the acoustic phase region over which simple expressions can be used for describing surface interactions.

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