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Complex loading and simulation of acoustic thickness shear mode resonator

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Abstract

During the last decades thickness shear mode resonators (TSM, QCM) have been object of comprehensive research. Many approaches were made to describe the behavior and physical effects when loaded. We present a physical model that describes the TSM in the full frequency range, including overtones for a large variety of loadings (e.g. gases, liquids or solid materials). By using an automated curve fit algorithm, absolute values for the loaded material (e.g. thickness, viscosity) can be extracted. The model has been validated with a large number of experiments including liquids with complex viscosities, biomolecule interactions, electrochemisty or vacuum deposition techniques. Additionally, the appearance of layer resonances have been predicted and verified. Layer resonances are remarkable because they appear at even-numbered overtones, which have been considered to be impossible.

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Keywords: Thickness shear mode resonator; complex viscosity; layer resonance; TSM; QCM

1. Introduction

Our research group studies acoustic sensors (TSM, SAW) together with biological processes and biomolecule interactions, e.g. blood coagulation, cell adhesion or DNA adsorption. The desired determination of physical properties has led to substantial work on modeling and describing the sensors [1]. In the recent years many approaches have been made to describe thickness shear mode resonators (TSM). Most of them, e.g. the well known Sauerbrey- or Kanazawa-equation or the dissipation measurement only describe certain aspects like the shift of resonant frequency. Equivalent circuit models (BVD-model) are well advanced but still need certain assumptions or exotic components like negative capacitors [2]. Furthermore, they can not describe the periodicity. Our new model describes the impedance of a loaded TSM-resonator in the full frequency range, including all overtones. Loadings ranging from gases, liquids to solids as well as stacked materials can be calculated.

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2. TSM-model

The new TSM-model is a complete analytical approach and consists of three major parts:
(1) The impedance of the thickness shear mode resonator,
(2) the geometry of the loading (e.g. half space, stack) and
(3) a description of the loaded material (e.g. Maxwell-model of complex liquids).
The parts are described in detail in the following sections.

2.1. Impedance of the TSM

Based on a one dimensional approach, the propagation of a shear wave is written in terms of the acoustic impedance Z_q of the resonator, the piezoelectric coupling coefficient K^2 and the acoustic load Z_l. Formula (1) shows the electric admittance $Y = \frac{1}{Z}$ of a TSM

$$Y = \sum_{i=0}^{n} \frac{i\omega C_i}{1 - K^2 \dfrac{\tan(\zeta_i)/\zeta_i}{1 + i \dfrac{Z_l \tan(\zeta_i)}{2Z_q - i\dfrac{Z_l}{\tan(\zeta_i)}}}} + i\omega C_s \tag{1}$$

where $\omega = 2\pi f$ denotes the frequency and $\zeta = \frac{\pi f}{2 f_a}$ the frequency normalized to the resonance frequency f_a. The summation accounts for the various modes (main mode plus additional spurious modes) in one resonance region, C_i describes the corresponding capacity of each mode and C_s an additional parasitic capacity. The periodicity is represented by the $\tan(\zeta)$ expression.

2.2. Geometry of the loading

The most general case of loading for this approach is a stack of layers. Of importance for the TSM-resonator is the effective acoustic impedance Z_l at the boundary surface between the loading and the TSM. Figure 1 shows the general case for a loaded TSM. The effectic acoustic impedance Z_l can be calculated as follows:

$$Z_l = \frac{P1}{P2}, \begin{pmatrix} P1 \\ P2 \end{pmatrix} = \prod_{m=1}^{n} M_m \begin{pmatrix} Z_F \\ 1 \end{pmatrix}, M_m = \begin{pmatrix} 1 & i\tan(k_m d_m)\cdot Z_m \\ i\tan(k_m d_m)/Z_m & 1 \end{pmatrix},$$

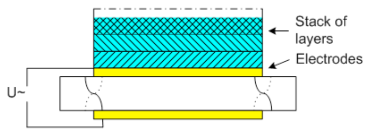

Figure 1, Stack of layers as general case for TSM loading

where M_m is a Matrix containing the parameters for a propagating shear wave within the layer m, d_m the layer thickness, $k_m = \omega/v_m$ the wave number and v_m the propagation speed of the shear wave. $Z_m = \rho_m \cdot v_m$ is the acoustic impedance of the corresponding layer and Z_F the acoustic impedance of a halfspace concluding the stack of layers (can be zero for vacuum).

2.3. Loaded material

Since the presented model describes the TSM-impedance in the full frequency range, it is necessary take the frequency behavior of the loaded material into account. Various types of loadings can be calculated. It is common to use equivalent models to describe the behavior of the material e.g. Maxwell- or KelvinVoigt-model for liquids. The properties of the loaded material must be written in terms of density and complex shear modulus to be used in the above formulas. A complex viscosity η^* is transferred to the shear modulus G^* by $G^* = i\omega\eta^*$.

2.4. Derived properties

Since our model yields most of the common approaches, their parameters (like frequency shifts, dissipation factor or series resistance) can be derived from our simulation. The desired derivation is made by applying specific boundary condition for the above mentioned three parts of the TSM-model. Table 1 shows the boundary conditions and approximations for selected specific solutions to be applied to the TSM-model.

Table 1, boundary conditions to derive specific solutions from the general TSM-model

Part of TSM model	SAUERBREY equation	KANZAWA equation	Dissipation monitoring
(1) TSM impedance	Change of resonance frequency	Change of resonance frequency	Change of Eigenfrequency
(2) loading geometry	Layer + vacuum	Halfspace	Halfspace
(3) loaded material	Solid	Newtonian liquid	Complex viscosity
Further approximations	Thin layer	Small viscosity, small piezoelectricity	

2.5. Complex loadings

The new TSM model has been validated with numerous experiments including liquids with complex viscosities, bio molecule interactions, electrochemistry or vacuum deposition techniques. By using an automated curve fit algorithm during measurements it is possible to directly determine absolute values for the loaded material properties. Compared to existing models no reference condition is needed. Figure 2 shows the measured and simulated impedance of a 5MHz TSM-resonator, loaded with a complex viscous solution of 30% PEG6000 (polyethylenglycol) in water. The determined viscosity is $\eta' = 13\text{mPas}, \eta'' = 7\text{mPas}$. To achieve an accurate result it is important to take spurious modes into account. Especially at higher viscosities they influence the main resonance and may cause measurement deviations. Since the new TSM model calculates the complete impedance curve of the thickness shear mode resonator, specific values (e.g. shift of resonance frequency, quality factor or dissipation) can be derived. Table 2 shows selected parameters calculated for the liquid loading shown in figure 2.

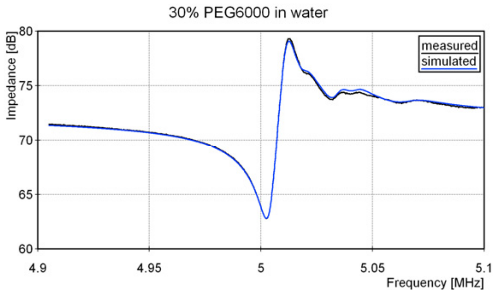

Figure 2, Measured and automatically fitted impedance curve of a 5MHz TSM loaded with a complex viscous liquid of η=13.0+i7.0mPas. The simulated curve matches the measurement very well and almost no variations can be seen.

Table 2, TSM and derived material properties

TSM properties	
Static capacity	$C_s = 8.0\text{pF}$
Parallel capacity	$C_p = 4.1\text{pF}$
Fundamental frequency	$f_a = 5.022\text{MHz}$
Liquid loading of 30% PEG6000 in water	
Assumed density	$\rho = 1.0\frac{g}{cm^3}$
Determined viscosity	$\eta' = 13.0\text{mPas}$
	$\eta'' = 7.0\text{mPas}$
Derived properties corresponding to common models	
Frequency shifts	
Shift of resonant frequencies[b]	$\Delta f_{r1} = -2853\text{Hz}$
	$\Delta f_{r2} = -2099\text{Hz}$
Shift of Eigen-frequencies[c]	$\Delta f_{e1} = -2476\text{Hz}$
	$\Delta f_{e2} = -2476\text{Hz}$

Quality factor, dissipation	
Quality factor	$Q = 293$
Dissipation factor	$d = 3.413 \cdot 10^{-3}$
Equivalent circuit model	
Series resistance	$R_s = 4184\Omega$
Series inductivity	$L_s = 38.84\text{mH}$
Series capacity	$C_s = 2.60366\text{pF}$
Series resonant frequency	$f_{rs} = 5.005036\text{MHz}$

[b] Compared to air, Δf_{r2} is the shift of the corresponding antiresonant frequency, the maximum impedance

2.6. Layer resonances

In significant thick layers deposited on the TSM-resonator (approximately >10µm for metals), it is possible to excite shear oscillations within the layer. This is remarkable because these layer resonances occur between the main resonances at even numbered overtones, which was generally considered to be not possible. Figure 2 shows the impedance of a 5MHz TSM-resonator between the overtones 3 to 5 loaded with a 10µm Cu-layer, deposited by sputtering technique. As for explanation, such a thick heavy layer shifts the resonances far enough so that the layer resonance can be excited. The well known Sauerbrey equation to determine the layer thicknesses can not be applied anymore because the shear modulus of the deposited material must be taken into account. Table 3 shows the material properties determined by the complete modelling of the TSM-resonator. They show a good agreement to the corresponding properties taken from literature, respectively the manufactured thickness. By using the comprehensive TSM model it is now possible to both determine the shear modulus and layer thickness of such layers.

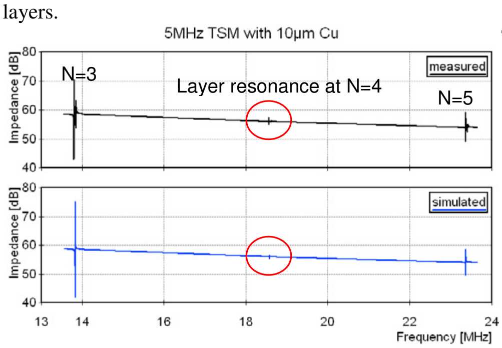

Figure 2: Measured and simulated layer resonance at the even numbered overtone N=4 in a 10µm Cu layer.

Table 3, TSM and determined material properties for a 10µm Cu-layer

TSM properties	
Static capacity	$C_s = 13.4\text{pF}$
Parallel capacity	$C_p = 4.0\text{pF}$
Fundamental frequency	$f_a = 5.015\text{MHz}$
Solid layer properties determined with TSM	
density	$\rho = 8.9 \frac{g}{cm^3}$
Shear modulus	$G' = 40\text{GPa}$
	$G'' = 0.14\text{GPa}$
Layer thickness	$d = 10.1\mu\text{m}$
Layer properties corresponding to literatur / manufactoring	
density	$\rho = 8.9 \frac{g}{cm^3}$
Shear modulus	$G' = 47\text{GPa}$
	$G'' \approx 0$
Layer thickness	$d = 10\mu\text{m}$

3. Summary

A general model of thickness shear mode resonators covering a large variety of loadings is presented. The properties of the loaded material can be determined by several algorithms. The occurrence of layer resonances at even numbered overtones has been predicted and detected.

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References

[1] Bruenig, More general model of quartz crystal microbalance response to viscoelastic loading, contribution to Eurosensors 2008.

[3] Johannsmann, viscoelastic analysis of organic thin films on quartz resonators, 1998.

[4] M. V. Voinova, M. Rodahl, M. Jonson, and B. Kasemo, "Viscoelastic acoustic response of layered polymer films at fluid-solid interfaces: continuum mechanics approach", Physica Scripta, Vol. 59 (1999) 391-396.

[c]Corresponds to QCM-dissipation (QCM-D) measurements. The shift of resonant frequency, Eigenfrequency and the output of the Kanazawa equation are only equal for small viscosities and neglected piecoelectricity.