ELECTROMECHANICAL COUPLING FACTOR k_{35}^2 OF THICKNESS-SHEAR MODE OF THE PIEZOELECTRIC THIN FILMS DEPOSITED ON SUBSTRATES

*Min-Chiang Chao, †Tsung-Ying Wu, Zuoqing Wang, and Chih-Lin Wang

TXC Corporation Ltd., No.4, Kung Yeh 6th Road, Ping-Cheng City, Tao-Yuan County, Taiwan, R.O.C.

Abstract **-** An experiment method for characterizing piezoelectric film, which is deposited on a substrate plate to form a thickness-shear wave High-overmode Bulk Acoustic Resonator (HBAR), will be presented in this paper. Based on the parallel and series resonant frequency spectra of the HBAR, the electromechanical coupling factor of the piezoelectric film operating in thickness-shear mode can be evaluated directly. Numerical simulation results of samples consisting of ZnO film on fused SiO_2 substrate are carried out to show the validity of the method. The effect of the electrodes is compensated by a modified formula.

I. Introduction

Piezoelectric thin films have been widely used in high frequency bulk acoustic wave (BAW) and surface acoustic wave (SAW) devices, such as filters, resonators, actuators and sensors. For self-supported single piezoelectric films, various measurement techniques have been developed to evaluate the properties of these films. However, for very high frequency devices, such as zinc oxide film on fused quartz [1] and AlN film on silicon [2], the films are not self-supported. Therefore, the methods recommended by the IEEE Standard [3] are not available.

Hickernell [1] and Naik, et al [2] developed a method to extract k_t^2 value by fitting the input impedance and admittance data with the equivalent circuit analysis results on multi-mode resonance of a thickness-extension mode composite resonator. More recently, a direct method was developed to characterize piezoelectric film coated on an isotropic substrate (form a kind of thickness-longitudinal HBAR) [4], [5]. In bulk acoustic resonator applications, however, thickness-shear modes are more often in use, for example, on AT-Quartz.

In this paper we present a method to evaluate the properties of the piezoelectric film based on the high overmode bulk acoustic resonator (HBAR) resonance frequency spectra directly. The configuration of the HBAR to be discussed is shown in Fig.1. The thin ZnO film within two Aluminum electrodes is deposited on a substrate, which is an AT-cut quartz in real samples, but in the simulation discussed in this paper it is a fused quartz for simplicity. It was reported that if the C-axis of the film is 40 degree declined from the normal (Z coordinate axis) of the principle plane and the electric field is applied along Z-axis, a shear wave resonator can be obtained [6]. For this configuration, the related parameters of the fused quartz substrate plate are the density, ρ_{sb}, the shear modulus, μ_{sb}, and thickness, b. For the piezoelectric film, the parameters describing the film material (poled ceramic ZnO) are quite complicate. Here, it is phenomenologically described as a "pure shear mode", i.e., the related parameters are formally described in Descartes coordinates -- the density, $\hat{\rho}$, the effective shear effective modulus, $\hat{C}_{55}$, thickness, l_f, and the effective coupling factor, k_{35}^2.

The objective of the paper is to show a method, by which we can directly evaluate the three effective parameters of the piezoelectric films, i.e., $\hat{\rho}$, $\hat{C}_{55}$, and k_{35}^2, from the HBAR spectra, by knowing the thickness of the film and the three parameters of the substrate. Due to the space limit of this article, only the procedure of determining electromechanical coupling coefficient is presented.

The principles of the measurement method, which is a set of explicit formulae derived from the input impedance of the composite resonator, are presented in the first part. Then the validity and accuracy of the method will be given by numerical simulation. To investigate the validity of the method, we will ignore the mechanical effect of the electrodes. Then we will discuss the effects of the electrodes by further simulations.

II. HBAR resonance frequency spectrum

Fig.2 shows the simulated input impedance of an HBAR consisting of a thin piezoelectric film on a substrate plate. In practice, hundreds of pairs of resonance frequencies appear in the "fundamental mode region" of the film. The method relays on the parallel and series frequency spectra, and the resonance frequency equations are derived from the input impedance formula.

For the composite resonator consisting of a piezoelectric layer on a substrate, the input electrical impedance can be obtained from Sittig's model [7], which is given in Eq.(1), by ignoring the electrodes.

$$Z_{in} = \frac{1}{j\omega C_0} \cdot \left[1 - \frac{k_{35}^2}{\gamma} \cdot \frac{(2 \cdot tan(\gamma/2) + z_b \cdot tan(\gamma_{sb}))}{(1 + z_b \cdot tan(\gamma_{sb})/tan(\gamma))} \right] \quad (1)$$

where $\gamma = 2\pi f \cdot l_f / \hat{V}_s, \quad \gamma_{sb} = 2\pi f \cdot b/V_{sb}$. (2)

$C_0 = \varepsilon_{33}^S \cdot A/l_f$ is the clamped capacitance of the resonator; $k_{35}^2 = h_{35}^2 \cdot \varepsilon_{33}^S / C_{55}^D$ is the effective coupling factor of the piezoelectric film; $z_b = Z_b/Z_0$, Z_b and Z_0 are the acoustic impedance of the substrate plate and the film layer, respectively, and $Z_b = \rho_{sb} \cdot V_{sb} \cdot A$, $Z_0 = \hat{\rho} \cdot \hat{V}_s \cdot A$, A is the surface area of the resonator.

In the calculation of Fig.2, an imaginary part (0.1 %) is added to the velocities for both the substrate and film to avoid the singularities. The response shows a series of resonances due to the finite substrate thickness, and an enveloped resonance of these resonances due to the effect of the piezo-film. To clarify the roles of these parameters, we briefly discuss the resonance frequency spectrum.

III. HBAR spectrum method

●*Parallel and series resonance frequency formulae*

The parallel and the series resonance frequency equations can be obtained from (1) by setting $|Z_{in}|$ to infinite, and to zero, respectively.

$$tan\ (\gamma) + z_b \cdot tan\ (\gamma_{sb}) = 0 \quad (3)$$

$$tan(\gamma) + z_b \cdot tan(\gamma_{sb}) = (k_{35}^2/\gamma) \cdot [2 \cdot tan(\gamma/2) + z_b \cdot tan(\gamma_{sb})] \cdot tan(\gamma) \quad (4)$$

It is shown in (3) that the parallel resonance frequencies are only determined by the mechanical properties of the two layers. When the thickness of the substrate is much larger than the film (as in practical use), many resonances appear. The spacing between resonances looks like uniform, but in fact it is periodically distributed. This property is important and the method developed in this paper is based on this phenomenon.

The period of the parallel resonance frequency spacing (PRFS) can be obtained by taking: $tan(\gamma) = 0$, or $tan(\gamma) - \infty$. The regions where $tan(\gamma) = 0$, i.e., $\gamma \approx n\pi$, are referred to as the normal regions while the regions where $tan(\gamma) - \infty$, i.e., $\gamma \approx (n - 1/2) \cdot \pi$, are referred to as the transition regions. There are $M - 1$ resonance frequencies in a period where $M = (\hat{V}_s/2l_f)/(V_{sb}/2b)$ is the ratio of the half wavelength resonance frequency of the film to that of the substrate.

For each parallel resonance frequency there is a corresponding series resonance frequency in the spectrum. Each pair of resonant frequencies, labeled by mode m , has a different relative difference, which is quantitatively related to the "effective coupling factor" of the m-th mode resonator.

● *Effective electromechanical coupling factor and its distribution*

The m-th mode parallel and series resonance frequencies are labeled by $f_m^{(p)}, f_m^{(s)}$. An "effective coupling factor" of the mode is defined by

$$k_{eff}^2(m) \approx (\pi^2/4) \cdot (f_m^{(p)} - f_m^{(s)}) \cdot f_m^{(s)} / (f_m^{(p)})^2 \quad (5)$$

It is interesting to observe the effective coupling factor distribution. For the sample given above the results are shown in Fig.3. The parallel and series resonance frequencies are calculated from Eq.(3) and (4), respectively, and the data of $k_{eff}^2(m)$ are evaluated from (5). It is noted that the peak of the effective coupling factor is near the frequency where $f = \hat{V}_s/2l_f$, and it is the position of the fundamental frequency when the piezoelectric film is both side-surfaces free.

The coupling factor of the film, k_{35}^2 , usually can be obtained by fitting the data of the measured k_{eff}^2 (m) and the data calculated from (2) and (3). In the following, we develop a method by which the k_{35}^2 can be directly evaluated by using the k_{eff}^2 (m) data at the center of the first normal region.

● *Principles of the direct measurement method*

Using the definition of the "effective coupling factor" in (5), we derived an explicit formula, which relate k_{35}^2 to the "effective coupling factor" of a special mode.

At the first normal region where $tan(\gamma) \approx 0$, we obtained

$$k_{35}^2 = (1 + \rho_{sb} b / \hat{\rho} l_f) \cdot (k_{eff}^2(m_N)) \quad (6)$$

where $m_N = 1 + round(\hat{V}_s b / V_{sb} l_f)$ is the mode order at the center of the region.

Formula (6) gives the principle of the measurement method--the k_{35}^2 value of the film can be determined from the $k_{eff}^2(m_N)$ value and the mass ratio of the two layers. The effective coupling factor $k_{eff}^2(m_N)$ is determined by the resonance frequency spectra while the mass ratio of the two layers is previously known.

IV. Validity verification of the method

Firstly, we concern the relation of the accuracy with the thickness of the substrate for a given film. Obviously, the accuracy in measuring k_{35}^2 is determined by the approximate formula and by the accuracy of the measured resonance frequencies, which determine the effective coupling factor, k_{eff}^2 . In simulation, the data of the resonance frequency spectra are calculated (that means the data are ideal), and the difference between the evaluated parameters by simulation and the input data is the accuracy of the approximate method. The parameters used in simulation are given in Fig.2, and the thickness of the substrate is changed from 0.85 mm to 0.025 mm, which correspond to m_N being 235 to 8. Results indicate that if m_N is an integer or it is larger than 50, the errors will not larger than 1 %; if the m_N is far away from an integer, the errors will increase with the m_N decrease.

Secondly, it is understood that the formula (6) was derived based on Eqs.(3) and (4) which pertain only to lossless materials. Any piezoelectric material, however, has mechanical, dielectric and piezoelectric losses. As such, the resonance frequencies have to be calculated directly from Eq.(1) or (2). For checking the validity of the method, we carried out a numerical simulation by taking the mechanical losses into account to show its effects on the k_{35}^2 measurement.

The parameters of the sample used in simulation are the same as given in Fig.2, except that the velocity of the film is a complex, i.e., $\hat{V}_s = c_r + j \cdot c_i$. We took $c_r = 2.830 km/s$ and c_i/c_r = 0.0%,0.1%,1.0%,2.0%,5.0%and 10.0%. The simulation results indicated that the method is available for practical materials, and the accuracy depends on the material Q-value. In the range of $Q \geq 20$, the resonant frequencies and so the k_{35}^2 values do not change significantly (less than 1.0 %).

V. Effect of electrodes

For high frequency BAW devices, especially for resonators, the effects of electrodes have to be taken into account. Following the same procedure as the case of ignoring the effects of electrodes, the impedance formula and the resonance frequency equations are given in (7), (8) and (9). The formula used to evaluate the electromechanical coupling factor is given by (10).

$$j\omega C_0 \cdot Z_{in} = 1 - \frac{k_{35}^2}{\gamma} \cdot \frac{(z_1 + z_2) \cdot sin(\gamma) + j \cdot 2 \cdot (1 - \cos(\gamma))}{(z_1 + z_2) \cdot cos(\gamma) + j \cdot (1 + z_1 \cdot z_2) \cdot sin(\gamma)} \qquad (7)$$

$$(z_1 + z_2) \cdot cos(\gamma) + j \cdot (1 + z_1 z_2) \cdot sin(\gamma) = 0 \qquad (8)$$

$$(z_1 + z_2) \cdot cos(\gamma) + j \cdot (1 + z_1 z_2) \cdot sin(\gamma) - \frac{k_t^2}{\gamma} \cdot (z_1 + z_2) \cdot sin(\gamma) + j \cdot 2(1 - cos(\gamma)) = 0 \qquad (9)$$

$$k_{35}^2 = \frac{\hat{\rho} \cdot l_f + \rho_{sb} \cdot b}{\hat{\rho} \cdot l_f + \rho_e \cdot (l_{e1} + l_{e2})} \cdot k_{eff}^2(m_N) \qquad (10)$$

Where, $\gamma = \omega l_f / \hat{V}_s$; $z_1 = Z_1/Z_0, z_2 = Z_2/Z_0$. Z_1 , Z_2 are the acoustic load impedances of the electrode presenting at the upper and lower side of the piezoelectric layer respectively. They are given by

$$Z_1 = j \cdot Z_{e1} \cdot tan(\gamma_{e1}) \qquad (11)$$

$$Z_2 = j \cdot Z_{e2} \cdot \frac{(Z_{sb}/Z_{e2}) \cdot tan(\gamma_{sb}) + tan(\gamma_{e2})}{1 - (Z_{sb}/Z_{e2}) \cdot tan(\gamma_{e2}) \cdot tan(\gamma_{sb})} \qquad (12)$$

Where $\gamma_{e1} = \omega l_{e1}/V_e, \gamma_{e2} = \omega l_{e2}/V_e$, $\gamma_{sb} = \omega b/V_{sb}$ are the wave number in the electrodes and the substrate, respectively; $Z_{e1} = Z_{e2} = S \cdot \rho_e \cdot V_e$, $Z_{sb} = S \cdot \rho_{sb} \cdot V_{sb}$, are the acoustic impedance of the electrodes and the substrate, respectively. ρ_{e2}, ρ_{sb} are the densities, V_{e2}, V_{sb} are the velocity of this two materials, respectively.

Eq.(10) is the modified formula of the method. Comparing with the case of ignoring the electrode, the mass of the electrodes will enhance the electromechanical coupling factor of the center mode. For investigating the validity of the formula, we simulated the effects of the electrode on the measurement method. In simulation, the data of the HBAR spectra are calculated by using (8) and (9), or directly by (7), and then using Eq.(5) to evaluate the effective coupling factors of the modes.

The data of the samples used in simulation are the same as before, except the substrate thickness is 0.25 mm and with different thickness of the electrodes. The results are shown in Fig.4. The dotted line is the data from Eq.(6) and the solid line is the results from Eq.(10). It can be found that the effects of electrodes can be properly compensated by the modified formula (10) in the limited range of considering the electrode as a mass loading.

VI. Conclusion

We presented a measurement method for characterizing the piezoelectric film, which is deposited on a substrate plate, to form a thickness-shear wave high-overmode bulk acoustic resonator (HBAR). Directly using the parallel and series resonant frequency spectra of the HBAR, the electromechanical coupling factor of the piezoelectric film k_{35}^2 can be accurately evaluated. Validity of the method was verified by numerical simulation on samples consisting of ZnO film on fused SiO2 substrate by taking the mechanical loss into account. Simulation further indicated that the mechanical effects of the electrodes can be corrected by a modified formula in the range of considering the electrodes as a mass loading.

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*e-mail: chaomk@txc.com.tw

† e-mail: bryanwu@txc.com.tw

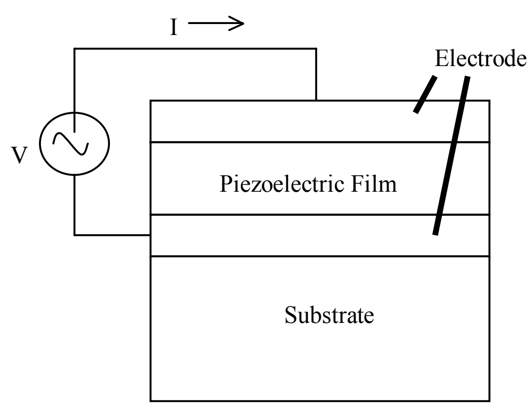

Figure 1 The schematic simulation model of the HBAR

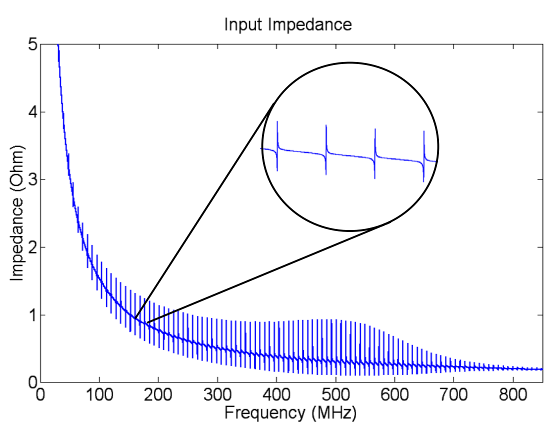

Figure 2 Input electrical impedance of HBAR. The Zno thickness =2.5µm, acoustic velocity=2831m/s, density= 5675kg/m3, k^2_{35}=0.029, the fused quartz thickness = 0.25mm, acoustic velocity=4100m/s, density= 2650kg/m3.

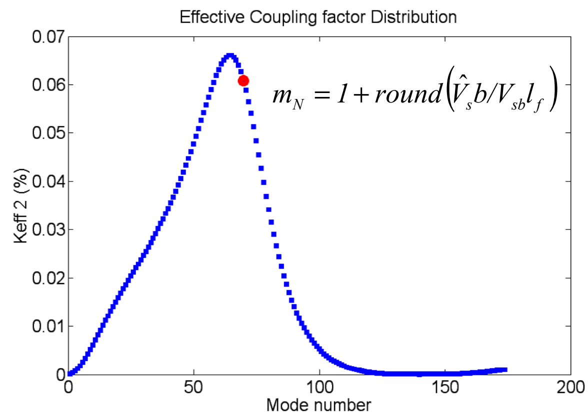

Figure 3 Effective coupling factor distribution.

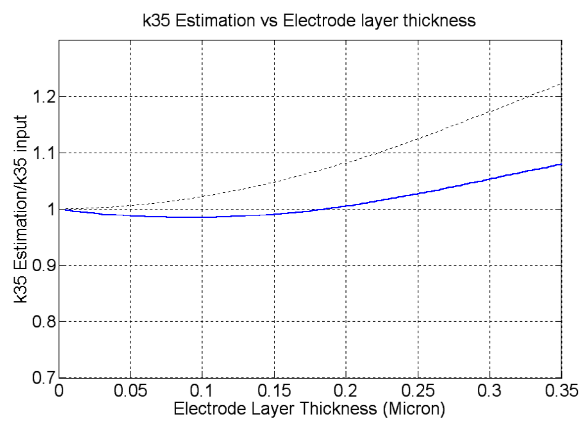

Figure 4 k^2_{35} estimation:Dotted :Calculation by Eq.(6)
Solid : Calculation by Eq.(10).