Mass Sensitivity of Thin Film Resonator Devices

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***Abstract*—A systematic study of the influence of the materials' properties and thickness in composite Thin Film Bulk Acoustic Resonators (FBAR) on the Mass sensitivity is presented. Calculations based on the Mason Transmission Line model are presented along with some preliminary experimental results. We present and investigate the concept of sensitivity amplification in the mass sensitive regime and show how this amplification correlates with wave reflection and interference within the composite structure. Asymmetrical resonators where the sensitivity differs between the two different surfaces are also presented.**

I. Introduction

The possibility for inexpensive mass production of miniaturized and highly sensitive sensors has made the thin film electro-acoustic technology very attractive for various sensor applications. A good understanding of the factors influencing the mass sensitivity is of importance for the design of Thin Film Bulk Acoustic Resonators (FBAR) for various applications. Recently, a number of experimental and theoretical investigations on the mass sensitivity of different FBAR devices both operating in the shear and the longitudinal thickness excited mode[1-5] have been presented. In a FBAR sensor, in contrast to QCM, the thickness of the electrodes is comparable to that of the piezoelectric film. It has been empirically shown that the mass sensitivity is affected by all the layers in the resonator structure and more specifically by their thickness and acoustic impedance. Recent studies of FBARs have indicated the existence of a sensitivity amplification effect if a layer of low acoustic impedance is added to the structure[4, 5]. It has also been shown in the case of QCM that a mass sensitivity amplification can be obtained with viscous layers [6] as well as with rigid thick layers of low acoustic impedance material added to the resonator [7]. However, there has not been a thorough study, to our knowledge, that shows in detail the influence of rigid non-viscous layers in composite FBAR structures, which is the subject of study in this work.

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II. Theory

A. Single material resonators

From the theory behind the QCM and other single material resonators it follows that the relative frequency shift is proportional to the relative mass change as

$$\frac{\Delta f}{f} \propto \frac{\Delta m}{m} \quad , \qquad (1)$$

or equivalently to the frequency of operation as

$$\frac{\Delta f}{f} \propto \Delta m\, f \quad . \qquad (2)$$

B. Definition of mass sensitivity

Only rigid masses attached to surface are considered here and the mass sensitivity (S) is defined here as the relative frequency shift, $\Delta f/f_0$, normalized to the mass of the rigid thin layer attached onto surface. Δf is the resonance frequency shift caused by the added mass and f_0 is the resonance frequency without the added mass. The mass sensitivity is then:

$$S = \frac{\frac{\Delta f}{f_0}}{\rho_m t_m}, \qquad (3)$$

where ρ_m is the measured material density and t_m the thickness of the measured material.

It is well known that as long the attached layer is sufficiently thin the phase shift within the layer can be neglected and hence only the mass of the layer will influence the resonance frequency; and not the stiffness of the material. Therefore, by normalizing to the surface density in (3), S will be independent of the type of material sensed.

C. Perturbation theory of acoustic waves

In an FBAR sensor, in contrast to QCM, the thickness of the electrodes is comparable with that of the piezoelectric film. Therefore, a FBAR must be considered as a multilayer structure. The acoustic path includes the piezoelectric film as well as acoustically "dead" material, e.g. electrodes and additional layers such as for instance Au, which is commonly used as a suitable surface for various biochemical applications, or SiO_2 which also is used for temperature compensation.[8] Under these conditions the simplified theory for single material resonators will not be adequate for describing the behavior of FBAR sensors.

Rayleigh stated that at resonance the peak kinetic energy equals the peak potential energy.[9] A thin layer of mass rigidly attached to the surface will move synchronously with the surface, not changing the amplitude of displacement nor the potential energy. The added mass at the surface will perturb the system causing the resonance frequency to change. From this fact one can easily derive an expression for the mass sensitivity.

$$S = \frac{\frac{\Delta f}{f_0}}{\rho_m t_m} = -\frac{1}{4}\frac{\omega^2 u_m{}^2}{U_{Kin}^{Total}} = -\frac{1}{2}\frac{u_m{}^2}{\int_0^h \rho u^2 dz}, \qquad (4)$$

where u_m is the displacement amplitude of the added layer (that is the displacement amplitude at the surface of interest) and h is the total thickness of the multilayer structure. ρ and u are the density and the amplitude distributions respectively in the multi layer structure.

From eq.(4) it is obvious that the sensitivity is determined by the amplitude of oscillation at the surface of interest. It is also evident from the integral in the denominator that the material in the resonator structure and the internal order of the including layers will influence the sensitivity. In an asymmetrical FBAR structure the sensitivity to a mass load will also vary depending onto which side of the structure the mass is added.

D. Models used for computing the Mass sensitivity

There are two dominating one-dimensional matrix based equivalent models for computing the response from a multilayer resonant structure; the Nowotny-Benes (NB) model and the Mason Transmission Line model. With the Mason model it is easier to obtain the displacement amplitude distribution and other information within the studied structure at the same time as calculating the electrical impedance. But to initially verify the validity of the perturbation model in eq. (4), the mass sensitivity was calculated directly using the NB model by adding thin layers of arbitrary material onto the resonating structure and then calculating the relative frequency shift. The results were then compared with those obtained with equation (4) using the amplitude distribution calculated from the Mason model.

It was concluded that the Mason transmission line model is convenient to derive the amplitude distribution within multilayer FBAR structures and subsequently calculate the mass sensitivity using eq. (4). In addition, the particle displacement, energy and strain distribution in the structure are also calculated. To avoid singularities in the calculations the latter were performed at parallel resonance frequency. The majority calculations were carried out for the pure shear mode. No energy losses in the materials have been considered.

III. Results and Discussion

Commonly used layers of non-piezoelectric material in the acoustic path of a FBAR are the metal electrodes and additional layers such as for instance Au, which is normally used as a stable surface for various biochemical applications, or SiO_2 which is used for temperature compensation.[8] The Au and SiO_2 have higher and lower acoustic impedance than AlN respectively, and are therefore also interesting to use as case study materials for illustrating how the sensitivity is influenced by both high and low acoustic impedance materials.

A. Influence of Acoustic impedances

As a starting point a simplified structure consisting of 2µm AlN clamped between two imaginary thin electrodes where one electrode is covered with a layer of Au or SiO_2 of varying thickness. The displacement amplitude distribution was calculated with the Mason model, for the first and second harmonic. The results are given in figure 1-4.

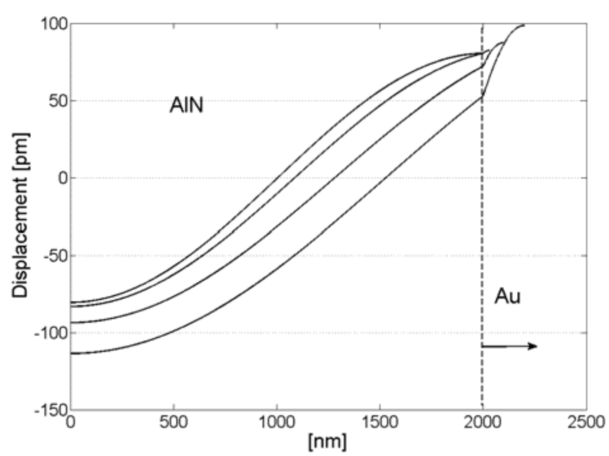

Figure 1. *Displacement amplitude calculated for the first harmonic pure shear mode of a 2µm AlN resonator, with imaginary thin electrodes on each side with an additional layer of Au with varying thicknesses on one side.*

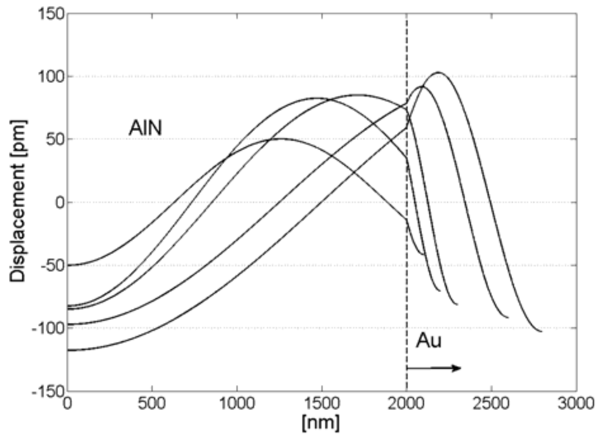

Figure 2. *Displacement amplitude calculated for the second harmonic pure shear mods of a 2μm AlN resonator, with imaginary thin electrodes on each side with an additional layer of Au with varying thicknesses on one side.*

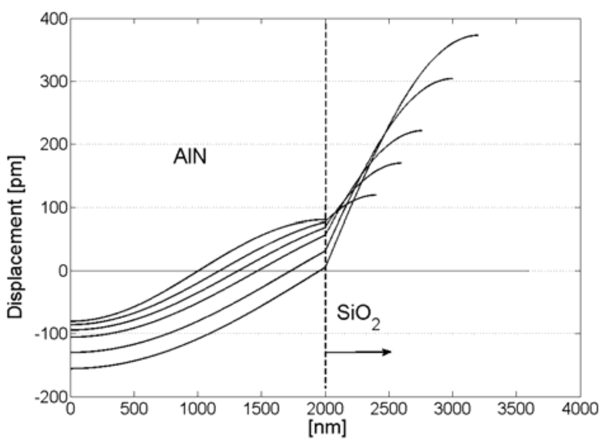

Figure 3. *Displacement amplitude calculated for the first harmonic pure shear mods of a 2μm AlN resonator, with imaginary thin electrodes on each side with an additional layer of SiO_2 with varying thicknesses on one side.*

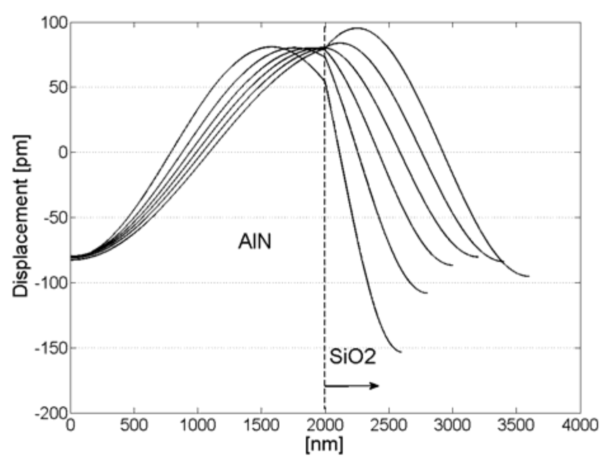

Figure 4. *Displacement amplitude calculated for the second harmonic pure shear mods of a 2μm AlN resonator, with imaginary thin electrodes on each side with an additional layer of SiO_2 with varying thicknesses on one side.*

The mass sensitivity was then calculated by applying eq.(4) for both the AlN surface and the added material's surface, respectively. Both the first and the second harmonic resonance are shown in Fig. 5 and Fig. 6 for the SiO_2 and Au case respectively.

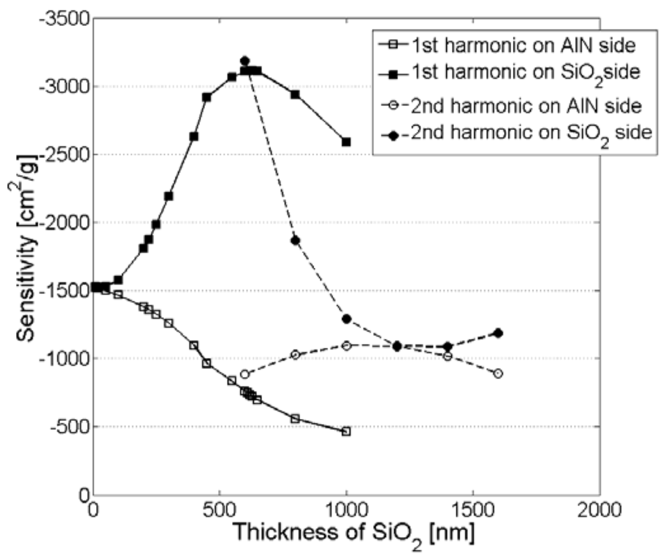

Figure 5. *Mass sensitivity calculated for the first and second harmonic pure shear modes of a 2μm AlN resonator, with imaginary thin electrodes on each side with an additional layer of SiO_2 with varying thicknesses on one side.*

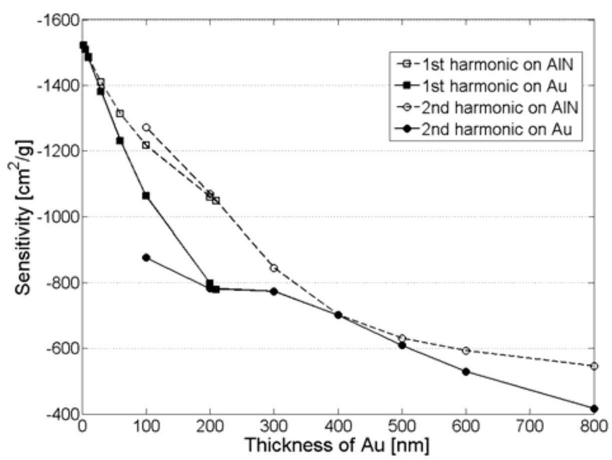

Figure 6. *Mass sensitivity calculated for the first and second harmonic pure shear modes of a 2μm AlN resonator, with imaginary thin electrodes on each side with an additional layer of Au with varying thicknesses on one side.*

It is seen in figure 5 and 6 that by adding only a small fraction of a non piezoelectric material, roughly 1% of the AlN thickness, there is a decrease in mass sensitivity at both surfaces independently of the acoustic impedance of the added material. This is expected since we are still in the regime where the theory for the single material resonator (eq. 1 and 2) is valid. But already at 100nm of added SiO_2 the mass sensitivity at the SiO_2 surface is amplified compared to the pure AlN case and reaches a maximum at a SiO_2 thickness of around 600 nm. The sensitivity to mass load at the bare AlN surface however decreases continuously. And at 600 nm of SiO_2 we see a 6-fold difference between the two surfaces and a maximum of sensitivity at the SiO_2 surface twice that of the bare AlN case. This sensitivity amplification is seen when material is added to the FBAR structure, even though the total mass is increased and hence the resonance frequency is decreased, which goes against eqns. (1) and (2). Similar results as above were observed for other low acoustic impedance materials such as Al. The calculations were then repeated replacing the SiO_2 with other materials that have equal or higher acoustic impedance than the AlN. In all these cases only a decrease of the sensitivity was observed. This is illustrated in Fig. 6 where the SiO_2 is replaced by an Au layer. In both cases the side where no extra material was added only the expected decrease due to the lowering of the frequency was observed.

B. Reflection and interference of Acoustic waves

It is evident that there is a fundamental difference between the cases of high and low impedance materials. The structures studied above could be described as AlN/Au/ambient and AlN/SiO_2/ambient, where ambient could be air or water, both having lower acoustic impedances than both Au and SiO_2. The basic difference between the two cases is the jump in impedance at the AlN/layer interface. In the first case it is from low to high impedance, whereas in the second case it is from high to low impedance. The implications are that the transmitted wave in the AlN/SiO_2 case will have a relative amplitude larger than one while in the AlN/Au case it is smaller than one, since the amplitude ξ_2 of the transmitted wave is given by:

$\xi_2 = \dfrac{2}{1 + z_2/z_1}\,\xi_1$, where ξ_1 is the amplitude of the incident wave, while z_1 and z_2 are acoustic impedances of the AlN and the added layer respectively. In a finite structure, however, the amplitude is determined by superposition of the transmitted and reflected waves at the two interfaces together with their corresponding phases, which in our case means that the amplitude is also a function of the thickness of the added layer. For this purpose a numerical calculation with the Mason model of a composite structure consisting of a semi-infinite AlN slab and an added layer of finite thickness is performed. The frequency of the incident wave is chosen to be equal to the resonant frequency of the resonator under consideration. Figure 7 shows the peak amplitude at the surface of the added layer as a function of its thickness for both Au and SiO_2.

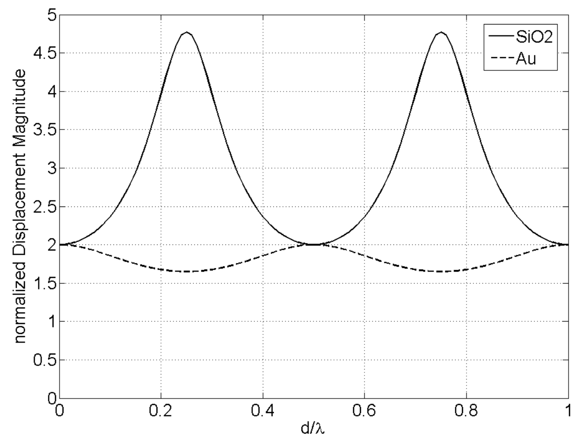

Figure 7. *The displacement magnitude at the surface of an layer of SiO_2 and Au respectively addied on an infinite AlN slab, normalized to the incoming wave amplitude.*

At ¼ of a wavelength a clear maximum of the amplitude at the surface is seen for the case of SiO_2 and a minimum for the case of Au. This result indicates that the sensitivity amplification in the case of low acoustic impedance material is related to a constructive interference in the structure, giving rise to an increased amplitude at the surface. It is also seen in the case of the SiO_2 a minimum at ½ wavelength, corresponding roughly to the minimum observed for the second harmonic at the SiO_2 surface in fig 5.

Revisiting eq. (4), it is seen that there are three main quantities influencing the mass sensitivity; frequency, amplitude at surface and the total energy within the system respectively. Since the AlN thickness was kept constant in the calculations the frequency decreases and this effect will also influence the sensitivity, causing a shift of the peak sensitivity from ¼ of a wavelength towards smaller SiO_2 thicknesses, as indicated in fig 8. In the case of the Au added layer this effect is much stronger and hence determines the overall behavior of the mass sensitivity versus thickness.

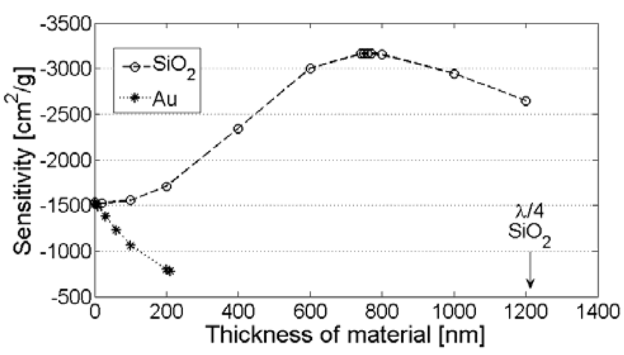

Figure 8. *Mass sensitivity calculated for the first harmonic pure shear mode of a 2μm AlN resonator, with imaginary thin electrodes on each side with an added layer of SiO_2 or Au respectively. The presented sensitivity is for the side of the resonator onto which material is added. The position of the quarter wavelength is marked for the SiO_2.*

C. Combination of low and high acoustic impedance materials

The qualitative arguments in the previous arguments were sufficient to prove the existence of sensitivity amplification whereas for the precise determination of the position of the peak sensitivity a complete Mason computation must be made. Such complete calculations were then made for realistic FBAR structures consisting of 2μm AlN, with 220 nm thick electrodes on either side. By virtue of the above arguments and as seen in figure 9 the addition of Al electrodes will actually result in a sensitivity magnification, equally on both sides. Thus, a sensitivity of $1620 cm^2/g$ is obtained for a resonator with Al electrodes as compared to $1530 cm^2/g$ for 2μm AlN only. Similar calculations to those above by including an additional SiO_2 or Au layer were also performed. The results for the sensitivity of the 1^{st} harmonic on the SiO_2 and Au side respectively are shown in fig 9.

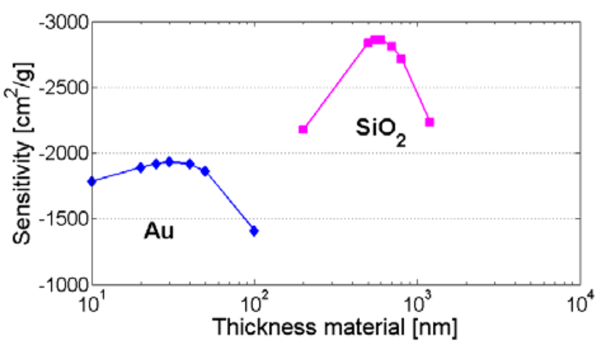

Figure 9. *Mass sensitivity calculated for the first harmonic pure shear mode of a 2μm AlN resonator, with 220 nm Al electrodes with an additional layer of Au and SiO_2 respectively. The presented sensitivity is for the side of the resonator onto which material is added.*

Thus in the case where real (low acoustic impedance) electrodes are included in the calculations, a sensitivity amplification is observed in both the SiO_2 as well as the Au case. The effect responsible for getting a sensitivity magnification also for the high acoustic impedance case is believed to be due to low effective acoustic impedance of the combined Al and Au layers.

IV. EXPERIMENTAL

Some preliminary experimental studies were made to illustrate the validity of the above calculations. A well controlled reactive sputtering process was used to repeatedly deposit 2nm of Al_2O_3 onto different resonators and measure the frequency shift after each deposition. The electrical measurements were performed using a HP 8720D network analyzer. The parallel resonance frequency was used in the measurements since the measurement procedure demanded repeated probing of the devices and the parallel resonance frequency less sensitive to electrode scratching.

Table 1 shows the results for two particular resonators - one consisting of 2μm thick AlN with 200 nm Al on either side operating at the first harmonic, while the other has an additional layer of 1.22μm SiO_2 for temperature compensation [8] operating at the second harmonic. The highly textured AlN films were specifically grown [10] with a mean tilt of the c-axis of around 25^o degrees, allowing therefore the excitation of both the quasi shear mode and the quasi longitudinal mode at 1.3GHz and 2.3GHz respectively.

Table 1: Comparison between theoretical (Theory) and experimental (Exp.) values of the relative mass sensitivity [cm^2/g] for a temperature compensated ($Al/AlN/Al/SiO_2$) resonator and a non-compensated (Al/AlN/Al) resonator operating at the 1.3 GHz quasi-shear mode and the 2.3 GHz quasi longitudinal mode respectively.

	Theory	**Exp.**	**Theory**	**Exp.**
	1^{st} Harmonic without additional material	1^{st} Harmonic without additional material	2^{nd} Harmonic with 1.22μm SiO_2	2^{nd} Harmonic with 1.22μm SiO_2
shear	1520	1410	950	935
long	1470	1310	990	980

It is noted that the comparison between theory and experiment given in Table 1 is presented here to illustrate the excellent agreement between the two. It does not, however, experimentally demonstrate the existence of a maximum in the sensitivity. A comprehensive experimental study is in progress to that effect and will be published in a follow up article.

V. CONCLUSIONS

Systematic theoretical studies of the mass sensitivity of both composite and non-composite FBAR resonators have been performed. It has been predicted that the inclusion of a layer with a low acoustic impedance (lower than the piezoelectric material) in a FBAR sensor results in an enhancement of the mass sensitivity, which passes through a maximum for the 1^{st} harmonic. The above enhancement is observed on the surface of the added layer and is complemented by a corresponding decrease in sensitivity on the opposite side. With respect to the 2^{nd} harmonic the maximum is observed on the opposite side while the sensitivity on the added layer surface goes through a corresponding minimum. Finally, for a realistic FBAR resonator with “thick” Al electrodes operating at the 1^{st} harmonic the sensitivity exhibits a maximum for both high and low impedance of the added layer. In all cases the behavior of the sensitivity is argued to be a direct consequence of the interference pattern in the added layer formed as a result of the superposition of the reflected and incident waves.

Preliminary experimental measurements show an excellent agreement with theoretical predictions. Full experimental confirmation of the predicted behavior of the sensitivity is yet to be performed. It is finally noted, that for brevity the discussion has been solely confined to sensitivity variations and has not illuminated the effects of including additional materials on both the Q value and the electromechanical coupling. For optimal design of a sensor all three parameters need to be considered simultaneously.

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