Effects of compensating the temperature coefficient of frequency with the acoustic reflector layers on the overall performance of solidly mounted resonators

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Keywords:

Solidly mounted resonators
Temperature coefficient of frequency
Acoustic reflectors
Finite Element Analysis

A B S T R A C T

Thin film acoustic wave resonator based devices require compensation of temperature coefficient of frequency (TCF) in many applications. This work presents the design and fabrication of temperature compensated solidly mounted resonators (SMRs). The characteristics of each material of the layered structure have an effect on the device TCF but depending on the relative position with respect to the piezoelectric material in the stack. The influence of material properties of the different layers composing the device on the TCF is discussed in detail. TCF behavior simulation is done with Mason's model and, to take into account the deterioration of overall performance due to the finite lateral size and shape of the resonator, we have used 2D and 3D finite element modelling of the resonators. The overall behavior of the device for external loads is predicted. SMRs are designed according to simulations and fabricated with different configurations to obtain TCF as near to zero as possible with an optimized response. Resonators are made by depositing Mo/AlN/Mo piezoelectric stacks on acoustic reflectors. As reflector materials, conductive W and insulating WO_x films have been used as high acoustic impedance materials. SiO_2 films are used as low acoustic impedance material.

1. Introduction

Bulk acoustic wave resonators (BAW) based sensors are gaining much attention for chemical and physical sensing applications, because of their simple and robust structure, interconnection with electrical systems, the possibility of low-cost mass production and high sensitivity [1,2]. Their potential application in mobile communication, as competitors of surface acoustic wave (SAW) and dielectric filters, and in biological and gas sensing, are widely reported [3–5]. The thickness-excited longitudinal wave mode in bulk acoustic wave resonators (both suspended and solidly mounted (SMR)) has been used in gravimetric chemical and physical sensors working in gas phase and they show encouraging results for bio and smart gas sensor applications [6,7]. Some attempts [8,9] have been made to operate these resonators for biochemical sensing handling liquid samples. FBAR based on *c*-axis-inclined ZnO [10] and AlN [9] operating in the thickness shear

mode have been successfully used in liquid media, indicating a great potential for chemical and biochemical sensors as high sensitivity transducers.

Temperature stability in FBAR and SMRs for sensor applications is another non-resolved critical issue. The thermal stability of the resonator can be evaluated by the temperature coefficient of the resonant (or anti-resonant) frequency (TCF), which measures the relative variations of resonant frequency with temperature ($\text{TCF} = (1/f) \cdot (df/dT)$). Since there is no piezoelectric material available which is temperature compensated, it is compulsory to use composite structures in such a way that some materials compensate the negative coefficients of the common piezoelectric materials. The variation of the resonant frequency with temperature can be due to the variation of material properties such the acoustic velocity, which depends on the elastic coefficients, and the variation of the geometry due to dilatation processes. Reducing TCF in a resonator is usually achieved by adding films which have properties that compensate the rifts of those that move with temperature. The most common material used for this purpose is SiO_2 , which has a positive coefficient of the elastic constants and compensates the

negative one of the other materials composing the resonator [11]. ZnO and AlN are both sensitive to temperature variation having a negative coefficient. The typical temperature coefficient of frequency (TCF) of suspended ZnO and AlN SMRs are $-60 \text{ ppm}/^\circ\text{C}$ and $-25 \text{ ppm}/^\circ\text{C}$ respectively [12]. To compensate this negative TCF, an additional layer of material having positive TCF in the acoustic path is needed. Successfully compensation of thickness shear mode by [13] in ZnO/Si and AlN/Si composite FBARs has been reported. In this case, Si was p+ doped to achieve a positive TCF, but it results in a significant reduction of both electromechanical coupling coefficient (k_t^2) and resonant frequency. The TCF of AlN is reduced to $-15 \text{ ppm}/^\circ\text{C}$ [14] by using SiO_2 films (which display a TCF of $+85 \text{ ppm}/^\circ\text{C}$) as a compensating material. The added material also results in a substantial reduction of coupling and resonant frequency.

This paper reports the simulation at different temperatures and the electrical characterization of fabricated SMRs using SiO_2/W and SiO_2/WO_x reflectors. Different kinds of the reflector are simulated and fabricated with different thickness from the ideal symmetric $\lambda/4$ to asymmetric with AlN as a piezoelectric material. We report the influence of the different thicknesses of the layers composing the acoustic reflectors on the TCF. All the simulations are done with Mason model and Finite Element Modelling (FEM) through acoustic velocity dependence on temperature and thermal expansion respectively. It is worth to note that in this work, SiO_2 layers are part of the reflector. This preserves the performance of the resonators (coupling and quality factor).

2. Simulation methods

The one dimensional simulation method based on Mason's model [15] is proposed for determining the influence of different materials and their thicknesses in the reflector stack on the TCF of SMRs. The accurate design of the resonator is needed before fabrication. Mason's model provides a good tool for driving the resonant frequencies of the different modes at a time. It can also be used as designing tool to determine the thicknesses of the different layers of the acoustic reflector to minimize the TCF and their influence on the performance of the resonator.

The energies associated with the transmitted and reflected wave can be easily calculated, if we consider that a wave is propagating from the piezoelectric layer towards the sandwiched reflector layers. The transmitted and reflected wave energy can be computed with the help of the effective acoustic impedance Z_b of the bottom layer stack of Mason's model. For this purpose, the mirror reflectivity is given by

$$R = \frac{Z_p - Z_b}{Z_p + Z_b} \quad (1)$$

where Z_p and Z_b is the acoustic impedance of the piezoelectric layer and the effective acoustic impedance of the layer stack underneath it respectively. R , Z_p and Z_b are complex numbers, which also take into account acoustic losses. In order to study the in band reflectivity, it is more convenient to use the inverse of R (transmittance T).

The reflector transmittance is affected when the typical symmetric configuration (all layers of a $\lambda/4$ thickness) are changed to asymmetric (some layers with a thickness different to $\lambda/4$). Variation in the thickness of any one of the layers of the reflector below the AlN layer leads to deformation in the reflector T . This causes the variation of the leakages of energy from the piezoelectric stack and the possible degradation of overall performance. Increasing the thickness of SiO_2 (top reflector layer) causes the shear and longitudinal resonances into this layer to appear in the transmission band of the reflector. The deformation generated in this layer is transmitted to the AlN film causing a piezoelectric field that is

measured as impedance variations as shown in Fig. 1. For simulating the transmittance spectrum of the different reflectors in Fig. 1, material constants are taken from [16–18].

Fig. 1 shows that increasing the uppermost SiO_2 layer thickness of the reflector distorts its transmittance and inaugurates overtone modes in the electrical spectrum at frequencies in the band of interest and causes to decrease the acoustic reflectance at major frequencies. It can be seen that further increase in reflector uppermost layer thickness leads to higher distortion in the reflectance. The additional energy loss due to the reduction of the acoustic reflectance can be reduced by carefully designing the whole layer stack and a maximum reflector response can be achieved at the desired frequencies as shown in Fig. 1. It is also notable that this increase of the SiO_2 thickness also causes the decrease of the resonant frequencies generated in the AlN film as the effective mass of the whole resonator varies (gravimetric effect). This, of course, can be corrected by redefining the thickness of the AlN layer. If the increase of the thickness of the uppermost SiO_2 layer is high enough, the frequencies of the resonances in it, the overtones, appear at lower values than those corresponding to the main resonances (shear and longitudinal) generated in the AlN film. This situation is observed in Fig. 1(d). To identify the origin of these resonances is not straightforward and only by measuring their TCF one can definitively make this identification. TCF of the modes originated in SiO_2 are much more positive than those generated in AlN. All these behaviors are present not only in simulation, but also in experimental results. Maximum reflectivity of the acoustic reflector at the resonant frequency is essential because radiation of acoustic waves to the substrate represents energy losses that decrease the quality factor of the device [19]. To maximize reflectivity, it is essential to increase the acoustic impedance ratio between the acoustic layered materials, but also to modify the thickness of all layers when the uppermost SiO_2 layer is made thicker for TCF compensation. The design of the piezoelectric stack (AlN and electrodes) has also to take into account all these issues. Mason's model is a very efficient tool to do this. However, this is a one-dimensional model and no lateral effects are taken into account. To do it on the overall performance of the stack, we use precise 2D and 3D numerical simulation through Finite Element Analysis using COMSOL Multiphysics software. In 2D and 3D models, the finite element method in COMSOL software is used to solve the interaction between mechanical displacement and electrical potential by employing following constitutive piezoelectric equations [20].

$$T_i = c_{ij}^E S_j - e_{ij} E_j \quad (2)$$

$$D_i = \epsilon_{ij}^S E_j - e_{ij} S_j \quad (3)$$

where T_i and S_j are the stress and strain components. c_{ij} is the stiffness constant, e_{ij} is the piezoelectric stress constants and, E_j is the electrical field component. ϵ_{ij} is the permittivity constants and D_i the electrical displacement field. The superscripts S and E indicate that the respective constants are measured at a constant strain and electric field respectively. The frequency response of the resonators and the displacement profile of the wave in the resonator stack are evaluated with 2D FEM. Perfectly matched layers (PMLs) are used at the boundary edges of the stack to avoid energy leakage due to the reflection of waves from the boundaries. The bottom electrode is set to ground, and the frequency dependent potential of 1.0 V is applied to the top electrode. At the boundaries of the PMLs domain, the fixed constraint condition is applied. The other layers are set as free. The meshing is done with mapped mesh having several distributions.

The displacement profile of longitudinal waves of the asymmetric resonator (W reflectors) with $1.21 \mu\text{m}$ thick layer of SiO_2 at the resonant frequency is simulated with 2D finite element model as

Fig. 1. Simulated response of AlN based SMR with W/SiO₂ SMR (black line) and transmittance of the acoustic reflectors for the shear modes (red line) and the longitudinal modes (blue line) centered at 3.0 GHz. (a) Symmetric reflector (all layers of $\lambda/4$ thickness) and asymmetric reflectors with the uppermost SiO₂ layers of different thickness, (b) 600 nm, (c) 1000 nm and (d) 1210 nm. It is also shown the frequency response (black line) of SMRs made with those reflectors. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

shown in Fig. 2. It can be seen that no significant energy is radiated to the substrate or edges, and all energy is confined inside the resonator, which confirms a good performance of the reflectors in the stack. However, further increase causes the energy to leak into the substrate.

Although 2D FEM provides a good approach to evaluating the frequency response of the SMRs, a 3D FEM model has also been developed to calculate the overall response of the resonator. In this model, symmetric boundary conditions are applied to the relevant boundaries. Similar kind of boundary and electric conditions are applied as in 2D model. To reduce the computational time, only a quarter of the original structure is simulated with 3D geometry and for appropriate boundaries, symmetric conditions are applied. The ground and electric conditions are employed in the same way

as in 2D geometry. The spurious response of the SMRs is also calculated by the 3D model. As very thin layers are used in a 3D model, a swept mesh and triangular mesh elements are used to mesh the entire model. The displacement profile is same as obtained with 2D model. The following expression is used to simulate the electrical impedance using the *pzd* interface.

$$Z = \frac{V}{j\omega Q} \quad (4)$$

where Z , V , ω and Q represent the electrical impedance, applied voltage, angular frequency and the charge on the top electrode surface, respectively. The stress profile and impedance simulated with CONSOL Multiphysics is shown in Fig. 3.

Fig. 2. (a) Displacement profile at the resonant frequency, (b) amplitude of standing wave as a function of depth for asymmetric acoustic reflectors with 2D finite element model.

(a)

(b)

Fig. 3. 3D simulation of stress profile of a symmetric W-based resonator at the resonant frequency (~ 2.98 GHz) figure (a) and calculated impedance of the same resonator figure (b).

It can be seen from the stress profile that most stressful region is the bottom area of the piezoelectric layer and the top region of the first SiO_2 layer. Fig. 3(b) shows the impedance spectrum calculated with 3-D finite element model and it is the same as the one calculated with Mason's model.

3. Experimental

Test devices for measuring the TCF and the influence of the reflector design on it were fabricated by depositing the piezoelectric layer sandwiched between the electrodes on top of the acoustic reflector. The bottom electrode consisted in 100 nm thick sputtered Mo film and the top one in 150 nm thick Mo layer. The thickness of the AlN was always 1000 nm. Although this stack is not optimum for the different used reflectors, we used it in all the experiments to compare the influence of the thickness of the uppermost SiO_2 layer of the reflector in the values of TCF. Acoustic reflectors with different configurations made of alternating layers of low (SiO_2) and high (W or WO_x) acoustic impedance materials have been used. As substrate, (1 0 0) oriented Si wafers 100 mm in diameter were used. AlN films were sputtered in an ultra-high-vacuum system pumped to a base pressure below 1.3×10^{-6} Pa. A high purity aluminum target 150 mm in diameter was sputtered in Ar/N_2 atmospheres (40:60) using a pulsed-DC source (MKS ENI RPG-50E) working at 250 kHz. To study shear and longitudinal modes, tilted c-axis and pure c-axis oriented AlN films were used. Pure c-axis oriented films were sputtered at low pressure (0.27 Pa) and 1.2 kW power. During deposition the substrate temperature was kept at 400 °C and for biasing the substrate to a DC voltage of -60 V, an RF power of 15 W was used. This substrate biasing is intended to adjust the in plane residual stress to values lower than 200 MPa. This stress is important to be maintained as low as possible because it can generate delamination of the structure when temperature changes. Under these conditions, the rate of film growing at the center of the substrate was 45 nm/min. To deposit AlN films with tilted grains, before the main AlN film deposited under the same conditions, an AlN seed layer was deposited at high pressure (0.66 Pa) and 600 W without deliberately biasing or heating the substrate. The seed layers of AlN exhibit a (1.03)-preferred orientation, which is crucial to stimulate the growth of the consequent AlN tilted films provided by these

conditions [21]. Additionally, directional deposition of the active piezoelectric layer is needed, therefore the samples were located at 4 cm from the center of the substrate holder and only 34 nm/min of deposition rate was achieved. Using these conditions, AlN films with the wurtzite c-axis tilted around 24° with respect to the surface normal are obtained. The Mo bottom electrode is continuous while the top one is dry-etching patterned. The geometry of the resonator consist in a top electrode surrounding by an extend ground plane in a ground-signal-ground (GSG) configuration. Ground plane contacts the bottom electrode by a strong capacitive coupling.

The acoustic reflectors comprised three layers of high acoustic impedance material (W or WO_x) alternated with four layers of low acoustic impedance material (dense SiO_2). Pulsed-DC sputtering of 150 mm targets in a Leybold Z550 system was used to deposit all layers. To get uniform thickness across the 100 mm silicon wafer, a system of screens between the rotating substrate and the targets was used. Si target was used to deposit SiO_2 layers in Ar/O_2 mixtures with low pressure to ensure a dense material with positive temperature coefficient of the acoustic velocity. The sputtering of high impedance layers (W and WO_x) was done at low pressure (0.13 Pa). 100 μm pitch RF-probes Picoprobe from GGB Industries with an Agilent N5230A network analyzer was used for on wafer measuring the electrical impedance of the SMRs as a function of the frequency and temperature. We use segmented frequency scans to acquire 4000 samples around each resonance for accurately determining the resonant and antiresonant frequencies. During measurements, the sample temperature was varied from 25 °C to 100 °C in steps of around 10 °C by a heater in the sample holder and a temperature controller. A type-K thermocouple was used to measure the temperature of the surface of the sample by attaching it with a high thermally conductive.

4. Results and discussion

In the present work, a theoretical model for the temperature compensated solidly mounted resonator is presented. We start with a symmetric configuration (i.e. $\lambda/4$ -thickness reflector) and we continue with the asymmetric configuration in which the thickness of top two reflector layers is varied to observe its effects on the TCF of SMRs. With the increase in temperature, there is a

decrease in the stiffness constant of most of the materials. It reduces the acoustic velocity, which leads to the negative TCF. However, SiO₂ [22] has a positive temperature coefficient of its elastic constants, which results in an increase of the acoustic velocity with temperature, thus showing a positive TCF. The use of SiO₂ as low impedance material in acoustic reflectors helps to compensate the TCF of the negative temperature coefficient of other materials. With the increase in temperature, the acoustic velocities decrease and as a result, the resonant frequency shifts to lower values. This can be partially compensated by increasing the thickness of SiO₂ layer. To observe this effect, thermal expansion is applied in COMSOL Multiphysics software using the following expression.

$$\varepsilon_{inel} = \alpha(T - T_{ref}) \quad (5)$$

where ε_{inel} is the fractional change in length by thermal expansion, α is the coefficient of thermal expansion, T and T_{ref} are the actual and reference temperatures respectively. However, the major contributing source to the TCF is the thermal variation in the elastic constant of materials, which directly affects their acoustic velocities. From COMSOL simulations, it is observed that other thermal effects such as thermal expansion can also affect the TCF as in Fig. 4. It shows a decrease in the resonant frequency with every 20 °C rise in temperature.

An increase in SiO₂ thickness loads the resonator, which not only reduces the resonance frequency but also k_{eff}^2 and Q values. A careful design of the whole stack helps to recover the frequency values and also to avoid the degradation due to energy loss.

Fig. 5 displays the normalized resonant frequency as a function of temperature for shear and longitudinal modes. Asymmetric W-based acoustic reflectors are used in this configuration with AlN as a piezoelectric material with a non- $\lambda/4$ -thickness of SiO₂ of 1.21 μm .

Measured TCF values are $-15.2 \text{ ppm}/^\circ\text{C}$ and $-6.6 \text{ ppm}/^\circ\text{C}$ for the shear and longitudinal wave modes of AlN and $+3.4 \text{ ppm}/^\circ\text{C}$ and $+23.2 \text{ ppm}/^\circ\text{C}$ for the shear and longitudinal overtones wave modes of SiO₂ layers.

The TCF variations of both shear and longitudinal wave mode of the resonator made on SiO₂-W reflectors are achieved by increasing the thickness of the SiO₂ layer as shown in Fig. 6.

The negative values of the TCF decrease when the thickness of the uppermost low impedance SiO₂ layer increases. However, the values of the quality factor Q and electromechanical coupling

Fig. 5. Measured values of normalized resonant frequency vs. temperature of shear and longitudinal wave modes with asymmetric W-reflectors.

Fig. 6. Measured TCF values of the main (AlN) and secondary (SiO₂), shear (S) and longitudinal (L) modes for asymmetric resonators as a function of the thickness of SiO₂ in SMR reflectors.

coefficient k_{eff}^2 decrease simultaneously. The relation of the Q factor and the k_{eff}^2 as a function of thickness of the layers in the W-SiO₂ based resonator is shown in Fig. 7.

Fig. 4. Simulated spectra of a resonator at different temperatures with Finite Element Modelling (FEM).

It can be seen that there is a constant decrease in the values of both Q and k_{eff}^2 with the increase of SiO_2 thickness. Above $1 \mu m$ thick SiO_2 , there is a sudden decrease in both Q and k_{eff}^2 values. At this thickness of SiO_2 , the TCF for longitudinal and shear modes of SiO_2 is also positive. Further increase in SiO_2 thickness compensates TCF but at a huge cost for the Q and k_{eff}^2 values.

A similar behavior was found in resonators made of insulating WO_x/SiO_2 reflectors. It is important to note that a redesign of the piezoelectric capacitor, which do not do in this work for only change a variable and making the comparison easy, can improve the values of both Q and k_{eff}^2 values and recover the resonant frequency values. The data of the TCF of the W/SiO_2 and WO_x/SiO_2 based symmetric and asymmetric reflectors with resonators operating in the shear and the longitudinal mode while varying the thicknesses of the corresponding uppermost layer (SiO_2 , W or WO_x) are given in Table 1.

There are only two, AlN shear and longitudinal, modes in symmetric reflectors. An increase in the thickness of the SiO_2 layer leads

to the generation of two overtone modes, shear and longitudinal, that appear into the SiO_2 layer. This increase in the thickness of SiO_2 also causes the reduction of negative temperature coefficient of frequency (Table 1). A further increase in the thickness turns the TCF for shear and longitudinal of SiO_2 to positive values (in the case of $W-SiO_2$) based reflectors. The best possible TCF compensation is achieved when the thickness of the uppermost SiO_2 layer reaches $1.21 \mu m$. The further increase also reduces the TCF but causing a great degradation of the reflectance, which leads to energy leakage from the device to the substrate and a decrease in the Q factor.

Similarly, to count the effect of the thickness variations of the first high impedance layer (W or WO_x in this case), we also increase the thickness of this layer. It is observed that by increasing the thickness of W up to $0.65 (\mu m)$, the TCF shows a decrease of the negative values compared to the symmetric configuration. Further increase in W thickness causes the increase in negative values of TCF shown in Fig. 8. This shows that a careful design of the resonator reducing the thickness of the uppermost W layer enables to decrease the TCF without a heavy layer of SiO_2 .

Fig. 7. Measured values of Q factor and k_{eff}^2 as a function of increasing thickness of SiO_2 layer in the W -based reflectors.

Fig. 8. Measured values of TCF of the main (AlN) and secondary (W) shear (S) and longitudinal (L) modes for asymmetric resonators as a function of the thickness of W in SMR reflectors.

Table 1
TCF measurements of several resonators with symmetric and asymmetric $W-SiO_2$ and WO_x-SiO_2 based reflectors varying W , WO_x or SiO_2 uppermost acoustic reflector layers.

Thickness	S-AlN	S- SiO_2	L-AlN	L- SiO_2
Symmetric W -reflector	-30.2	-	-31.1	-
Asymmetric W -reflector $SiO_2 = 0.71 \mu m$	-26.6	-13.3	-18.5	-15.8
Asymmetric W -reflector $SiO_2 = 1.01 \mu m$	-24.4	2.6	-10.6	16.4
Asymmetric W -reflector $SiO_2 = 1.21 \mu m$	-15.2	3.4	-6.6	23.2
Symmetric WO_x -reflector	-23.4	-	-19.6	-
Asymmetric WO_x -reflector $SiO_2 = 0.85 \mu m$	-19.9	-18.5	-14.6	-12.5
Asymmetric WO_x -reflector $SiO_2 = 0.95 \mu m$	-18.2	-17.4	-12.2	-5.5
	S-AlN	S-W	L-AlN	L-W
Asymmetric W -reflector $W = 0.65 \mu m$	-10.3	-28.8	-21.8	-38
Asymmetric W -reflector $W = 0.73 \mu m$	-19.1	-34.1	-13.8	-32.1
Asymmetric W -reflector $W = 9300$	-32.9	-30.8	-32	-32.7
	S-AlN	S- WO_x	L-AlN	L- WO_x
Asymmetric WO_x -reflector $WO_x = 0.95 \mu m$	-33.4	-46.7	-28.4	-30.4

All the mechanical coupling acoustic reflector layers accommodate in determining the resonant frequency in a layered structure. The position of the layer in the stack matters greatly because only the first two uppermost layers show significant influence on the TCF. This is due to the low amount of acoustic energy that reaches the deeper layers. To verify this, the thickness of other layers has also been varied to see their effects on TCF but it is found that these are negligible. Only the influence of the two uppermost layers and electrodes is significant. It is also confirmed, from the transmittance response of reflectors, that more thickening of the layer of SiO₂ can reduce TCF but causing excessive degradation of the response of the reflectors. Fully compensated or even positive TCF for longitudinal mode can be achieved. However, in the case of shear mode, it is very hard to obtain fully compensated TCF due to the dramatically worsening in the response of the resonator.

5. Conclusion

A theoretical model with experimental results for temperature compensated solidly mounted resonators is presented here. In the 2-D model, the displacement parameter for energy dissipation while increasing the thickness of different layers of the reflector is presented. The 3-D model displays the overall response of the resonator. The TCF of both the shear and longitudinal mode for different thicknesses of the uppermost layers of the acoustic reflector are calculated. The TCF of longitudinal modes can be fully compensated. The increase in the thickness of the reflector layers leads to the decrease in Q value and k_{eff}^2 , if no redesign of the piezoelectric capacitor is made. An increase in the number of layers does not affect the TCF (except the first two uppermost layers), but it enhances the reflector performance, and improves the response of the resonator.

Acknowledgements

This work was partially supported by the European Commission through the 7th Framework Programme by the RaptaDiag project HEALTH-304814 and by the Ministerio de Economía y Competitividad del Gobierno de España through project MAT2013-45957-R.

The authors would also like to thank for the financial support by of the Ministry of Higher Education (MOHE) Malaysia and Universiti Teknologi Malaysia (UTM) Skudai, Johor, Malaysia under Grant No. 12H75 and 4F736.

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