TEMPERATURE STABLE, POST-PROCESS TUNABLE, HIGH Q HBARS AT 3~5 GHZ

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ABSTRACT

This paper describes a temperature-compensated High-overtone Bulk Acoustic Resonator (HBAR) with a loaded quality factor (Q) of 801 and 545 at 3.427 GHz and 4.597GHz, respectively. The HBAR is composed of an Al/ZnO/Al resonator on a SiO₂/Si/SiO₂ diaphragm where a thermally grown SiO₂ with positive temperature-coefficient-of-frequency (TCF) compensates the negative TCF of the rest of the resonator layers. The HBAR's TCF reaches zero at a specific temperature, and is lower than 1ppm/°C over a 30°C temperature span, where the TCF is about 100 times better than the value obtainable with an un-compensated Al/ZnO/Al Film Bulk Acoustic Resonator (FBAR). Also, the resonant frequency of the HBAR as well as its TCF is shown to be tunable by adding additional SiN and/or SiO₂ layer after fabrication.

INTRODUCTION

There are three types of Bulk Acoustic Wave (BAW) resonators based on piezoelectric film: micromachined Film Bulk Acoustic Resonator (FBAR), Solidly Mounted Resonator (SMR) and High-overtone Bulk Acoustic Resonator (HBAR) [1~4]. Most BAW resonators are composed of metal/piezofilm/metal on top of a thin diaphragm or a thick substrate, and have shown a quality (Q) factor greater than hundreds (even tens of thousands in case of HBAR) at a resonant frequency of 0.5 to 10 GHz. The resonant frequency is predominantly determined by the thickness of the piezoelectric film. With their inherently high Q, BAW resonators are ideally suited for filters and oscillators at GHz, since the Q determines the insertion loss and phase noise for filters and oscillators, respectively.

Since Agilent mass-produced FBAR-based duplexer filters for mobile phones in 2000, FBARs are widely used for RF front-end filters for mobile phones. Similar filters based on SMR recently have joined the mobile phone market. On the other hand, HBAR remains to be used only for niche oscillator applications, though its Q can be made much higher than FBAR and SMR, mainly due to its multiple resonances and low electromechanical coupling coefficients.

Chip-Scale Atomic Clock (CSAC) enables miniature (and low power consuming) time reference for high security communication and jam-resistant global-positioning-system receiver. Since CSAC requires a very high Q resonator for its local oscillator, HBAR-based voltage controlled oscillators (VCO) is ideally suited for CSAC, where the oscillation frequency of particular interest is 3.4GHz or 4.6GHz for different system design topologies.

However, for HBAR-based VCO to be used for CSAC's local oscillator, the resonator must be very stable in temperature. For example, the resonant frequency shift of the resonator should not exceed 20ppm over 60 to 80°C, which means the temperature coefficient of frequency (TCF) of the resonator should be less than

1 ppm/°C (a conventional Al/ZnO/Al stand-alone resonator has a TCF of about -70 ppm/°C [5]).

To reduce HBAR's TCF, the following techniques have been explored and reported. A heater was embedded into an HBAR [6] to tune the resonant frequency to compensate the TCF. But this approach consumes large power and lacks repeatability. Another technique for HBAR is to use a capacitor (having a temperature coefficient in opposite sign to that of the HBAR's clamped capacitance) in series with the HBAR. The achievable TCF of an HBAR with this approach is limited by available capacitor.

The most promising technique for temperature compensation of a bulk acoustic resonator is to use a support layer (e.g., SiO₂ or Elinvar) that has TCF opposite to that of the piezoelectric layer for FBAR [7, 8]. No literature is found on temperature compensating HBAR with this method of incorporating a temperature-compensating layer. This paper describes HBAR with temperature-compensating SiO₂ layer, particularly their measured TCF's, timing stabilities and the post tuning ability.

THEORY

The resonant frequencies of a HBAR resonator is predominantly determined by acoustic-wave traveling time in the resonator, and are

$$f_r \approx \frac{N}{2(d_{\text{piezo}}/V_{\text{piezo}} + d_{\text{elec}}/V_{\text{elec}} + d_{\text{substrate}}/V_{\text{substrate}})^{-1}}$$

where d_{piezo} , d_{elec} , $d_{\text{substrate}}$ are the thicknesses of the piezomaterial (ZnO), electrodes (Al), and diaphragm (SiO₂) (or substrate (SiO₂/Si/SiO₂)), respectively, while V_{piezo} , V_{elec} and $V_{\text{substrate}}$ are the acoustic velocities in the piezomaterial, electrodes, and diaphragm (or substrate), respectively. The dependence of the resonant frequency on temperature mainly comes from the acoustic velocity's dependence on temperature. The acoustic velocity is equal to $\sqrt{E/\rho}$ where E and ρ are Young's modulus and mass

density, respectively. For most materials (such as Al, Si and ZnO) Young's modulus decreases as temperature increases, causing negative TCF for a BAW resonator.

However, due to the unique crystalline structure, the Young's modulus of SiO₂ increases as temperature increases, resulting in a positive TCF. Thus, SiO₂ layer can be used for compensating a negative TCF of Al/ZnO/Al/Si HBAR.

We build an HBAR with Al/ZnO/Al on SiO₂/Si/SiO₂ substrate (which is actually a diaphragm). Most of the resonator's acoustic energy is stored in the relatively thick single crystalline Si layer where the acoustic loss is much less than ZnO or Al. Hence, the resonator's Q is mostly determined by the single crystalline Si, and can be much higher than FBAR. The thermally grown SiO₂ layers below and above the Si layer are to compensate the negative TCF's of ZnO, Al and Si. Due to the complicated structure and acoustic energy distribution in the HBAR, there has not been an effective model to accurately predict the TCF of the HBAR, and

we have fabricated HBARs with various multilayer thickness ratios to obtain optimum TCF experimentally.

FABRICATION AND TESTING

The temperature compensated HBARs are fabricated on a Silicon-on-Insulator (SOI) wafer with the fabrication steps shown in Fig. 1. After obtaining a silicon diaphragm (out of the silicon device layer of SOI) by TMAH, XeF_2 and buffered HF etching (in that order) on an SOI wafer, we thermally grow wet SiO_2 on the device silicon layer to form $\text{SiO}_2/\text{Si}/\text{SiO}_2$ diaphragm. Then bottom $0.1\mu\text{m}$ Al is evaporated on the SiO_2 layer and patterned, followed by deposition of $0.68\mu\text{m}$ thick ZnO in a RF sputtering system with 10mTorr Argon and Oxygen gas mixture (50%/50%) at 300°C and 300W. After patterning the ZnO, $0.1\mu\text{m}$ thick top Al electrode is evaporated and patterned. The bottom Al, ZnO, and top Al on top of the diaphragm form the wave-generating layers of an HBAR.

Figure 1 Brief fabrication process for the temperature compensated HBAR

The fabricated resonators are characterized with HP8753D network analyzer with Cascade microwave micropositioner and probes (for impedance measurement) and Instec's hot/cold chuck (for temperature variation). We have developed a Labview program to acquire data from the network analyzer and analyze it by curve fitting to monitor HBAR's resonant frequencies. The noise floor of this method is around 0.5ppm, which is good enough for measuring the dependence of the HBAR's resonant frequency on temperature.

RESULTS AND DISCUSSION

HBARs with various top-view shapes and sizes (Fig. 2) along with various thickness ratios have been fabricated and tested. The testing results show little difference among different top-view shapes, but the top-view dimension of the HBAR affects the Q much. The HBAR with $100\mu\text{m}$ long sides is measured to have the highest Q at 3 to 5 GHz.

Figure 2 Top-view photos of the fabricated HBARs on $\text{SiO}_2/\text{Silicon}/\text{SiO}_2$

The TCF of the HBAR is directly related to the thickness ratios among various structure layers. Figure 3 shows the measured TCF's at about 80°C for different thickness ratios for the $\text{SiO}_2/\text{Si}/\text{SiO}_2$ multi-layers for the HBAR with Al/ZnO/Al having thicknesses of $0.1\mu\text{m}/0.68\mu\text{m}/0.1\mu\text{m}$ (for 3.4 GHz) and $0.1\mu\text{m}/0.48\mu\text{m}/0.1\mu\text{m}$ (for 4.6 GHz), respectively. The measured TCFs depend linearly on the thickness ratio between the positive TCF layer (SiO_2) and the effective negative TCF layer (obtained by converting the Al, ZnO and Si layers to an equivalent Si layer). The ratios of 0.28 and 0.35 produce zero TCF's for the 4.6 and 3.4GHz HBARs, respectively.

Figure 3 Measured TCF (ppm/ $^\circ\text{C}$) at 4.6GHz(top) and 3.4GHz (bottom) vs. the ratio of the +TCF layer thickness to the -TCF layer thickness.

The zero TCF HBAR with Al/ZnO/Al/ $\text{SiO}_2/\text{Si}/\text{SiO}_2$ ($0.1\mu\text{m}/0.68\mu\text{m}/0.1\mu\text{m}/1.7\mu\text{m}/9.9\mu\text{m}/1.7\mu\text{m}$) is measured to have eight resonant frequencies between 3 and 5 GHz (Fig.2). The HBAR has different TCF's at these frequencies, which are shown in the Table 2. The reason for the different TCF's is the different acoustic energy distribution along the HBAR thickness. The more acoustic standing wave energy in the positive TCF layer (SiO_2), the more positive of the whole HBAR's TCF.

Figure 4 Measured S_{11} vs. frequency of the HBAR.

Table 1 TCFs at five different resonant frequencies of the HBAR on SiO₂/Si/SiO₂

Resonant Frequency (GHz)	3.208	3.427	3.636	3.873	4.124	4.366	4.597
TCF (ppm/°C) at 72.5°C	-1.87	0	-3.95	-10.1	-10.7	-6.5	-1.84

The HBAR is measured to have impedance variation from 3.416 to 3.428GHz as shown in Fig. 5. The highest loaded Q's at the parallel resonant frequency (3.4271 GHz) and series resonant frequency (3.4215 GHz) are measured to be 801 and 660, respectively. The electromechanical coupling coefficient (K_t^2) is 0.41%. If the series resistance is de-embedded [9], the unloaded Q's are 821 and 1045 at the parallel and series resonant frequencies, respectively.

At the parallel and series resonant frequencies near 3.4 GHz, the HBAR is measured to have a TCF of 1.0 to -0.8 ppm/°C between 60 and 90°C, where the zero TCF point is at 72.5°C. The parallel resonant frequency vs. temperature (from room temperature to 125°C) is shown in Fig. 6. The total parallel resonant frequency change between 53 and 90°C (over 37°C range) is 36.6kHz, mere 10.7ppm. And from room temperature (27°C) to 120 °C, the total resonant frequency change is 312kHz, which is 91ppm.

Figure 5 Measured Smith-chart impedance from 3.416 to 3.428GHz.

Figure 6 Measured resonant frequency vs. temperature for the HBAR at 3.427GHz.

Figure 7 Measured resonant frequency vs. temperature for the HBAR at 4.597GHz

The same HBAR yields a zero TCF at 32.8°C (Fig. 7) with a loaded parallel Q of 545 for a parallel resonant frequency of 4.597 GHz. The HBAR's parallel resonant frequency varies a total of 228ppm at 4.597 GHz over a wide temperature span of 24 to 125°C. Note that the resonant frequency of a typical silicon-supported ZnO HBAR varies about 3,700ppm over 24 – 125°C.

The TCFs at the parallel and series resonant frequencies of the HBAR are measured to vary with temperature as shown in Fig 8. The measurement shows that the TCF changes linearly from 4ppm/°C at 23°C to around -4ppm/°C at 122°C, with a slope of -0.079ppm/°C/°C. With this linear variation of the TCF, we cannot obtain a very low TCF from -50°C to 120°C. Thus, in an effort to obtain an "S-shape" in the resonant frequency vs. temperature curve, we have applied a DC voltage to piezoelectrically stiffen the HBAR to see if the voltage can affect the TCF vs. temperature curve. As can be seen in Fig. 9, the DC voltage is measured to change the resonant frequency of the HBAR. However, we have observed no change in the TCF curve by an applied DC voltage.

Figure 8 Measured TCF at parallel resonant frequency (gray) and series resonant frequency (black) vs. temperature of the HBAR.

Figure 9 Measured HBAR's resonant frequency vs. applied DC voltage.

Figure 10 Post-process tuning by additional layers of PECVD SiN and SiO₂ on the backside of HBAR

Due to the sensitivity of HBAR's resonant frequency and TCF to the structure's multilayer thicknesses, the fabrication process needs to be controlled critically to meet the frequency and TCF demand for the devices. Thus, we have developed a post-process, frequency and TCF tuning method by depositing PECVD SiN and SiO₂ layers on the backside of the HBAR (Fig. 10). The measured data show that the additional layers change the HBAR's resonant frequency and TCF at a different rate. Thus, any desired resonant frequency and TCF can be obtained by combining different thicknesses of the SiN and SiO₂. For example, an

additional 0.6 μm thick SiN and 0.4 μm thick SiO₂ on Al/ZnO/Al/SiO₂/Si/SiO₂(0.1 μm /0.68 μm /0.1 μm /1.7 μm /3.9 μm /1.7 μm) HBAR makes the HBAR have a 3.427GHz resonant frequency and zero TCF at 75°C with a same high Q (a fine tuning from a resonant frequency of 3.601GHz and TCF of 13.9ppm/°C).

For CSAC, an HBAR-based voltage controlled oscillator (VCO) can be used for keeping a short-term stability of the clock, while the atomic emission unit keeps the long-term stability. Nevertheless, the long-term (as well as short-term) stability is still very important for HBARs. For testing the short-term stability, we keep the temperature compensated HBAR at 72.5°C, where the TCF of HBAR is 0, to minimize the effect from the temperature fluctuation. Figure 11 shows that the parallel frequency fluctuation is measured to be about 3.3ppm and 6.7ppm within 90 minutes and 8 hours, respectively.

Figure 11 Measured short-term stability of the temperature compensated HBAR.

Figure 12 Measured long-term stability of the temperature compensated HBAR.

To test the long-term stability we place the HBAR on a printed circuit board (PCB), and connect it to the network analyzer through an SMA connector. The network analyzer applies a constant power of -3.8dBm to the HBAR to obtain the S₁₁. Though the HBARs used for the short-term and long-term stability tests are from the same wafer and have similar TCF parameters, their resonant frequencies are different. Figure 12 shows that the parallel resonant frequency remains constant (within the measurement error of 11ppm) over 330 hours, but the series

resonant frequency varies about 33ppm over the same period of time. The reason for the fluctuation of the series resonant frequency is that there is a spurious resonance very near the series resonant frequency, which may have much higher TCF than the series resonant frequency.

CONCLUSION

In this paper we describe the experimental verification that using SiO₂ layer to compensate the HBAR's TCF is effective. A single HBAR supported on a SiO₂/Si/SiO₂ substrate/diaphragm (made on an SOI wafer) possesses a very low TCF and a high Q of about 800 and 545 at 3.4 GHz and 4.6GHz, respectively. Also the post-process tuning method is shown to be effective in meeting the frequency and TCF specifications without having to optimize the complicated thickness ratios for mass production. Therefore, using SiO₂ to compensate the HBAR's TCF is a very promising method to obtain a low TCF and high Q resonator at 3 - 5 GHz. Thus temperature-compensated HBAR is particularly suited for a voltage controlled oscillator for a local oscillator of a chip-scale atomic clock.

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