Temperature Coefficient of Frequency in Silicon-Based Cross-Sectional Quasi Lamé Mode Resonators

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Abstract— **Temperature coefficient of frequency (TCF) is studied in silicon-based cross-sectional quasi Lamé modes (CQLMs). Such modes are demonstrated in thin-film piezoelectric-on-silicon (TPoS) resonators and the TCF curves are modeled using eigenfrequency analysis in COMSOL for highly n-type doped silicon. It is shown that the ratio between the finger-pitch and the resonator thickness affects the turnover temperature of these resonators which could be predicted using this model. The CQLM-TPoS resonators fabricated on a 40µm thick SOI substrate, are characterized and the measured TCF values are confirmed to be in close agreement with the prediction. A relatively high turnover temperature of >100°C is reported for a third-order CQLM-TPoS resonator aligned to <100> silicon plane while a turnover temperature of <20°C is recorded for the <110> counterpart.**

Keywords— Lamé mode; MEMS resonator; temperature coefficient of frequency (TCF); piezoelectric actuation

I. Introduction

Bulk acoustic wave MEMS resonators have been used in filter blocks and also as sensors in many commercial applications. These resonators offer advantages such as low power consumption, small size, and since the silicon is the substrate of choice in microelectronics batch fabrication, the manufacturing process of MEMS resonators is compatible with the existing infrastructure developed for microelectronics industry.

However, the most important drawback of these resonators is their relatively high temperature coefficient of frequency (TCF). The center frequency of these resonators are dependent on the resonator's material properties and dimensions, and both features are dependent on the ambient temperature. The temperature coefficient of elasticity (TCE) is around -60 ppm/°C (TCF is around -30 ppm/°C) for lightly-doped silicon-based MEMS resonators [1] and around -50 ppm/°C (TCF is around -25 ppm/°C) for AlN-based resonators [2]. For such values of TCF, the frequency fluctuation would be large within the commercial temperature range (-40 °C to -80 °C) making it a challenge to utilize these resonators in ultra-stable clocks or frequency control applications.

To reduce frequency drift, active and passive methods are employed. The most widely studied passive temperature compensation methods are degenerate doping of the silicon device layer [3] and using a composite structure which contains a material with positive TCE (such as silicon dioxide) in the form of an over layer [4] or pillars [5]. With latter method, the fabrication complexity would be increased while the quality factor is negatively impacted. In addition to the above mentioned draw back, with passive temperature compensation methods, sub ppm temperature stability is out of reach which is required for many ultra-stable clock applications.

In active temperature compensation methods, resonance frequency would be tuned in real-time to compensate for the frequency drift due to the ambient temperature variations. Tuning the termination impedance [6], inducing a mechanical stress [7] and operating the resonator at a constant elevated temperature [8] (e.g. oven controlled oscillators) are amongst the most common methods for active TCF compensation of MEMS resonators. With these active methods, sub ppm frequency variation is achievable within commercial temperature range for the price of higher power consumption. Oven controlled oscillators are widely studied in the literature. Oscillator would be operated at a constant elevated temperature slightly above the desirable temperature range. A significant performance improvement is achieved if the resonator is heated to its turnover temperature (temperature at which the TCF changes polarity) by the oven. Designing resonators with turnover temperature values above commercial range (80 °C) is crucial in oven-controlled oscillators.

Turnover temperature in silicon resonators is dependent on the doping concentration and the resonance mode excited within the resonant body as reported in [9]. Based on the data reported in this study, turnover temperature of the planar Lamé mode silicon resonator is higher than any other conventional resonance mode for the same silicon doping concentration. Planar Lamé modes are commonly excited capacitively in silicon resonators at low-frequencies (MHz regime) [9]. The motional impedance of such capacitive resonators are relatively large and to reduce the motional resistance, extremely narrow gaps are required. On the other hand, such narrow gaps would negatively impact the power handling of such resonators. In the oscillator application, phase noise is directly related to the drive power and motional impedance of the resonator. With piezoelectric actuation the motional resistance would be substantially lower and the power handling could be improved

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by adding a substrate layer such as single crystalline silicon or diamond to the structure as is the case for thin-film piezoelectric-on-substrate (TPoS) resonators [10].

However, a planar Lamé mode can't be effectively excited in silicon using a thin overlaid piezoelectric film. This is because sputtered piezoelectric thin-films such as AlN are isotropic in the plane of the substrate and therefore, the opposing in-plane stress components of a planar Lamé mode (Fig. 1) would result in near-zero charge accumulation on metal electrodes placed across the thin film.

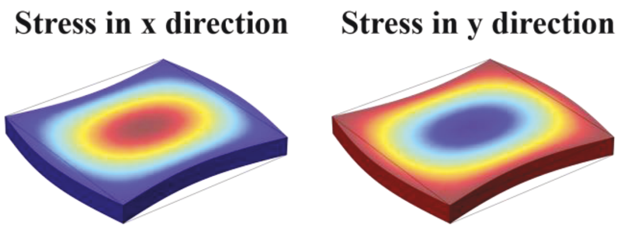

Fig. 1. The simulated stress field in x and y direction for planar Lamé mode silicon resonator. The stress field is tensile in one direction and compressive in the other direction. Due to in-plane isotropy of common thin-film piezoelectric materials such as AlN, such modes cannot be excited piezoelectrically.

Cross-sectional Lamé mode resonators (CLMR) have been demonstrated recently in thin-film AlN resonators [11,12] by targeting Lamé modes in the cross section of an AlN slab. These resonators offer coupling factors larger than what is achievable in lateral-extensional mode (contour-mode) resonators due to the fact that for CLMRs both d_{31} and d_{33} piezoelectric coefficients constructively contribute in the excitation of the Lamé mode in the cross section of the AlN film.

In this work we first demonstrate that cross-sectional *quasi*-Lamé modes (CQLM) could be piezoelectrically actuated in TPoS resonators. Then, temperature dependency of frequency is modeled and studied for CQLM TPoS resonators for highly n-type doped silicon layer using COMSOL, confirming that turnover temperature above 100°C is achievable in these resonators at moderately high doping concentrations. Then, it is shown using the same COMSOL model that the turnover temperature is tunable by varying the ratio of the resonator thickness to the electrode width. Finally, the frequency response and TCF curves are measured for the TPoS resonators fabricated on a relatively thick highly n-type doped single crystalline silicon. Measured data confirms that the CQLM could be effectively excited piezoelectrically in TPoS resonators with relatively high quality factor featuring high turnover temperatures suitable for oven controlled applications.

II. CQLM TPoS Resonators

In lateral-extensional TPoS resonators the d_{31} piezoelectric coefficient is mainly responsible for inducing in-plane xy stress and exciting the lateral mode vibration in the resonator slab. Interdigitated electrode pattern is used to excite higher harmonics in such resonators. The distance between two adjacent fingers is called the finger pitch (*FP*) and is equal to the half wavelength. *FP* is typically chosen larger than the thickness of the silicon block in lateral extensional mode resonators Fig. 2.

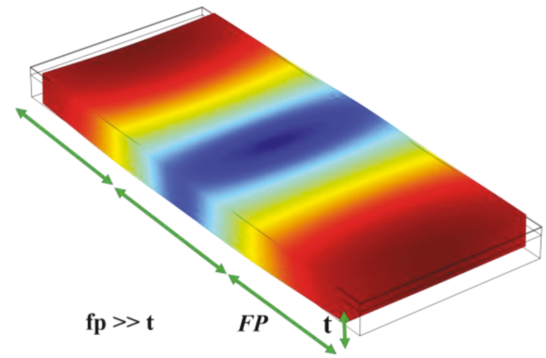

Fig. 2. The simulated stress field for lateral extensional mode TPoS resonator. The FP should be larger than the thickness of the silicon block for a clean lateral extensional mode.

As the thickness of the resonator increases and approaches the FP, mode shape similar to the one presented in Fig. 1 emerge on the cross section of the resonator slab hence the name cross-sectional Lamé modes [11]. Due to opposite signs of d_{31} and d_{33} piezoelectric coefficients in AlN, Lamé-mode could be excited piezoelectrically in the entirety of the composite structure of (Mo/AlN/Si). Caused by the presence of AlN and Mo layers, the acoustic symmetry of the medium is disrupted and the mode shape deviates from pure Lamé-mode consequently Fig. 3. Therefore, we will refer to this mode shape as Cross-Sectional *Quasi* Lamé mode (CQLM).

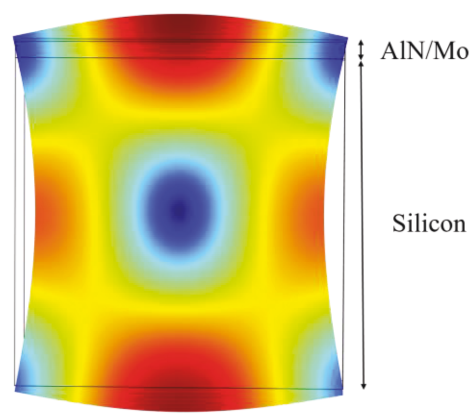

Fig. 3. The simulated mode shape of a cross-sectional *quasi* Lamé mode (CQLM) in a composite structure. Due to the presence of AlN and Mo layers, acoustic symmetry is disrupted and the mode shape is slightly different from pure Lamé, hence the name cross-sectional *quasi* Lamé mode (CQLM).

The same interdigitated pattern which is commonly used for excitation of a lateral-extensional mode is used to excite CQLM in TPoS resonators. Third order CQLM in a 126 μm (3×42 μm) × 50 μm × 42 μm (40μm silicon+2μm AlN) TPoS slab is presented in Fig. 4. A schematic view graph of the third-order CQLM TPoS resonator is also shown in Fig. 5.

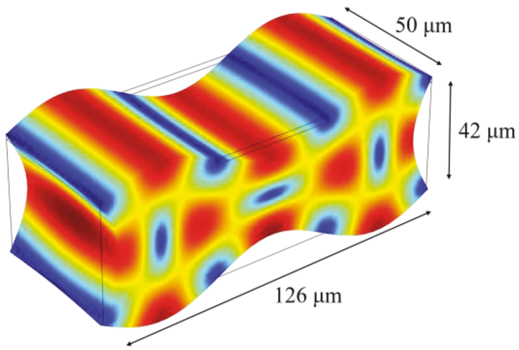

Fig. 4. The simulated third-order CQLM in a TPoS resonator.

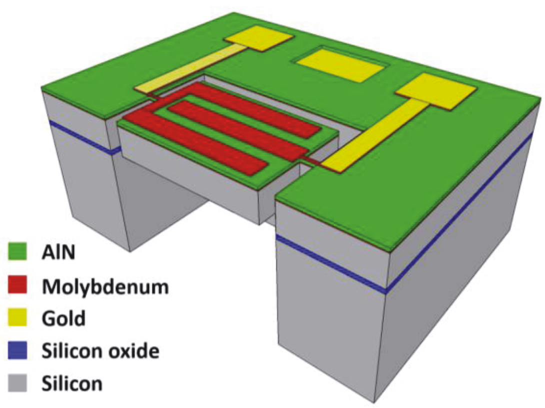

Fig. 5. A schematic view graph of a third-order CQLM TPoS resonator. Electrode patterns are the same as the ones for lateral extensional mode.

III. TCF IN CQLM-TPOS RESONATORS

Due to their high turnover temperature, Lamé mode resonators in highly n-type doped silicon are considered an excellent choice for oven controlled oscillator applications. For [100] aligned Lamé-mode devices since all the faces of the resonator block are aligned to [100] (Fig. 6), it is predicted that the frequency temperature dependency of CQLM TPoS resonator would be similar to the TCF curves of a planar Lamé mode resonator (TCF>100 °C for moderately high n-type doping). On the other hand, since the resonator block faces of a [110]-aligned CQLM device are different from the [110]-aligned planar Lamé mode resonator, it is predictable that the TCF curves of such device would be different.

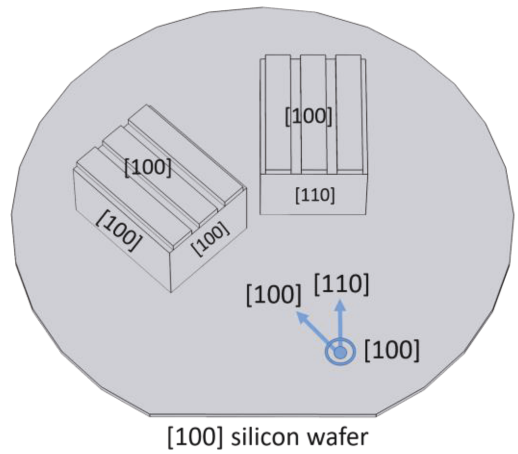

Fig. 6. On a [100] silicon wafer, for the resonators to be aligned to [100] crystalline plane, the device should be rotated 45 degrees. All the faces of the resonator block are [100] which would be similar to the Lamé mode.

To predict the frequency drift versus temperature for CQLM TPoS resonators, eigenfrequency analysis is utilized in COMSOL. Frequency drift versus temperature curves are generated for CQLM TPoS resonators aligned to [100] and [110] crystalline planes.

In order to develop TCF curves, silicon stiffness and their temperature coefficient are borrowed from [9] (TABLE I) for phosphorus doped single crystalline silicon ($n=6.6\times10^{19}\ cm^{-3}$). The stiffness matrix is then calculated for each temperature using Eq.1, Eq.2 and Eq.3. The new stiffness matrix is then used to repeat the modal analysis and calculate the shifted resonance frequency.

$$C11_T = C11_0 + TC11^{(1)} \times C11_0 \times 10^{-6} \times (T - T_0) + TC11^{(2)} \times C11_0 \times 10^{-9} \times (T - T_0)^2 \quad (1)$$

$$C12_T = C12_0 + TC12^{(1)} \times C12_0 \times 10^{-6} \times (T - T_0) + TC12^{(2)} \times C12_0 \times 10^{-9} \times (T - T_0)^2 \quad (2)$$

$$C44_T = C44_0 + TC44^{(1)} \times C44_0 \times 10^{-6} \times (T - T_0) + TC44^{(2)} \times C44_0 \times 10^{-9} \times (T - T_0)^2 \quad (3)$$

Where $C11_T$, $C12_T$ and $C44_T$ are the single crystalline

TABLE I
ELASTIC CONSTANTS OF PHOSPHORUS-DOPED ($N=6.6\times10^{19}\ CM^{-3}$) SILICON AND THEIR CORRESPONDING FIRST AND SECOND ORDER TEMPERATURE COEFFICIENTS [9]

Dopant	C11 (GPa)	C12 (GPa)	C44 (GPa)	$TC11^{(1)}$ (ppm/°C)	$TC12^{(1)}$ (ppm/°C)	$TC44^{(1)}$ (ppm/°C)	$TC11^{(2)}$ (ppb/°C^2)	$TC12^{(2)}$ (ppb/°C^2)	$TC44^{(2)}$ (ppb/°C^2)
Phosphorus 6.6×10^{19}	164.0	66.7	78.2	-34.2	-135.2	-67.8	-103	-1	-40

silicon stiffness coefficients at an arbitrary temperature T and $C11_0$, $C12_0$ and $C44_0$ are the stiffness coefficient at T_0.

As shown in Fig. 7 , the turnover temperature for [100]-aligned CQLM resonators are above 100 °C. This conforms that the temperature-frequency dependency of these resonators are similar to the planar Lamé mode resonators.

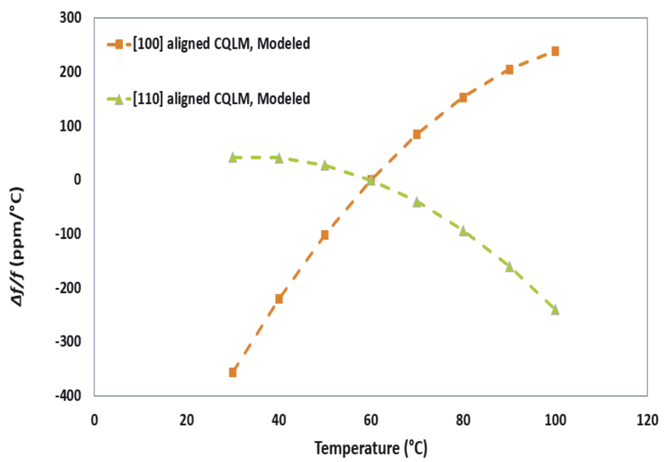

Fig. 7. The simulated temperature-frequency dependency for CQLM silicon resonator with a highly n-type doped silicon device layer.

As mentioned, CQLM would substitute the conventional lateral mode as the finger pitch to stack thickness ratio (FP/t) approaches one. Correspondingly, the simulated turnover temperature for a CQLM resonator starts from the values expected for a pure Lame mode resonator and approach that of the lateral-mode resonator as shown in Fig. 8. Therefore, finger pitch over thickness ratio could be used as a design parameter in CQLM TPoS resonators to achieve a certain turnover temperature given a specific doping concentration. This feature could be used to adjust the turnover temperature slightly above the operational temperature range to optimize the power consumption in oven controlled oscillator applications.

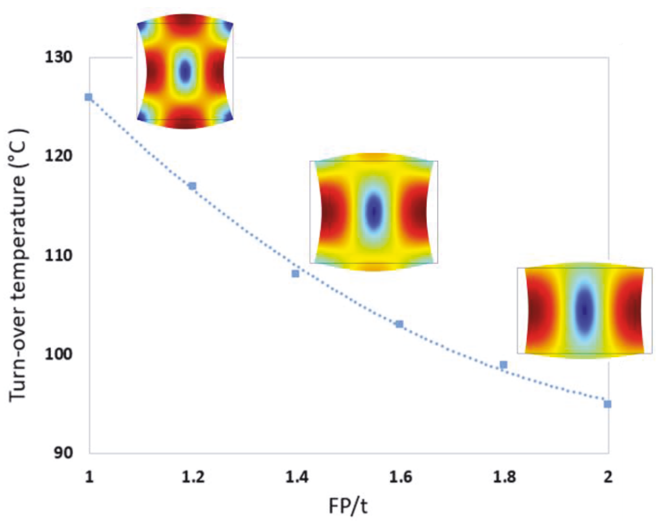

Fig. 8. The Turnover temperature of a CQLM TPoS resonator as a function of finger pitch to stack thickness ratio. The turnover temperature would be higher when the ratio gets closer to one. Turnover temperature could be tuned by adjusting the FP/t ratio.

IV. Fabrication and Experimental Results

CQLM-TPoS resonators are fabricated on a relatively thick (40µm) degenerately n-type doped (4.7×10^{19}) [100] SOI substrate in a five mask process. The sputtered AlN film is 2µm thick and is sandwiched between two 100nm thick layers of Molybdenum. The detailed fabrication process could be found in [13].

The frequency response for the fabricated devices are measured in partial vacuum (1 mTorr). Third-order CQLM-TPoS resonators with a finger pitch (FP) of 51 µm are characterized using a Rohde & Schwarz *ZNB 8* network analyzer and a pair of GSG probes (Cascade Microtech Inc) at ambient temperature. The loaded quality factors (Q_{loaded}) are measured and the unloaded quality factors are extracted based on the results. The frequency response for a third-order CQLM TPoS resonator with the highest measured quality factor (14,500 at 67 MHz) is shown in Fig. 9. This specific device is supported by a circular acoustic isolation structure to minimize the anchor loss the details of its design is described elsewhere [13].

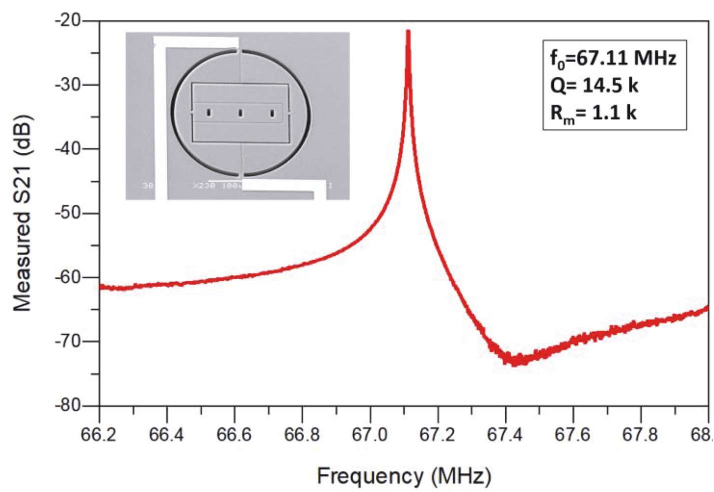

Fig. 9. The frequency response measured for third order CQLM TPoS resonator. The acoustic isolation frame used in this resonator is described in details elsewhere [13].

The measured temperature-frequency curve is then measured for CQLM TPoS resonators aligned to [100] and [110] planes (Fig. 10). The center frequency drift is measured in the range of 30 °C to 100 °C in a Janis cryogenic vacuum probe station in which liquid nitrogen could be used to cool down the stage below ambient temperatures. The measured TCF curves of Fig. 10 are plotted alongside the modeled TCF curves for comparison purposes. As predicted by the simulation results of section III the turnover temperature for the [100]-aligned CQLM TPoS resonator is above 100 °C. However, the measured turnover temperatures are slightly different from the simulated values. This is mainly because the available stiffness coefficients used in the simulation section are reported for a doping concentration higher than what was used for fabrication of the CQLM TPoS resonators of this work. As shown in the figure the TCF curves for [100]-aligned CQLM resonator is resembling what was expected for planar Lamé mode.

Properties such as relatively high quality factor, low motional resistance and high turnover temperature, suggest CQLM TPoS resonators as great candidates for implementation of oven-controlled oscillators.

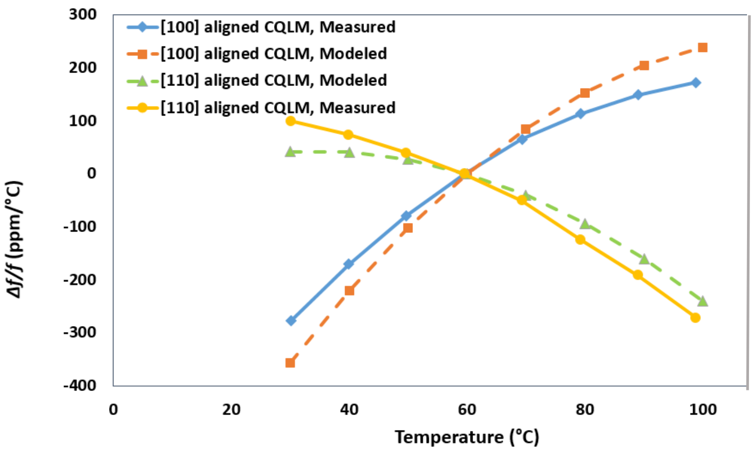

Fig. 10.The measured temperature-frequency dependency for CQLM TPoS resonator fabricated on a SOI wafer with 4.7×10^{19} doping concentration. As predicted with COMSOL modeling the turnover temperature is above 100 °C.

V. CONCLUSION

Lamé mode resonators are commonly excited capacitively and offers properties such as high turnover temperature. This mode cannot be excited piezoelectrically by thin film piezoelectric materials such as sputtered AlN in TPoS resonators. Cross-sectional quasi lame mode is excited piezoelectrically in TPoS resonators and turnover temperature of above 100 °C is measured for CQLM TPoS resonators fabricated on degenerately n-type doped SOI wafers. The turnover temperature is tunable with adjusting the resonator's finger pitch to thickness ratio. CQLM TPoS resonator could potentially be the resonator of choice in high performance Oven controlled Oscillators due to the unique properties of this mode shape.

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