TEMPERATURE-COMPENSATED EXTENSIONAL-MODE MEMS RESONATORS ON HIGHLY N-TYPE DOPED SILICON SUBSTRATES

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ABSTRACT

For the first time, lateral-extensional micromachined resonators fabricated on highly n-type doped silicon substrates and aligned to the [100] crystalline orientation are shown to exhibit an adjustable turnover temperature. This behavior commonly observed in quartz resonators is a key to achieving exceptional temperature stability in oven-controlled crystal oscillators.

To demonstrate the effect of doping concentration and resonator alignment to different crystalline orientations, the thin-film piezoelectric-on-silicon (TPoS) platform is utilized. It is shown through combined theoretical analysis and finite element simulation that the turnover temperature is a sensitive function of doping concentration and also can be adjusted by changing the thickness of the resonant structure. In order to experimentally validate these results, similar resonators are fabricated on three silicon-on-insulator (SOI) substrates and the temperature variation of frequency for several devices are measured and the trends are shown to agree with theory. The minimum temperature variation of frequency is measured for a ~25MHz TPoS resonator aligned to the [100] crystalline orientation showing a maximum frequency variation of 148ppm over the -40°C to 85°C temperature range. This is more than 20x reduction compared to the earlier results from similar uncompensated devices.

INTRODUCTION

Silicon microresonators are poised to gain widespread use in timing and frequency control applications due to their small size and ease of integration. Significant improvements have been made recently with respect to many critical performance factors including quality factor, operating frequency, phase noise, spurious modes, and insertion loss [1–3]. However, one of the most significant drawbacks to using single-crystal silicon MEMS resonators has continued to be their relatively high and constant temperature coefficient of frequency (TCF) (about -30ppm/°C). This results in more than an order of magnitude larger temperature-induced frequency variation compared to quartz crystals. In addition, quartz resonators benefit from a turnover temperature at which point the TCF is zero. Therefore, very stable quartz oscillators are attainable within the industrial operating temperature range (-40°C to 85°C) by biasing the temperature of an oven-controlled crystal at the turnover temperature [4].

Previous work has shown that the TCF in silicon resonators can be reduced by including materials with opposing TCF coefficients (i.e. silicon dioxide) [5] or by doping the silicon with boron and aluminum [6]. These methods have demonstrated significant improvement in overall frequency variation but they commonly sacrifice the resonators' quality factor or processing simplicity. In this work, it is shown that n-type doped extensional mode silicon resonators aligned to the [100] direction can exhibit a zero TCF at a certain temperature (i.e. turnover temperature) much like quartz crystal resonators. In addition, it is proved that turnover temperature can be adjusted by doping concentration and the device thickness within a certain temperature range and, therefore, can be designed to produce a minimal frequency shift over a targeted operational temperature range. This approach is very valuable in the sense that it does not require any alteration of the

device fabrication process instead the doping concentration of the starting substrate need to be tightly controlled.

We have chosen TPoS resonators [7] to serve as the platform to analyze the effect of thickness, doping concentration and crystal alignment on TCF. TPoS resonators offer low motional impedance while maintaining high quality factors in air due to the single-crystal silicon resonant structure [1]. A schematic of a typical two port TPoS resonator with input and output pads separated by a ground pad can be seen in Fig. 1. A piezoelectric material is sandwiched between two metal layers and is utilized to both drive a single-crystal silicon structure into resonance and to sense the resulting vibration. A thin metal bottom electrode serves as a ground plane while the patterned, top interdigitated metal electrodes provide the input and output pathways. Using this structure, a 25MHz resonator aligned to the [100] crystalline orientation is presented to exhibit an overall frequency variation of less than 150ppm over the -40-85°C temperature range.

Figure 1: Schematic of a micromachined thin film piezoelectric-on-silicon resonator.

THEORY

The electronic free energy is an important factor in defining the bonding forces between individual atoms and therefore it largely contributes in the elastic properties of solids. The electrons redistribute among the available energy levels in many-valley semiconductors such as silicon so that the total free energy in the crystal is minimized. Since these energy levels vary with the introduction of doping impurities in the crystal, the total free energy of the system also changes. This change in free energy consequently changes the elasticity matrix(c) of the material according to (1), where G is the total Gibbs free energy, V_0 is the volume of non-deformed crystal and S is the strain.

$$c_{ij} = \frac{1}{V_0} \cdot \frac{\partial^2 G}{\partial S_i \partial S_j} \quad (1)$$

For free electrons, Keyes has presented several expressions describing the electronic contributions in the elastic coefficients [8]. In the case of n-type silicon, the contribution of free electrons on the elastic coefficients is calculated as [9]:

$$\delta c_{11} = -\frac{2}{9} N \frac{\Xi_u^2}{E_f} X, \delta c_{12} = \frac{1}{9} N \frac{\Xi_u^2}{E_f} X, \text{ and } \delta c_{44} = 0 \quad (2)$$

where,

$$X = \eta F_{1/2}'(\eta) / F_{1/2}(\eta) \quad (3)$$

and N is the electron concentration, $\mathcal{E}_u$ is the uniaxial deformation potential constant, E_f is the Fermi energy, η is E_f/kT and F is the Fermi integral.

Using (2), the contribution of doping levels on the elastic coefficients, c_{11} , c_{12} and c_{44} (i.e. δc_{11} , δc_{12} and δc_{44}) at any temperature can be calculated. These values and the temperature dependent elastic constants of pure silicon are then utilized to compute the elastic coefficients of doped silicon at every temperature. Then, the Young's modulus (E) for the directions [100] and [110] are calculated using:

$$E_{[100]} = c_{11} - 2c_{12} \frac{c_{12}}{c_{11} + c_{12}} \quad (4)$$

$$E_{[110]} = 4c_{44} \frac{c_{11}^2 + c_{11}c_{12} - 2c_{12}^2}{2c_{44}c_{11} + c_{11}^2 + c_{11}c_{12} - 2c_{12}^2} \quad (5)$$

Once the Young's moduli are calculated, the temperature induced variation of frequency can be plotted assuming that the frequency (f) of the extensional resonator approximately follows the equation below:

$$f = \frac{1}{2w} \sqrt{\frac{E}{\rho}} \quad (6)$$

where ρ is silicon's density and w is the width of the fundamental mode lateral-extensional resonator. The simulated frequency vs. temperature at three different doping concentration are plotted in Fig. 2 for devices aligned to [110] and [100] orientation respectively. From these plots it is clear that TCF for the devices aligned to [110] direction is approximately linear and does not strongly depend on the doping concentrations (N) when N ranges from $3e19$ to $5e19 \text{ cm}^{-3}$. In contrast for the devices aligned to [100] direction the curves exhibit a quadratic dependency on temperature with a zero TCF at a turnover temperature.

Figure 2: Theoretical temperature-induced frequency variation in two extensional silicon resonators aligned to [110] (top) and [100] (bottom) for three different n-type doping concentrations.

It is observed that the turnover temperature in the [100] plots are a sensitive function of doping concentration. We have used these results to choose a doping concentration for our starting substrates that helps us in validating the existence of turnover temperature in a TPoS resonator aligned to the [100] direction. Although, in preparation of these plots the effect of device thickness and the piezoelectric film (i.e. aluminum nitride) are not considered, the silicon properties are assumed to dominate the overall performance of the device.

SIMULATION

To better predict the effect of doping concentration in a TPoS resonator and specifically examine the effect of device thickness on the temperature-induced frequency variation, finite element eigenfrequency analysis is utilized. A single-crystal silicon slab with an aluminum nitride layer on top is oriented in the chosen crystalline directions, [100] and [110] in COMSOL. As the temperature is swept from -40°C to 85°C , the material properties for the single-crystal silicon are changed in accordance to the previously described theory while the AlN Young's modulus is modified as described by Bruls [10].

The plots in Fig. 3 are created for the same three doping concentrations used earlier and show the frequency variation vs. temperature for a TPoS resonator made of $15\mu\text{m}$ silicon and $1\mu\text{m}$ AlN. Compared to plots presented in Fig. 2 the TCF appears to be a less sensitive function of doping concentration. This is a more accurate prediction of what is observed in practice considering that the resonance frequency is not a simple function of the uni-directional Young's modulus. Also the turnover temperature has moved to the left for the devices aligned to [100] direction which is expected considering that the TCF of AlN is negative. The turnover temperature is at -30°C , -5°C , and 40°C for the doping concentrations of $3e19$, $4e19$, and $5e19 \text{ cm}^{-3}$ respectively.

Figure 3: COMSOL-Simulated temperature-induced frequency variation in two TPoS resonators aligned to [110] (top) and [100] (bottom) for three different doping concentration. The silicon and the AlN thicknesses in the device are assumed to be $15\mu\text{m}$ and $1\mu\text{m}$ respectively.

Next, we have also studied the effect of the device thickness on the temperature-induced frequency variation. The two simulated thicknesses, 8 and 40 μm , are the actual thicknesses of the wafers that are used to fabricated devices. According to the simulated data shown in Fig. 4 the TCF (the slope of the plot) will slightly increase for the devices aligned to [110] direction as the silicon thickness increases. Also, the turnover temperature will gradually shift to the right as the thickness increases for the devices aligned to [100] direction. For example a 20°C shift from 20°C to 40°C is predicted when the thickness is changed from 8 μm to 40 μm assuming a doping concentration of $4.75 \times 10^{19} \text{cm}^{-3}$. These results suggest that doping levels and the device thickness can be used as design parameters to minimize the overall frequency variation over a given operating temperature range in [100]-aligned resonators.

Figure 4: COMSOL-simulated TCF data for two TPoS resonators with the silicon thicknesses of 8 and 40 μm aligned to [110] (top) and [100] directions. The doping concentration for both resonators are assumed to be $4.75 \times 10^{19} \text{cm}^{-3}$.

FABRICATION

The lateral-extensional mode TPoS resonators are fabricated using a five-mask process (Fig. 5). To begin, a stack of molybdenum (Mo), aluminum nitride (AlN), and molybdenum is sputtered on top of the silicon device layer of a silicon-on-insulator (SOI) wafer as seen in Fig. 5a. After deposition, the top Mo layer is dry etched with fluorine-based plasma to form the top electrodes. Access to the bottom electrode is then gained through a wet alkaline etch of the AlN (Fig. 5b). The resonator body is then defined with a series of dry etches through the AlN/Mo and then through the device layer silicon (Fig. 5c). The handle-layer silicon is etched from the backside using a DRIE process. Finally, the structure is released with a buffered oxide etch of the buried silicon dioxide layer (Fig. 5d).

A fabricated resonator can be seen in Fig. 6. Note that the starting substrate in all our experiments are [100] SOI wafers. Therefore resonators aligned to the wafer flat are oriented in the [110] direction. By rotating the resonator 45° in-plane the device will be aligned to [100] direction.

Figure 5: Schematic process flow for TPoS resonators.

Figure 6: The SEM of a fabricated TPoS resonator aligned to the [110] direction. The arrows in the figure indicate the crystal orientations (this device is a [110]-aligned resonator).

RESULTS

Three wafers with different device thicknesses, dopants, and dopant concentrations were used in this work (Table 1). As seen in the table the absolute value of the doping concentration is not known for these wafers. However, the 8 μm and the 40 μm wafers are made from the same starting silicon substrate and their actual doping concentration are expected to be close to each other. Similar resonators were fabricated on each of these wafers oriented in differing crystalline directions. The devices were tested in a Janis cryogenic vacuum probe station using an Agilent network analyzer.

Table 1: The device silicon properties for the utilized SOI wafers.

Thickness (μm)	Dopant	Resistivity (Ωcm)	Doping Concentration (cm^{-3})
8	P	0.001 – 0.0015	4.97×10^{19} – 7.85×10^{19}
15	As	0.001 – 0.003	2.52×10^{19} – 9.67×10^{19}
40	P	0.001 – 0.0015	4.97×10^{19} – 7.85×10^{19}

Typical frequency responses for two devices fabricated on the 40 μm substrate and aligned to [110] and [100] directions are shown in Fig. 7.

Figure 7: Experimental frequency responses for [100]- (left) and [110]- aligned (right), 40 μm , P- doped TPoS resonators at 25°C.

Note that the lower quality factor (and higher motional impedance) of the [100]-aligned resonator is believed to be due to the fact that the dimensions of these resonators are optimized for [110] alignment. As expected, the frequency of the [100]-aligned resonator is lower than the [110]-aligned device.

The resonance frequency is measured over the temperature range of -40 to 85°C for the devices fabricated on all three substrates and aligned to both [110] and [100] directions. The results are plotted in Fig. 8. Considering that the effect of thickness on the TCF has been shown to be relatively small, the substantial difference in the measurement from the [100]-aligned 15μm device is considered to be a result of discrepancy in doping concentration. Based on the predictions of Figs. 2 and 3 it can be concluded that the doping concentration of the 15μm wafer is lower than the other two. Also, the difference between the turnover temperatures of the [100]-aligned 8μm resonator (22°C) and the 40μm device (33°C) is believed to be a result of the thickness difference. Therefore, the prediction in Fig. 4 is experimentally validated. One may argue that this shift could be a result of a slightly higher doping concentration in the 8μm wafer. This conclusion can be dismissed upon investigation of the results from the [110]-aligned devices. A higher doping concentration should have resulted in a lower TCF for the [110]-aligned 8μm device compared to the 40μm counterpart based on the theoretical analysis shown in Fig. 2 and Fig. 4. This is in contrast with the measurement. Therefore, the data presented in Fig. 8 validates that the turnover temperature shifts to the right as the device thickness and the doping concentration increases. More importantly, the [100]-aligned 8μm thick resonator exhibits an overall frequency variation of 148ppm.

Figure 8: Experimental TCF data for three [110]-aligned and three [100]-aligned resonators fabricated on SOI wafers with varying thicknesses. The results are the first observation of turnover temperature in silicon resonators and agrees with the theoretical prediction about the effect of doping and the device thickness.

CONCLUSION

In this work, we have investigated the effects of doping levels, device thickness, and device orientation on temperature stability in n-type doped lateral-extensional silicon resonators. The theoretical analysis and simulated data predict that a turnover temperature exists for highly-doped silicon resonators and that the turnover temperature is a function of orientation and doping concentration. We have also shown that for a given doping concentration the turnover temperature can be adjusted by device thickness. Moreover, we have experimentally validated that these theoretical predictions using thin-film piezoelectric-on-silicon (TPoS) resonators as the implementation platform. We have reported a 25MHz TPoS resonator that exhibits a turnover temperature at 22°C and an overall frequency variation of less than 150ppm over the industrial temperature range (-40°C to 85°C). This is a significant reduction in the previously reported frequency variations from uncompensated silicon resonators which is more than 3000ppm over the same range of temperature.

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