Turn-over Temperature in Lateral-Field-Excited Thin-Film Lithium Tantalate Contour-Mode Resonators

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***Summary*— In the present work, the possibility of designing thin-film lithium tantalate bulk resonators that exhibit a turn-over temperature in their frequency-temperature characteristic is explored. The simulation results suggest that contour-mode resonators carefully aligned to a specific crystalline orientations on an X-cut $LiTaO_3$ (LT) film exhibit a turn-over temperature. The exact location of the turn-over temperature could be adjusted by rotation within the X-cut. Preliminary experimental results measured from resonators fabricated on a 1.8um LT film bonded to a Si substrate confirm the existence of the predicted turn-over temperature. A zero-temperature coefficient of frequency (TCF) has been observed at 100 ˚C in resonators rotated 40 degrees with respect to -Y-axis in X plate of LT.**

Keywords—TCF; Thin-film LT Resonators; Lateral-field-Excited; Contour-mode resonators; MEMS.

I. Introduction

Microelectromechanical system (MEMS) resonators are increasingly being adopted for timing applications because of their distinguished advantages of small size, the potential for integration with CMOS technologies, and low power consumption. However, MEMs resonators' sensitivity to the temperature, mainly from the temperature coefficient of elasticity (TCE), is considered as an inherent disadvantage of these resonators. In fact, most of the materials utilized in MEMs resonators, such as pure silicon, aluminum nitrate (AlN), and lithium niobate (LN) resonators have negative frequency drift versus temperature that causes large frequency drift (more than 1000 ppm) [1,2] over the industrial range (-40 - 80 ˚C). This large frequency variation could be a serious problem, especially in timing applications in which frequency stability is the main concern [1].

Several solutions have been proposed in the previous research to improve the frequency performance of MEMS resonators, mainly categorized into an active and passive methods. In passive compensation approaches, the intrinsic property of the resonating structure is manipulated, such that the frequency sensitivity due to temperature change is reduced [2], while active compensation techniques are usually based on electrical tuning or ovenization of the MEMS resonators [2,3]. Oven-controlled frequency stabilization is considered as one of the common active methods in which the resonator is heated and maintained at a high temperature, usually at its local zero TCF (also known as turn-over temperature), to minimize the influence of fluctuation of ambient temperature. Therefore, to actualize this method, resonators with a local zero TCF are required. As mentioned earlier , most of the materials used in MEMS resonators have negative frequency drift versus temperature. However, there exist two exceptions; highly n-type doped silicon resonators [4] and thickness shear mode of X-Cut Lithium Tantalate (LT) resonators that exhibit turn-over temperature [5,6]. The combination of relatively strong piezoelectricity and zero TCF of X-Cut LT film, could enable low-loss thermally-stable acoustic resonators .

In most previous efforts, the TCF of LT resonant structures has been examined for thickness shear mode resonators [5], in which the resonant frequency is determined by the thickness of the piezoelectric material, hence incompatible with achieving multi-frequency functionality on a single chip [7]. Recently, thin-film lateral bulk extensional (i.e., contour mode) resonators have gained much attention since they enable dispersed-frequency designs on the same substrate and for their capacity to target higher operational frequency with relatively high-quality factors. In this study, the existence of zero TCF have been investigated for contour-mode thin-film LT resonator through simulations, and a turn-over temperature around 100 ˚C is reported for fabricated device 40 degrees rotated with respect to -Y-axis (Fig.1(a)). The S_0 lamb waves are excited using lateral field interdigitated fingers on an X-cut film.

II. Design and Simulations

In order to investigate our hypothesis on turn-over temperature in contour-mode LT resonators, several simulations have been executed in COMSOL Multiphysics software using eigenfrequency analysis for the slab of X-Cut Lithium tantalite that is rotated with some specific angle (θ) with respect to -Y-axis. The resonator's orientation, the conceptual view of proposed one port resonators and the stress profile are shown in Fig. 1. The dimension of the simulated resonator is listed in Table 1.

To predict the frequency shift as a function of temperature and to find TCF curves, the stiffness matrix is calculated for each temperature using (1).

$$C = C_{ref} + a_1 C_{ref}(T - T_{ref}) + a_2 C_{ref}(T - T_{ref})^2 \qquad (1)$$

where C is LT elastic constant at an arbitrary temperature

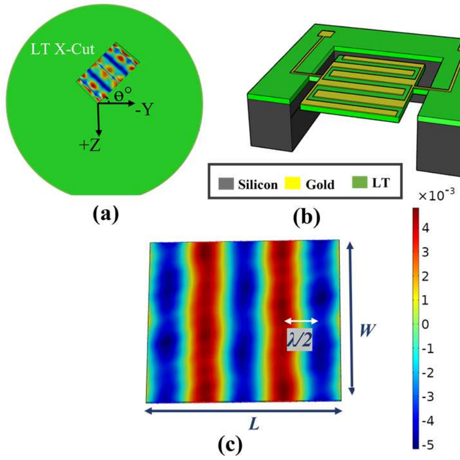

Fig. 1: (a) The orientation of contour-mode resonators fabricated on LT substrate (b) conceptual schematic of the device structure (c) Stress profile of 5th order resonator in y-direction.

referenced to the room temperature (T_{ref}), and C_{ref} is elastic constant at room temperature. a_1 and a_2 are first and second-order temperature coefficient corresponding to each elastic constant respectively which their values are borrowed from [8] and brought in Table 2.

Table 1: geometrical parameters of the simulated X-cut LT resonator

Parameter	*Value*
Plate length *(L)*	120 µm
Plate Width *(W)*	108 µm
Order number of S_0 mode (*N*)	5
LT slab thickness	1.8 µm
Wavelength (λ)	48 µm
Target resonant frequency	123 MHz

Table 2: Elastic constants of LT and their corresponding first and second-order temperature coefficients [8]

Elastic constant ($* 10^{12}$**Pa**)		a_1 ($* 10^{-4}/°C$)	a_2 ($* 10^{-7}/(°C)^2$)
C_{11}	**0.22**	**-1.03**	**0.77**
C_{12}	**0.044**	**-3.41**	**-1.18**
C_{13}	**0.0812**	**-0.5**	**6**
C_{14}	**-0.014**	**6.67**	**16.7**
C_{33}	**0.279**	**-0.96**	**-3.21**
C_{44}	**0.096**	**-0.43**	**1.67**
C_{66}	**0.092**	**-0.47**	**1.24**

The simulated frequency variations versus temperature for the 5th order resonator (with dimension listedin Table 1) are depicted for several values of θ (=40, 43, 45 deg) in Fig.2. As seen, the frequency versus temperature plots resemble upward parabolic curves and a zero TCF is observed between 80 ˚C - 110 ˚C depending on the rotation angle (θ). This property could be useful and exploited in the case of micro-oven control oscillators in which a turn-over temperature higher than the operation range is desired [9].

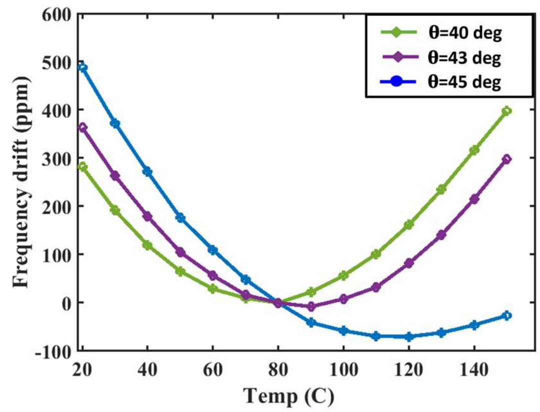

Fig. 2: Frequency drift versus temperature for different angles with respect to -y axis.

Lamb wave in piezoelectric materials could be excited through either a lateral-field excitation or a thickness field excitation [2]. However, based on piezoelectric coupling coefficient of LT (2), in X-plate d_{12} and d_{13} are zero. Therefore, S_0 lamb wave could not be excited through application of a thickness field. Therefore to apply a lateral field IDT are should be placed on the surface of LT. Fig. 3 demonstrate the resonators' displacement in an LT resonator for which the electrodes are placed at anti nodes of the resonance mode shape. Previous publications have suggested that less spurious mode can be achieved by putting IDT at anti-nodes [10].

$$\begin{bmatrix} 0 & 0 & 0 & d_{15} & -d_{22} \\ -d_{22} & d_{22} & d_{15} & 0 & 0 \\ d_{31} & d_{31} & d_{33} & 0 & 0 \end{bmatrix} \quad \begin{matrix} d_{15} = 2.65 * 10^{-11} \\ d_{22} = 0.7 * 10^{-11} \\ d_{31} = -0.3 * 10^{-11} \\ d_{33} = 0.57 * 10^{-11} \end{matrix} \qquad (2)$$

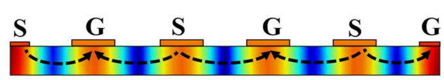

Fig 3: displacement of resonator with electrodes placed at anti-nodes.

III. Fabrication process and experimental resultas

Using the simulation results as a guide, the fabrication process was performed in 4 steps which are detailed in Fig. 4.

4 inch LT X-Cut wafer was sent for bonding (this step accomplished by "NGK insulator"company) on 500µm silicon handle wafer and polished to 1.8um thickness. After that, Cr/Gold (30nm/120nm) was deposited by Ebeam evaporator

and patterned using lift-off process to form the electrodes. The next step is defining the boundary of resonators by etching LT in an Argon plasma utilizing silicon oxide as a mask. Lastly, the backside of the resonators is etched by Bosch process. The SEM of one of the fabricated resonators is shown in Fig.5. The acoustic isolation frame around the device is employed here to reduce the anchor loss and consequently improve the quality factor [9,11].

A typical frequency response of the resonators (Y_{11}) has been measured and depicted in Fig. 6. The electromechanical coupling coefficient (K_t^2) is calculated to be ~2% based on the measured frequency response.

The TCF measurement is conducted in a Janis cryogenic vacuum probe station using high-frequency probes and the

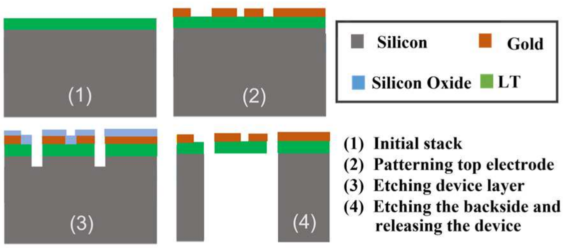

Fig. 4: Fabrication process of the proposed resonator

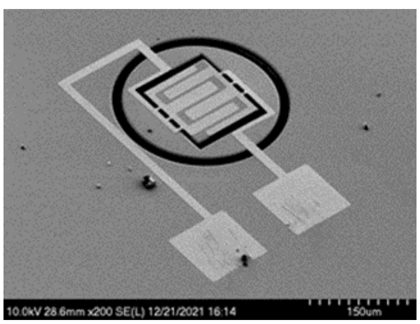

Fig. 5: SEM of the device

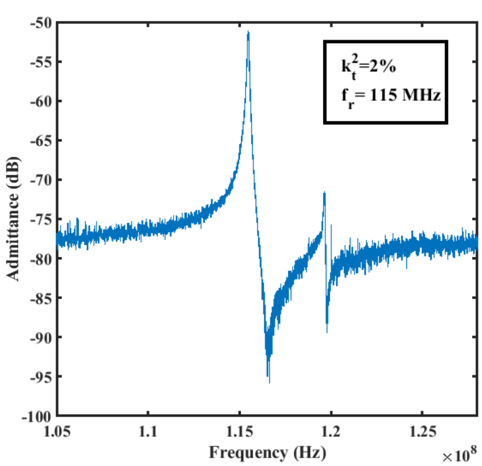

Fig. 6: Frequency response of the device

Agilent E5061A ENA network analyzer. The sample holder is heated by a resistive heater and controlled by a PID controller. The variation of the resonance frequency is measured for 7th order (N=7) resonators at θ=40 deg at 115 MHz operation frequency and is fitted by second-order polynomial (shown in Fig. 7). As it is seen, zero TCF have been observed around 100 ˚C and 110 ˚C that verifies the initial theory. The observed discrepancies between the measured and simulated data in terms of the turn-over temperature (in simulation result for θ=40 deg, turn-over temperature happens around 80 ˚C) might be rooted in the tolerance of rotation angle, which would cause some shifts in turn-over temperature as mentioned in previous parts. Another sourse of error might be that the gold electrodes were not considered in simulation to reduce the computations load.

IV. Conclusion

In this study, the frequency-temperature characteristic of lamb wave LT resonators with different rotation angles along -y-axis in x-cut plate has been simulated and also measured for devices rotated 40 degrees off the -y-axis. Upward parabolic frequency-temperature plots and a zero TCF at 100°C has been observed for ~θ=40 deg. Relatively high coupling coefficient along with a local zero TCF temperature in these resonators make them a suitable candidate for oven-controlled oscillator application.

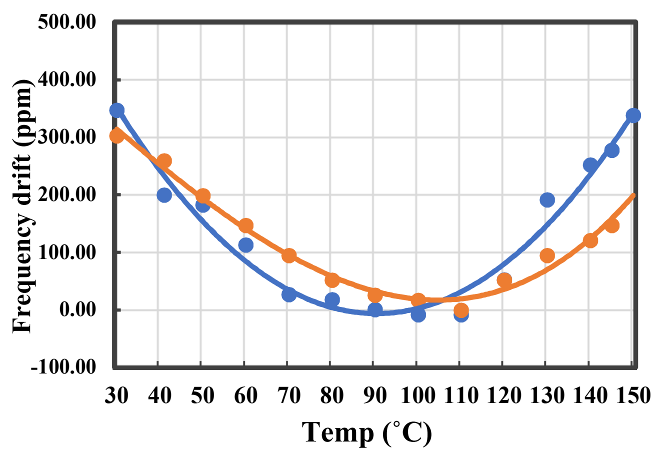

Fig. 7: Measured frequency drift of 7th order resonators versus temperature at θ =40 deg

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