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Dependence of temperature coefficient of frequency (TCf) on crystallography and eigenmode in N-doped silicon contour mode micromechanical resonators

Haoshen Zhu [a,*], Cheng Tu [a], Guangcun Shan [b], Joshua E.-Y. Lee [a,c,d]

[a] Department of Electronic Engineering, City University of Hong Kong, Kowloon, Hong Kong
[b] Department of Physics and Materials Science, City University of Hong Kong, Kowloon, Hong Kong
[c] City University of Hong Kong Shenzhen Research Institute, Shenzhen, Guangdong, China
[d] State Key Laboratory of Millimeter Waves, City University of Hong Kong, Kowloon, Hong Kong

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ABSTRACT

This paper reports the effects of crystal orientations on the temperature coefficient of frequency (TCf) of single crystal silicon square-plate micromechanical resonators vibrating in two distinct contour modes: Lamé mode and square extensional (SE). For the Lamé mode, the same TCf was found over several devices aligned to the ⟨1 1 0⟩ direction, while much greater variation in the TCf was observed among the devices aligned against the ⟨1 0 0⟩ direction. For the SE mode, the devices in both ⟨1 0 0⟩ and ⟨1 1 0⟩ orientations exhibit similar TCf values for varying doping levels. The sensitivity of TCf to doping concentration is also investigated. The TCf of Lamé ⟨1 0 0⟩ device is more easily influenced by n-type doping concentration than SE mode devices in both orientations while the Lamé ⟨1 0 0⟩ device is almost immune to doping variation. Devices with different dimensions are tested, and the TCf values are proved to be free of size scaling. Quantitative study based on free carrier contribution on elastic constants is performed and supports our observations. Close agreement among experiments, theoretical predictions and simulations is achieved.

1. Introduction

As a possible alternative to conventional quartz crystal oscillators, silicon micromechanical resonator (microresonator) based oscillators (or in general MEMS oscillators) have attracted increasing degrees of interest from both academia and industry [2] in the recent decade. Compatible with the modern IC fabrication process, these silicon-based microresonators are well suited for batch production and can be packaged together with ICs in standard plastic packages, which leads to lower cost, higher integration level and better reliability than the quartz counterpart. MEMS oscillator products are now entering the timing market, but certain barriers still exist.

One of the major obstacles preventing MEMS oscillators from high-end applications (like GPS and wireless communications) is their frequency stability over temperature. For instance, the newly released MEMS oscillator from Integrated Device Technology exhibits ±50 ppm shift over the industrial temperature range (−40 to 85 °C) [3], which is generally much higher than quartz oscillators and cannot at present meet GPS/4G specifications (±2.5 ppm). This problem derives from the relatively large negative linear temperature coefficients of elasticity (about −30 ppm/K) for intrinsic single crystal silicon (SCS), which results in a larger than 3000 ppm frequency drift over the temperature range of interest. Therefore, various temperature compensation techniques have **been** developed to alleviate this problem. For instance, one of the active techniques is to use the spring softening effect of the capacitive resonator to stabilize the resonant frequency via tuning the bias voltage [4]. Based on this method, a MEMS oscillator with a temperature-stabilized frequency of ±2.5 ppm has been demonstrated [5]. Additionally, a more general and powerful means of active compensation involves **the** use of a frequency synthesizer (i.e. phase-locked loop, PLL) [6]. To date, the state-of-the-art MEMS oscillator product adopting a PLL can achieve a frequency stability of 0.2 ppm over the industrial temperature range [7] (comparable to temperature compensated crystal oscillators, TCXO). Other methods include keeping the resonator in a temperature-stabilized micro oven [8]. Each of these approaches has its own limitations. For example, the bias voltage tuning method suffers from a

* Corresponding author. Tel.: +86 262161604.
E-mail addresses: haoshezhu2-c@my.cityu.edu.hk, zhuhaosheng@vip.sina.com (H. Zhu).

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limited tuning range and is normally only applicable to low frequency capacitive resonators. The PLL method of compensation on the other hand may degrade the phase noise performance. In general, the active compensation techniques complicate the electronics design and increase power consumption as well as cost to the system. As such, passive compensation techniques which address this problem from the bottom-up by engineering the material property of the resonators are still favorable.

Previous work has been done by using materials with opposite temperature coefficient of modulus (e.g. pairing Si and SiO_2), which has been shown to be capable of about 10 times improvement on the temperature stability [9,10]. But the same group of authors have also reported observing dielectric charging effects in these composite resonators which affect the long term stability of the oscillator and lead to large frequency drift [10]. On this note, modifying the temperature dependence of silicon via degenerate doping is regarded as a promising passive compensation approach. This approach reduces the complexity of fabricating a structure of composite materials, maintains high quality factor (Q) and eliminates the dielectric charging problem. Effective temperature compensation for MEMS resonators via both p-type [11,12] and n-type doping [13] has been demonstrated, showing that the temperature coefficient of frequency (TCf for short) could be lowered down to ~1 ppm/K. With the help of finite element (FE) analysis, quantitative studies based on Keyes' theory [14] on the contribution of free carriers to elasticity have been performed recently to predict the TCf of various MEMS resonators fabricated on n-type doped silicon wafers [15–17].

SCS bulk mode micromechanical resonators utilizing capacitive transduction exhibit superior Q and power handling capability [20], which makes them good candidates for realizing low phase noise reference oscillators. Advanced MEMS oscillator products (based on this kind of devices) aimed at communication applications have been reported recently [7]. In this work, square-plate SCS resonators fabricated on n-doped silicon-on-insulator (SOI) wafers are adopted as test vehicles to study the influence of both crystal orientation and vibration mode on the TCf of these MEMS resonators, which extends the preliminary results reported previously [1]. In addition to numerical studies, analytical predictions on the TCf for both the Lamé [18] and square-extensional (SE) [19] modes based on the square-plate resonators are presented herein and compared against the experimental results from multiple fabricated samples.

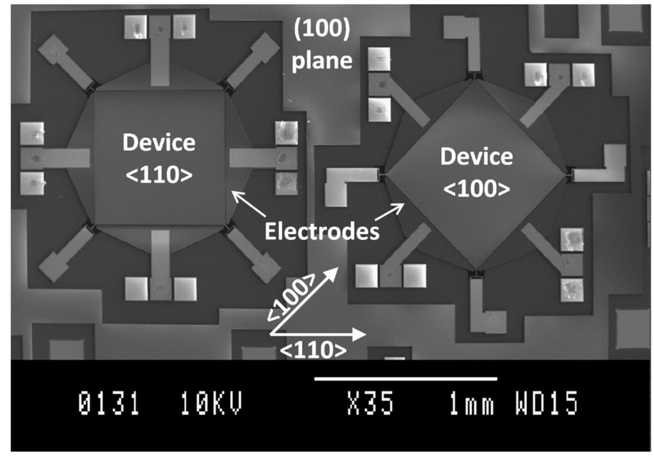

Fig. 1. Scanning electron micrograph (SEM) of the fabricated pair of identical resonators (edge length: $L = 800\ \mu m$) aligned to different crystal orientations in a single die.

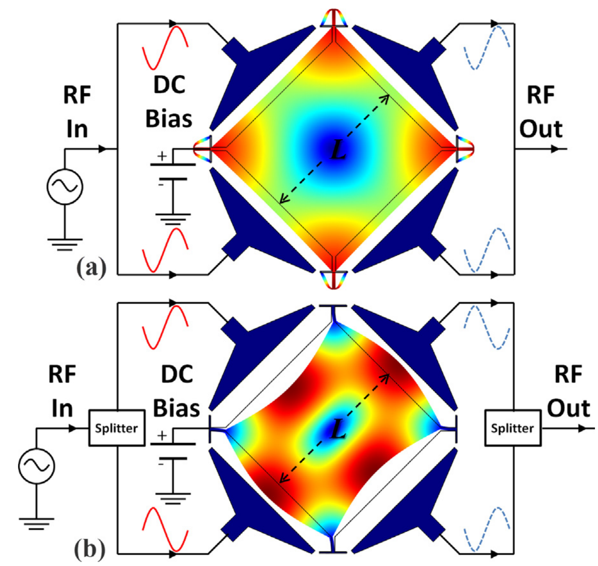

Fig. 2. Biasing configurations and their corresponding mode shapes: (a) SE mode; (b) Lamé mode. Mode shapes were simulated by finite elements (FE) using COMSOL.

2. Method and theory

Square-plate resonators of the same lateral dimensions were fabricated in pairs on the same sample die using a foundry SOI micromachining process. All devices were fabricated on (1 0 0) n-doped SOI wafers. The edge of one of the square-plates among each pair is aligned to the ⟨1 1 0⟩ direction (referred hereafter as Device ⟨1 1 0⟩) and the other to the ⟨1 0 0⟩ direction (referred hereafter as Device ⟨1 0 0⟩), all within the (1 0 0) plane. These pair of resonators are depicted in the scanning electron micrograph (SEM) shown in Fig. 1. As the square-plate resonators are placed alongside each other, negligible difference in doping concentration has been assumed. As such, the influence from different doping concentrations is ruled out, which allows for a direct comparison of the TCf on devices with different crystal orientations. The devices were characterized in a Janis cryogenic probe station via GSG probes using an Agilent E5061A vector network analyzer at a vacuum level of ~0.1 mTorr. The sample mount inside the chamber can be cooled by liquid nitrogen and heated up while the temperature is monitored and controlled by a PID controller with a resolution of up to 0.001 K. The resonators were excited in both the Lamé and SE modes (illustrated in Fig. 2) by electrostatic actuation and detected by capacitive sensing via the surrounding side electrodes. The corresponding biasing configurations used to actuate and detect the respective modes are also shown in Fig. 2.

The resonant frequency f of the SCS square-plate resonator in the fundamental Lamé and SE modes can be determined as follows [21,22]:

$$f_{\text{Lame}} = \frac{1}{\sqrt{2}L}\sqrt{\frac{G}{\rho}}, \tag{1}$$

$$f_{\text{SE}} = \frac{1}{2L}\sqrt{\frac{E_{bi}}{\rho}\left[1+\left(1-\frac{8}{\pi^2}\right)\left(\frac{\nu}{\nu-1}\right)\right]}, \tag{2}$$

where ρ is the material density, G is the shear modulus, E_{bi} is the biaxial Young's modulus, ν is the Poisson's ratio. It is well known that for an anisotropic material (like SCS), G, E_{bi} and ν are orientation dependent. With a cubic crystal structure, the mechanical properties (up to second-order elastic moduli) of SCS can be expressed by a stiffness matrix which consists of 3 elementary elastic constants: C_{11}, C_{12} and C_{44}. Other mechanical properties (like Young's modulus, shear modulus, Poisson's ratio) along different axis directions can then be derived from these elastic constants