Extraction of Material Properties of A Thin Silicon Membrane Embedded in A Piezoelectric Stack

Sagnik Ghosh
Institute of Microelectronics
Agency for Science, Technology and Research (A*STAR)
Singapore
Sagnik_Ghosh@ime.a-star.edu.sg

Prakasha Chigahalli Ramegowda
Institute of Microelectronics
Agency for Science, Technology and Research (A*STAR)
Singapore
Prakasha_Chigahalli_Ramegowda@ime.a-star.edu.sg

Duan Jian Goh
Institute of Microelectronics
Agency for Science, Technology and Research (A*STAR)
Singapore
Goh_Duan_Jian@ime.a-star.edu.sg

Jaibir Sharma
Institute of Microelectronics
Agency for Science, Technology and Research (A*STAR)
Singapore
sharmaj@ime.a-star.edu.sg

Yul Koh
Institute of Microelectronics
Agency for Science, Technology and Research (A*STAR)
Singapore
Koh_Yul@ime.a-star.edu.sg

Joshua E.-Y. Lee
Institute of Microelectronics
Agency for Science, technology and Research (A*STAR)
Singapore
Joshua.Lee@uts.edu.au

***Abstract*— We propose the use of a thickness extensional (TE) mode in a piezoelectric-on-silicon resonator to accurately extract the elastic stiffness constant (c_{11}) of a degenerately doped 2µm-thin silicon (Si) membrane with the piezoelectric stack in place. The frequency of this mode is discriminately sensitive to the Si membrane thickness and c_{11} of Si alone over the other layers in the stack. This presents a methodology to extract the properties of the elastic layer of a piezoelectrically transduced device with little influence from the other layers. The vertical stack of the TE mode resonator here is composed of 15% scandium doped aluminum nitride (ScAlN: ~0.3µm), molybdenum (~0.2µm) and thin passivation piezoelectric (~50nm) on the doped Si membrane formed by silicon migration. The methodology and test structure are validated by the close agreement of the extracted Young's modulus to literature values. We use Si as a well-studied material to validate the method, demonstrating that the method could be extended to other materials.**

Keywords—Piezoelectric-on-silicon resonator, elastic constant of heavily doped silicon, thickness extensional mode, thin silicon membrane, material property extraction

I. INTRODUCTION

Piezoelectric transduction is preferred for actuation and sensing among many microelectromechanical systems (MEMS) devices owing to the strong electromechanical coupling from piezoelectric material as compared to capacitive transduction. Piezoelectric materials in the form of thin-films are commonly deposited on an elastic layer, which includes but is not limited to silicon [1-3], silicon carbide [4] and diamond [5]. Piezoelectric-on-silicon technology [1-3] has been most widely explored to realize resonators and sensors given the wide availability of silicon (Si) wafers with high yield fabrication processes.

A set of piezoelectric MEMS resonators for timing and frequency reference applications require frequency stability across a wide range of temperature. Elastic constants of Si, heavily doped with either n-type or p-type dopants to a doping level of higher than 10^{19} cm^{-3} has shown reduced temperature dependence [6]. As such, passive temperature compensated MEMS resonators have been realized with piezoelectric-on-doped silicon [1]. Recently, thin, and heavily doped silicon membranes (≤ 5µm) have shown its promises for piezoelectric micromachined ultrasonic transducers (pMUTs) [3] and sub-GHz frequency temperature compensated MEMS resonators [2].

Existing methods to extract properties of doped Si employ capacitive transduction among MEMS resonators with thick Si device layer (≥ 20µm) [6,7] as motional resistance scales inversely with thickness to the 4th order. To date, there have been no reports on methods and structures to extract the material property of Si from structures transduced by a piezoelectric. Although using piezoelectric transduction on thin Si membranes allows for electrical characterization of resonance, it introduces a suite of additional variables in the extraction process from the additional layers. We herein coupled the electrical measurement results with our finite element (FE) models of a thickness extensional (TE) mode in a piezoelectric-on-Si resonator to accurately extract one elastic constant (c_{11}) of doped Si. Although Si has been used as a well-studied material to validate our method, this method can be extended to extract material properties of other elastic layers embedded in a piezoelectric stack.

II. METHOD OF EXTRACTION

A. Device description

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The TE mode resonator is fabricated using piezoelectric over silicon-on-nothing process [8] where a 0.3µm thick 15% scandium doped aluminum nitride (ScAlN) was sandwiched between a pre-released 2µm thick degenerately n-doped (doping level > 10^{20} cm^{-3}) Si membrane and a 0.2µm thick molybdenum (Mo). Here, doped Si membrane serves as the bottom electrode while Mo serves as the top electrode of the resonator. The top Mo electrode is further passivated with 50nm thick piezoelectric film.

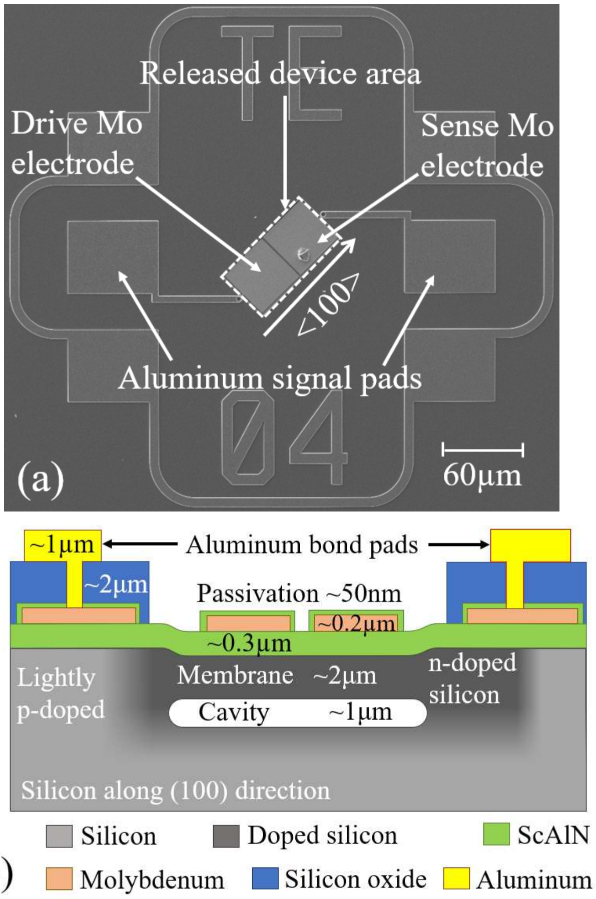

Fig. 1. (a) Top view scanning electron micrograph (SEM) showing the fabricated TE mode resonator aligned to <100> crystal axis of silicon substrate along (100) direction. (b) Cross-sectional view of the TE mode resonator showing the material stack forming the device.

Fig. 1a shows a scanning electron micrograph (SEM) of the TE mode resonator aligned to <100> crystal axis of the Si substrate along (100) plane, while Fig. 1b depicts the cross-sectional view with the vertical stack of materials forming the device. The TE mode resonator is built on a 120µm long and 60µm wide pre-released doped Si membrane which is clamped on all sides. As seen from Fig. 1a, the top Mo layer is patterned to provide drive and sense electrodes, whereas the bottom electrode remains floating.

B. *Elastic properties and their dependence on resonant frequency*

Resonant frequency of a TE mode resonator can be expressed as [9]:

$$f_n = (1/2t)\sqrt{(c/\rho)} \quad (1)$$

where t denotes the effective thickness of the released stack forming the device, c and ρ are effective elastic constant (or Young's modulus) and density of the stack respectively.

Here, we considered a cubic symmetry of single crystal silicon with three independent elastic constants (c_{11}, c_{12} and c_{44}) for the stiffness matrix according to [10]. As ScAlN has a hexagonal crystal structure with transverse isotropy, the stiffness matrix for ScAlN is composed of 5 independent elastic constants (c_{11}, c_{12}, c_{13}, c_{33} and c_{44}) according to [11]. Table-1 summarizes the values of elastic constants and Young's modulus applied in this study.

TABLE I. ELASTIC CONSTANTS AND YOUNG'S MODULUS USED IN THIS STUDY

Materials	**Elastic constant/Young's modulus**	**Value**	**Unit**
Si [12]	c_{11}	165.7	GPa
	c_{12}	63.9	
	c_{44}	79.5	
ScAlN	c_{11} [13]	351	
	c_{12} [14]	143	
	c_{13} [13]	109	
	c_{33} [15]	270	
	c_{44} [13]	111	
Mo	E	312	

We defined a term 'sensitivity' to quantify the dependence of the resonant frequency of the TE mode to a given elastic constant or Young's modulus of each respective layer. Given the non-linear dependencies with respect to elastic constants (or Young's moduli) on the resonant frequency according to equation (1), the sensitivity was calculated by linearizing the resonant frequency with respect to individual elastic constant (or Young's modulus) using Taylor's theorem of multivariable functions. Note that the sensitivity was calculated by obtaining the variation of resonant frequency due to a small change in a particular elastic constant (or Young's modulus) while the other elastic constants remained constant.

C. *Finite element modeling (FEM)*

We applied eigenfrequency analysis in COMSOL to simulate resonant frequency of TE mode using both two-dimensional (2D) and three-dimensional (3D) models. The thickness of respective layers was adopted from the SEM results in [2], and the properties of respective materials (defining the layers) were applied from Table-1. We used symmetric boundary condition for the 3D model. A rotated system was defined in both 2D and 3D models to employ <100> crystal axis alignment within Si substrate along (100) direction. Using the initial material parameters from Table-1, we obtained 1.2% higher resonant frequency for 3D model as compared to the 2D model for a TE mode given in Fig. 2.

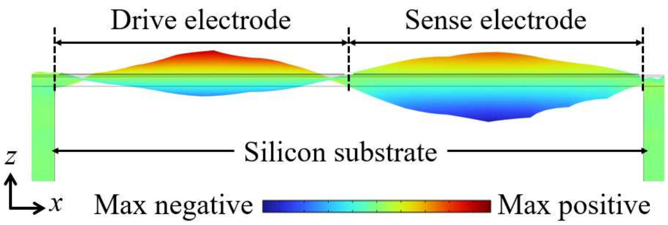

Fig. 2. FE simulated out-of-plane (along *z*-axis) displacement contour of TE mode showing the displacements around drive and sense electrodes sites are out-of-phase with respect to each other.

D. Experiemental validation

The fabricated TE mode resonator was electrically measured across a full wafer using Ground-Source-Ground (GSG) probes in a two-port configuration. Prior to the measurement of the actual devices, the GSG probes and the cables were calibrated using a standard calibration substrate in Short-Open-Load-Through (SOLT) configuration. We measured scattering (S) parameters of the devices using a vector network analyzer (VNA) inside a probe station. The admittance results, as converted from the measured S-parameters, were fitted with a Butterworth-Van-Dyke (BVD) model [16] to obtain resonant frequency (f_n), as shown in Fig. 3. Note that we obtained a 0.8% variation of resonant frequency across a wafer for the TE mode device depicted in Fig. 1a.

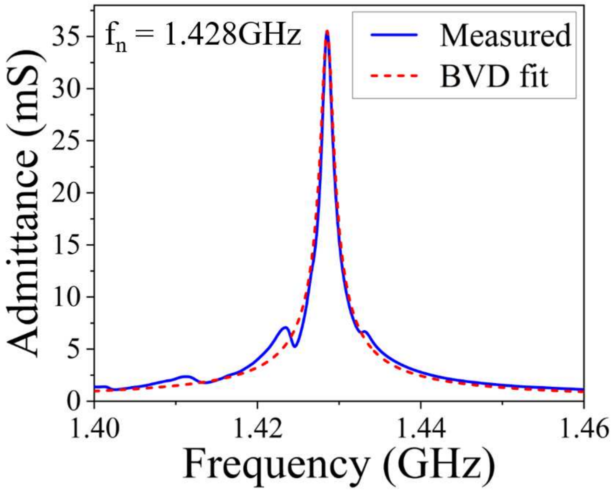

Fig. 3. Measured admittance (as converted from the measured scatternng parameters) of the TE mode resonator as a function of frequency sweep. Here, f_n denotes the resonant frequency of the TE mode resonator.

III. EXTRACTED MATERIAL PROPERTY

A. Simulated sensitivities and extracted material property

We obtained the sensitivity to the respective elastic constants of Si and ScAlN as well as the Young's modulus of Mo using COMSOL for both 2D and 3D models. To obtain the sensitivity to a particular elastic constant (or Young's modulus), the value for that given elastic constant (or Young's modulus) is swept around a small range and the corresponding variation in eigenfrequency was simulated using eigenmode analysis in COMSOL. Fig. 4 shows the sensitivity to individual elastic constant (or Young's modulus) to the eigenfrequency of the TE mode. As seen from Fig. 4, c_{11} of Si shows the highest sensitivity (45%) with respect to the eigenfrequency. A 4% contribution comes from c_{33} of ScAlN while the sensitivity due to remaining elastic constants are near-zero. Note that similar levels of sensitivities were obtained for both 2D and 3D models.

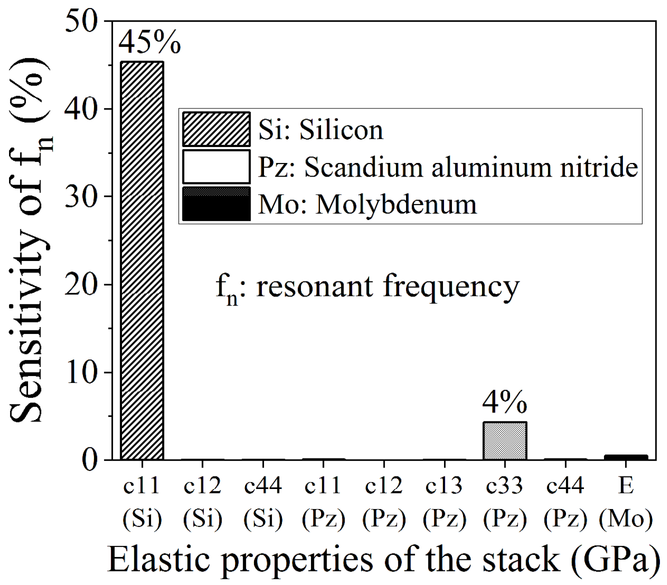

Fig. 4. Finite element simulated sensitivities of respective elastic constants (Si and ScAlN) and Young's modulus (Mo) of the released vertical stack to the resonant frequency of TE mode.

We applied an iterative gradient descent method using the sensitivity to c_{11} of Si, whereby c_{11} is initialized after each iteration until the difference between measured and simulated resonant frequencies converge. Table-2 provides an extracted range of c_{11} for doped Si as obtained using both 2D and 3D simulation models. It is worth noting that the range of c_{11} appears from the 0.8% variation in measured resonant frequency across a wafer.

TABLE II. EXTRACTED ELASTIC CONSTANT (C_{11}) OF DOPED SILICON

FEM	**Input to FEM: c_{33} of ScAlN (GPa)**	**Measured resonant frequency (GHz)**	**Extracted c_{11} of doped Si (GPa)**
2D	270 [15]	1.416 – 1.428	166.8 – 169.8
3D			162.3 – 165.3

B. Uncertainty in extracted c_{11} of doped Si due to c_{33} of ScAlN

As seen from Fig. 4, c_{33} of ScAlN shows a 4% sensitivity on the resonant frequency of the TE mode. Given the sensitivity of the other elastic constants to resonant frequency are near-zero, the only uncertainty in the extracted c_{11} of doped Si originates from the predefined value of the c_{33} of ScAlN. We further simulated a sensitivity of -11.12% for c_{33} of ScAlN to the extracted c_{11} of doped Si. Negative sign indicates a reduction in c_{11} of doped Si due to an increase in the c_{33} of ScAlN. As the upper bound of the reported c_{33} for ScAlN in literature is 310.7GPa [14], we further extracted the value of

c_{11} of doped Si factoring in the -11.12% sensitivity. Table-3 summarizes the extracted values of c_{11} of doped Si for a range of c_{33} of ScAlN reported in literature.

TABLE III. EXTRACTED ELASTIC CONSTANT (C_{11}) OF DOPED SILICON FOR A RANGE OF C_{33} OF SCALN

FEM	**Input to FEM: c_{33} of ScAlN (GPa)**	**Measured resonant frequency (GHz)**	**Extracted c_{11} of doped Si (GPa)**
2D	270 [15]	1.416 – 1.428	166.8 – 169.8
3D			162.3 – 165.3
2D	310.7 [14]		163 - 166
3D			161.6 – 158.6

IV. CONCLUSIONS

As there are no c_{11} of doped Si reported for a doping level of >10^{20} cm^{-3}, we extrapolated a c_{11} of 156GPa from [7]. The range of c_{11} values for doped Si extracted with the 3D model for a c_{33} of 310.7GPa for ScAlN [14] is more in tune with the extrapolated value for heavily doped Si from literature. The 1.2% difference between extrapolated and extracted values for c_{11} of doped Si can be attributed to the thickness and doping level variation across a wafer. Note that current analysis includes the thickness and doping information from only one site of a wafer. Above all, despite the small sensitivity to c_{33} of ScAlN, our fabricated resonators produced strong resonance characteristics which allowed our proposed method to accurately extract the c_{11} of heavily doped Si. It is worth noting that although Si has been used as a well-studied material to validate our extraction method, this method can be extended to the extraction of material parameters for other elastic layers embedded in a piezoelectric stack.

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