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Stress Fields Distribution and Simulation in 3C-SiC Resonators

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Abstract. In this paper the stress field distribution in 3C-SiC (111) resonators has been studied by micro-Raman measurements and COMSOL simulations. The measurements show that the asymmetry of the anchor points configuration produce an asymmetry in the stress filed distribution. This behavior has been confirmed also by the simulations. Furthermore, from the simulations the importance of the reduction of the under etching of the anchor points of the resonators has also been observed. In fact the reduction of this under etch produces a decrease of the stress in the double clamped beams, a small reduction of the resonance frequency, and a large reduction of the Q-factor and then of the oscillation frequency stability of the resonators in closed-loop operation.

Introduction

The cubic silicon carbide (3C-SiC) layers on silicon (or silicon-based) substrates are considered interesting materials for sensors and micro- and nano-electromechanical systems (MEMS and NEMS). The problem of stress control within the 3C-SiC film is crucial for both families of applications. Even though the micromachining techniques for silicon (Si) are well developed, Si-MEMS are not suitable for use in harsh environments (high temperature, high frequency, high wear, and corrosive environment). In extreme conditions, SiC appears to be a good candidate to replace Si due to its exceptional physical and chemical properties [1]. Furthermore, the high Young's modulus and the relatively low mass density induce a significantly higher resonant frequencies and quality factors in resonant devices at the same geometrical dimensions in comparison with Si or gallium nitride [2-3]. Recent results [4] have put into evidence that the presence of a high tensile stress on the 3C-SiC is crucial to obtain ultra-high Q-factor resonators on 3C-SiC/Si MEMS. Therefore, it becomes essential to be aware of the stress and its distribution within the material. The mean stress/strain in 3C-SiC/Si system and wafer deformation measurements were achieved by strain gauge approach [5] and X-ray diffraction (XRD) determination of quality and lattice parameters [6-7]. In this context, also Raman spectroscopy showed a great ability to characterize the residual stress of MEMS [8]. The present work is focalized on the study of the distribution of the stress fields within the epitaxial layer of a set of free-standing doubly clamped structures realized on 3C-SiC (111). In particular, micro-Raman measurements give a confirmation of the average stress obtained by microbalance measurements and show also that most of the stress is concentrated in the anchor points. The COMSOL simulations confirmed the experimental behavior and also gave the opportunity to understand the effect of the under etching that has been observed in our structures on several important parameters as the stress field along the beams and the anchor points, the resonance frequency and the Q-factor.

Experiment and Simulations

The 3C-SiC thin film was deposited in a previously described horizontal, low pressure, resistively heated hot wall chemical vapor deposition (CVD) system with a rotating sample holder [9]. Hetero-epitaxial 3C-SiC growth on Si substrates was achieved using a classical two-step process with a purified hydrogen (H_2)/argon (Ar) mix as carrier gas, and silane (SiH_4) and propane (C_3H_8) as Si- and C-precursors. Micro-Raman maps were acquired at room temperature using an HR800 spectrometer integrated system Horiba Jobin Yvon (Horiba, Lille, France) in a backscattering configuration. The excitation wavelength was supplied by a 325 nm He-Cd continuous-wave laser that was focalized on the sample by a 40 objective, with numerical aperture (NA) of 0.5. The scattered light was dispersed by an 1800 grooves/mm kinematic grating.

Simulations have been performed by COMSOL Multi-physics software [10]. Different parameters like beam displacement and stress over the beam have been calculated by finite element method after having defining the geometry, the material of the cantilever model (fixed at both ends) and his operational space. This work considered a calculating method for natural frequency in comparison with experimentally measured oscillation frequencies, Q-factor of micromechanical sensor; the numerical methods for solving the equation of resonance oscillation are considered for calculating the natural oscillation frequencies.

Results and Discussion

The process illustrated in Fig. 1(a) was adopted to realize surface micro-machined structures on SOI substrates with 10 µm SOL and 0.5 µm BOX. For more details see ref. [5]. For beams 11-15 three Raman maps were acquired: a single map on the left (which includes all five beams), a map in the middle (one for each bridge) and one at the right (one for each bridge), as illustrated in Fig. 1(b). Raman maps acquired in the central regions of the single beams prove a tensile stress of about 1.1 GPa, for all beams.

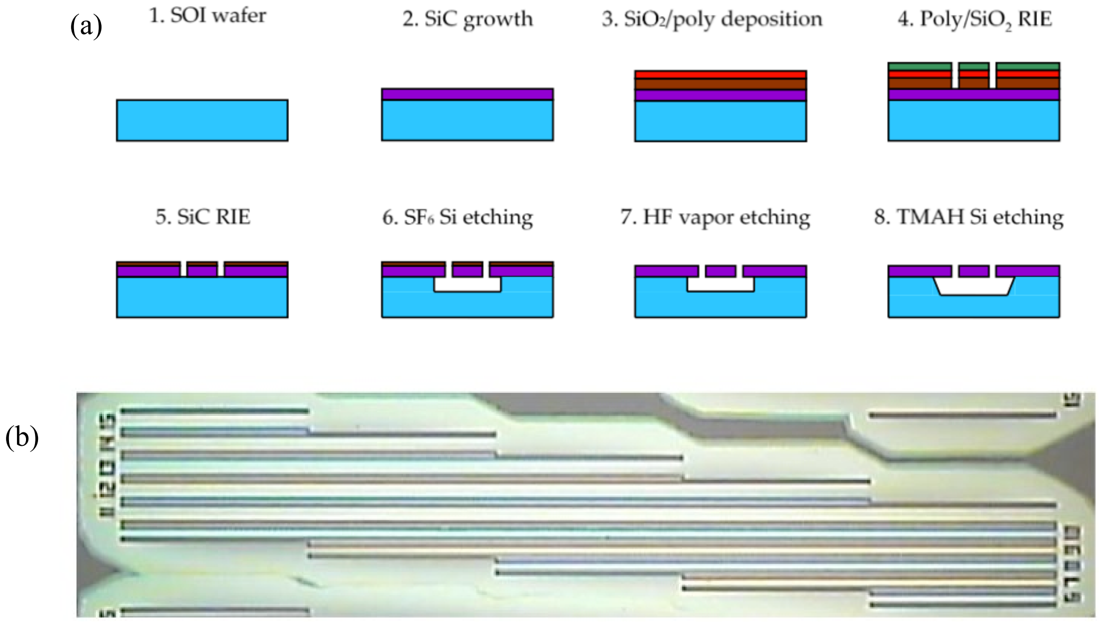

Fig. 1. (a) Scheme of the process used for the realization of the microstructures; (b) Optical image of the doubly clamped beams.

About the Raman maps acquired on the left and at the right of the beams, different trends were obtained depending on the position and on the length of the beams. As an example, Fig. 2(a) shows the shift of the Raman spectrum (TO-peaks) acquired above the beam (red spectrum), in the left achor point (black spectrum) and in the right anchor point (blue spectrum). Applying the equation proposed by Olego et al. [11-12], which links the shift of Raman phonon modes to stress relaxation within a

3C-SiC epitaxial layer, we obtained a particular trend of the stress. The stress always appears tensile, and, in the left anchor point it is about 1.6 GPa, in the beam is about 1.1 GPa, while in the in the right anchor point region is about 1.2 GPa.

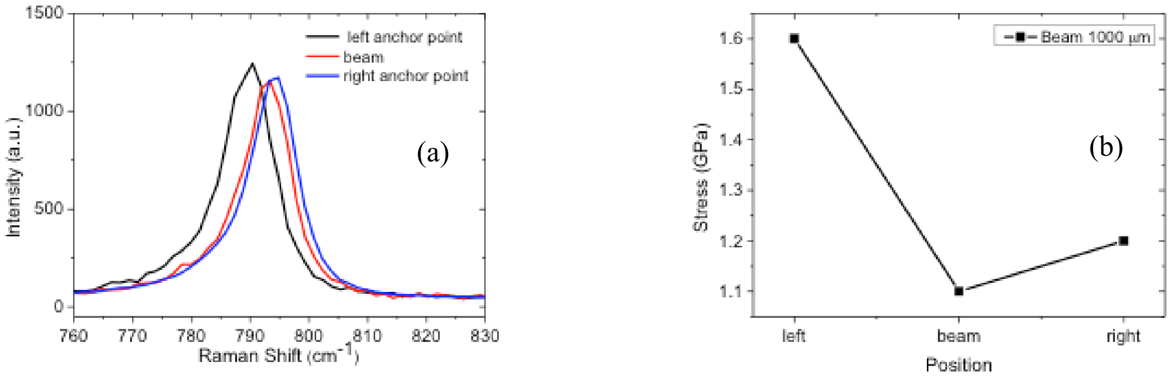

Fig. 2. (a) By μ-Raman measurements it is possible to observe the asymmetry of the anchor points due to the used design. (b) Stress at the anchor points and on the beam.

From these data it is also possible to observe that the different configuration between the different anchor points in the left region and in the right region of the beams produce different values of stress. This behavior can be observed also with the simulations with COMSOL where we can observe that the asymmetry of the configuration of the anchor points produces a large difference in the stress values as reported in Fig. 3.

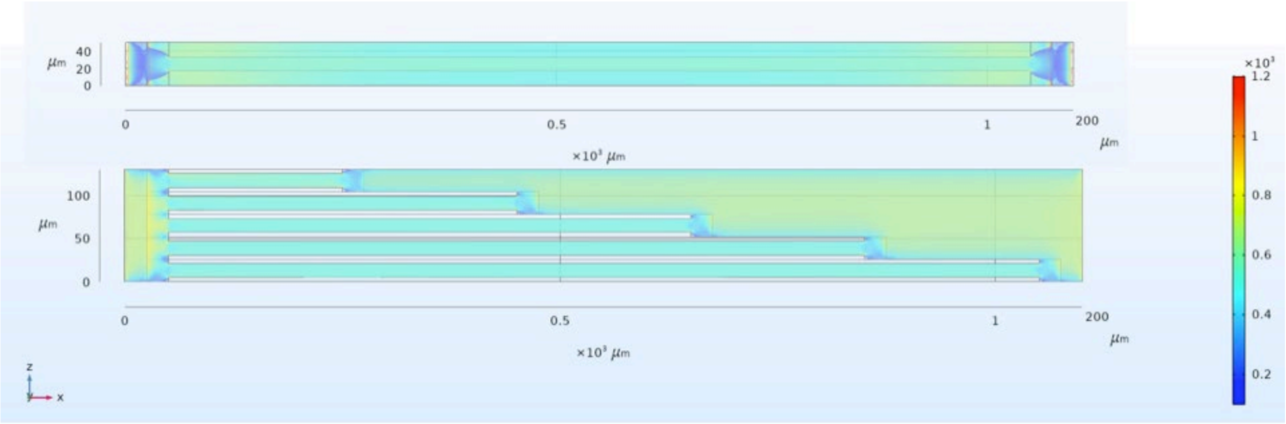

Fig. 3. Simulation of the stress profile of the double clamped beams.

Instead, along the double clamped beams the stress is almost constant, and no large variation can be observed between the different beam lengths. These values are in agreement with the mean stress value obtained by averaging all the values extracted from the Raman maps in the beam position and with the values obtained by microbalance.

Through the numerical simulation of these structures, it has been possible to understand the effect of the undercut of the anchor points. In fact, with the actual process, the release of the beams has been obtained by an isotropic etching that produces at the same time also the under etching of the anchor points. This feature produce, according to our simulations, both a considerable effect on the stress profile and on the resonance frequency and the Q-factor as reported in Fig. 4.

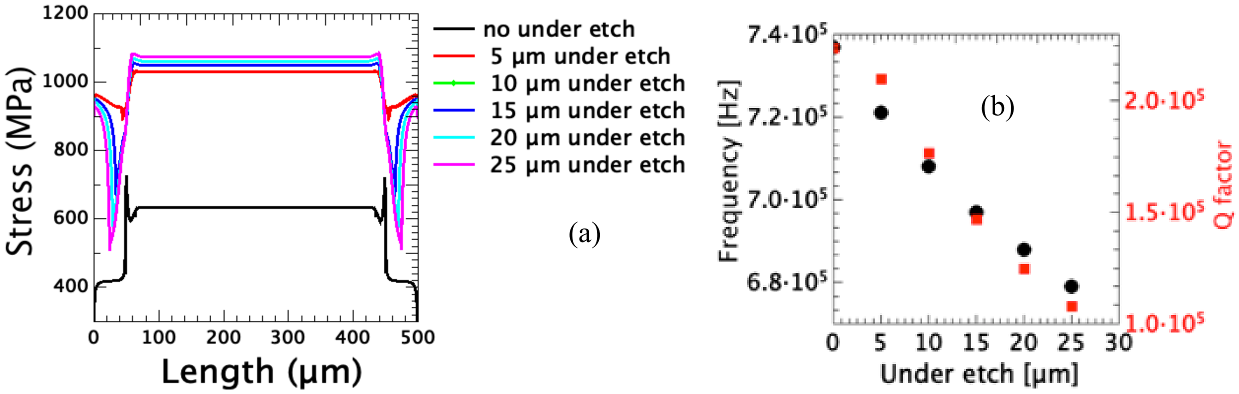

Fig. 4. (a) Stress profile along the beam with different under etch dimension from 0 to 25 microns. (b) Resonance frequency and Q-factor vs. the under etch region dimension.

In fact, Fig. 4(a) shows that the amount of the under etching has a large influence on the stress profile and that with only 5 microns of under etching the stress in the beam increases from about 600 MPa to more than 1 GPa. A further increase of the under etching produces only a marginal increase of the stress. The presence of the under etch has also a large influence on the resonance frequency and on the Q-factor value as reported in Fig. 4(b). Increasing the under etching from 0 to 25 µm we observe a reduction of 8% of the resonance frequency and of 52% of the Q-factor. Then according to our simulations, it is extremely important try to reduce as much as possible the under etching of the anchor points that is observed in our structures.

Summary

In this paper we have studied the stress profile in double clamped 3C-SiC beams by Raman spectroscopy. We have observed in our structure an asymmetry of the stress profile that is due to the asymmetry of the anchor points structures and this behavior can be observed also by COMSOL simulations. Finally, the simulations have pointed out the large effect of the under etching that we have in our structures on the stress profile, the resonance frequency and essentially the Q-factor.

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