# Analysis of Raman Spectra from Offset Spacer Region of Si-MOSFET Structure using Simulated Stress Tensor and Absorbed Light Intensity by FDTD Simulation

<sup>1</sup>Akira Satoh, <sup>1</sup>Tetsuya Tada, <sup>1</sup>Vladimir Poborchii, <sup>1</sup>Toshihiko Kanayama, <sup>2</sup>Shigeo Satoh, and <sup>1</sup>Hiroshi Arimoto <sup>1</sup>Nanoelectronics Research Institute

National Institute of Advanced Industrial Science and Technologies,

1-1-1 Higashi, Tsukuba, Ibaraki 305-8562, Japan

Phone: +81-29-849-1216 E-mail: ak-satoh@aist.go.jp

<sup>2</sup>Fujitsu Semiconductor Ltd., 50 Fuchigami, Akiruno, Tokyo 197-0033, Japan

## 1. Introduction

The variation of carrier mobility strongly depends on the strain distribution in the channel region of Si MOSFETs. However, it is impossible to make the nondestructive stress measurements in the channel region because this region is always hidden behind the gate electrode. Therefore, a precise stress simulation is indispensable for understanding the actual amount of stress in the channel region. We previously reported that a Raman shift predicted by three-dimensional stress simulation agreed with the measured Raman shift in the offset spacer region of a Si MOSFET [1]. Only the Raman signal from the restrictive offset spacer regions can be measured because the structure is covered with metallic silicide on the poly-silicon gate and source/drain region except for in the offset spacer region. We have determined the Raman shift in the offset spacer region by using the average values of stress tensor and light intensity, although they are not uniform. In this paper, we describe analysis of the Raman spectrum from the offset spacer region of a Si-MOSFET structure based on the simulated stress tensor and absorbed light intensity from a finite difference time domain (FDTD) simulation.

### 2. Experimental

We used a conventional three-dimensional TCAD simulator (Synopsys SENTAURUS) for the stress and FDTD simulation. Figure 1 schematically illustrates the top down UV Raman spectroscopy measurement [2, 3] of the Si-MOSFET structure. The offset spacer is transparent to the 364-nm-wavelength excitation. When the excitation polarization is set perpendicular to the gate structure (x-polarization), the excitation would efficiently reach the silicon beneath the offset spacer, although its width is 20



Fig. 1 Top down UV Raman measurement of Si-MOSFET structure.

nm, which is narrower than the wavelength of the excitation; this is in contrast to a case of polarization that is parallel to the gate structure (y-polarization) [4]. We carried out the FDTD simulation of the absorbed light intensity distribution on the silicon beneath the offset spacer to confirm this polarization effect using the same boundary used in the stress simulation. The structure was immersed into a medium with n=1.5 and k=0 as an immersion oil used in the Raman measurement. A plane wave light source (0.1 µm square) was placed 0.1 µm



Fig. 2. Light intensity distribution at 0.07  $\mu m$  above the top of the stress liner.



Fig. 3. 2D distribution of the light intensity calculated with the FDTD simulations for the light sources of (a) x-polarization and (b) y-polarization.

directly above the top of the contact etch stop layer (CESL). The resultant light intensity distribution at 0.07  $\mu$ m above the stress liner is similar to the actual excitation beam as shown in Fig. 2. Figure 3 shows a cross-sectional distribution of light intensity that was obtained by conducting three-dimensional FDTD simulations with different excitation polarizations. The light intensity for the *x*-polarization is relatively strong near the bottom corner of the gate structure, in contrast to that for the *y*-polarization.

The Raman shifts  $\Delta \omega$  of the optical phonons in the presence of strain are related to the eigenvalues  $\lambda$  of following secular equation [5],

$$\begin{vmatrix} p\varepsilon_{11} + q(\varepsilon_{22} + \varepsilon_{33}) - \lambda & 2r\varepsilon_{12} & 2r\varepsilon_{13} \\ 2r\varepsilon_{21} & p\varepsilon_{22} + q(\varepsilon_{33} + \varepsilon_{11}) - \lambda & 2r\varepsilon_{23} \\ 2r\varepsilon_{31} & 2r\varepsilon_{32} & p\varepsilon_{33} + q(\varepsilon_{11} + \varepsilon_{22}) - \lambda \end{vmatrix} = 0$$
(1)

where  $\lambda = \omega^2 - \omega_0^2$ , from which follows

#### $\Delta \omega = \omega - \omega_0 \approx \lambda / 2\omega_0 \,.$

*p*, *q*, and *r* are the deformation potential constants for crystalline silicon.  $\varepsilon_{ij}$  are the components of the strain tensor  $\varepsilon$ . In irradiation on a (001) surface, only longitudinal optical (LO) phonon is allowed to be excited. Consequently, the measured Raman shift  $\Delta \omega$  corresponds to the calculated Raman shift of  $\Delta \omega_3$ , which is obtained by solving Eq. (1).

#### 3. Results and discussion

Figure 4 (a) and (b) respectively show the simulated stress tensor  $\sigma_{xx}$  and light intensity distributions at the center of the Si-MOSFET structure with W=1.0  $\mu$ m. Figures 5 (a) and (b) show the calculated Raman shift and light intensity distributions of the Si in the offset spacer region, respectively. The Raman shift was obtained by solving the assigned Eq. (1) values of the stress tensors at each position. The Raman shift was uniform along the y direction and decreased monotonically from the gate edge to the boundary of the silicide along the x direction. Though the calculated Raman shift near the boundary of silicide was zero, each stress tensor component was not zero. The light intensity was uniform along the y direction and peaked at around 8 nm form the gate edge along the x direction.

For the top down Raman measurements, the actual Raman spectra involve all information about the distributions of the stress and light intensity in the offset spacer region that is narrower than the excitation beam size.

A Lorenz function with a 2.8-cm<sup>-1</sup> full width half maximum (FWHM) as a response function was assumed for the convolution. The synthesized Raman spectrum was calculated from the convolution using the Raman shift and light intensity distribution as shown in Figs. 5 (a) and (b). The peak position of 522.3 cm<sup>-1</sup> and FWHM of 5.5 cm<sup>-1</sup> of the calculated spectrum agrees well with those of the measured spectrum, as seen in Fig. 6. This result indicates that the top down UV Raman spectroscopy measurement is powerful enough for verifying the accuracy of the stress simulation.

#### 4. Conclusion

We analyzed the Raman spectra in the offset spacer region of a Si-MOSFET structure. The synthesized Raman spectrum was calculated from the convolution using the Raman shift and FDTD-simulated light intensity distribution. The peak position and FWHM of the calculated spectrum agreed well with those of the measured Raman spectra.

#### References

- [1] A. Satoh et al., Ext. Abst. of SSDM2010, pp. 295-296.
- [2] V. Poborchii et al., Appl. Phys. Lett., 89 (2006) 233505.
- [3] V. Poborchii et al., Appl. Phys. Lett., 91 (2007) 241902.
- [4] T. Tada et al., Ext. Abst. of SSDM2009, pp. 56-57.
- [5] I. De Wolf et al., J. Appl. Phys. 79 (1996) 7148.



Fig. 4. 3D distribution of (a) Stress tensor  $\sigma_{xx}$  and (b) simulated light intensity of Si-MOSFET.



Fig. 5. 2D distribution of (a) Raman shift and(b) simulated light intensity in the offset spacer region.Right side: gate edge. Left side: boundary of silicide.



Fig. 6. Comparison of Raman spectra by calculation and measurement.