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Raman Spectroscopic Study for Determining Stress Component in Single Crystal Silicon Microstructure using Multivariate Analysis

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1. Introduction

Stress evaluation in the nano-scale area of the semiconductor devices, such as ULSI, is strongly required recently. Especially, the control of stress/strain in a channel in the transistor and shallow trench isolation structures is becoming very important for high performance devices. Raman spectroscopy is a powerful tool for stress/strain evaluation of single crystal silicon (SCS), but it is difficult to apply to nano-scale area because its spatial resolution is around 1 μ m. Furthermore, Raman spectroscopy has a fundamental limitation on the stress/strain component evaluation. Generally, only the plane surface stress ($\sigma_{xx} + \sigma_{yy}$, or σ_{xx} only) is estimated from the peak shift position of Raman spectrum[1]. In this paper we suggest new Raman spectroscopic stress component evaluation method for single crystal silicon (SCS) micro/nano structure. An in-house tensile tester was employed to apply a uniaxial tensile stress the SCS boss in the gauge section. Raman spectra on the boss were measured under a constant tensile stress. To specify both the component and the magnitude, the analytical calibration curves for stress determination were newly constructed by the multivariate analysis with a partial least-square (PLS) method, which were performed using the stress components, estimated by finite element method analysis (FEA) and Raman spectral parameters, such as peak shift, amplitude, and width (FWHM).

2. Experiments

Figure 1 shows Raman spectroscopic measurement system (HORIBA, Ltd., FR-3000) with a handmade tensile tester [2, 3]. This system has a stage with piezo actuators, so that it is able to achieve a positioning precision of 20nm for the step measurement. The excitation line for Raman measurement was 363.8nm. All spectral parameters were derived by applying the curve fitting procedure with Gauss/Lorentz function.

Fig.2 represents the SCS specimen for tensile test. The specimen has 5x5 bosses with the dimensions of 4 μ m x4 μ m x270nm, fabricated by RIE.

3. Results and Discussions

Figure 3(a) shows typical Raman spectrum of SCS (100). The wavenumber at the peak in zero stress is 520.5cm⁻¹, which gradually shifts to the low side with increasing tensile stress, as shown in Fig.3(b). By the applying tensile stress to specimen, the distance between silicon

atoms increases, thereby binding and vibration energies decrease. Consequently, the peak shift of Raman spectrum shifts toward lower wavenumber. Fig.4 shows the peak shift depending on applied tensile stress. The linear relation is observed.

To specify the stress component, the Raman spectra were measured in a vicinity of SCS bosses at 50nm intervals on the line, as shown in Fig.5, along the tensile direction. Fig.6 depicts the obtained peak shift, amplitude, and width at various tensile stresses. As tensile stress increases, all the parameters on the boss, especially at the edge, change from that on a SCS flat part. This indicates that a nonuniform stress occurs due to the boss. Fig.7 compares the stress distribution calculated by Raman shift at 500MPa with that by FEA. The Raman and FEA stress over the boss and the flat part exhibit a good agreement, whereas those at the edge of the boss are quite different. So, only at the edge, two-curve fittings on Raman spectra, as shown in Fig.8, can be performed. Then, the multivariate analyses with a PLS method using the obtained Raman spectral parameters (Peak shift, Amplitude, Width in one-curve fitting and Peak shifts in two-curve fitting) as explanatory variable and FEA results as response variable conducted. Fig.9 shows the PLS calculation results for σ_{xx} , σ_{yy} , σ_{zz} , and σ_{xz} . The stress distributions calculated from Raman spectral parameters trace well the FEA distribution, especially, for σ_{xx} and σ_{yy} , both distributions became the magnitude very close.

4. Conclusions

We investigated the effectiveness of Raman spectroscopy for determining stress component in SCS microstructure using multivariate analysis with a tensile tester and FEA analysis. The nano-scale stresses distribution obtained from PLS method using measured Raman spectra were in very close agreement with those from FEA. The proposed evaluation method would be of great use for stress evaluation in nano-stress field of not only semiconductor devices but also MEMS.

References

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- [2] T.Namazu, S.Inoue, H.Takemoto, and K.Koterazawa, *IEEJ Trans. on Sens. Micromach.* **125** (2005) 374.
- [3] T. Namazu, S. Inoue, D. Ano, and K. Koterazawa, *Proc. MEMS 2004* (2004) 175.

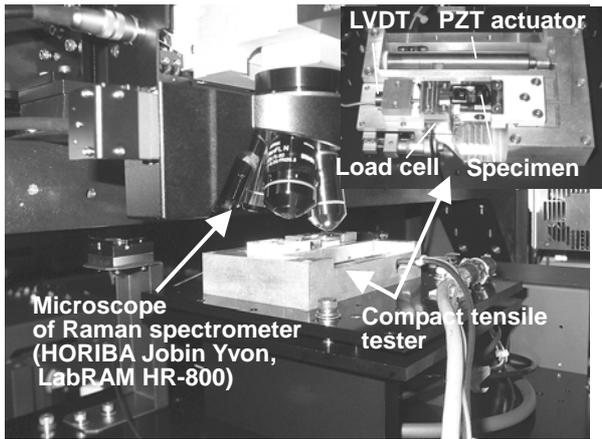


Fig. 1 Photographs of Raman Spectroscopic measurement system (FR-3000) with tensile tester.

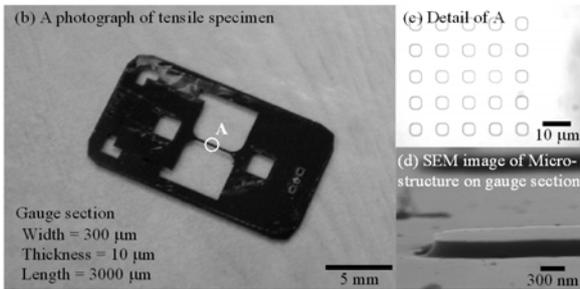


Fig. 2 Photographs of SCS micro specimen.

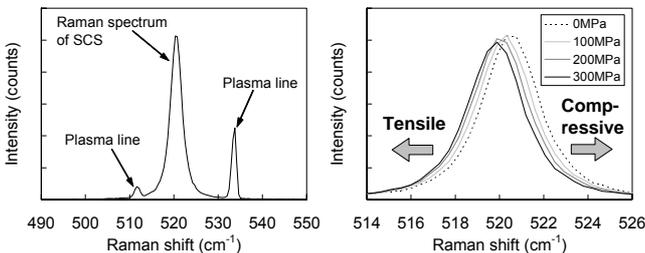


Fig. 3 Typical Raman spectrum of SCS and the shift of spectrum with increasing applied tensile stress.

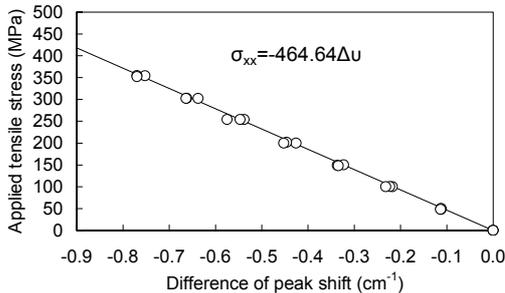


Fig. 4 Relation between the peak shift and applied tensile stress.

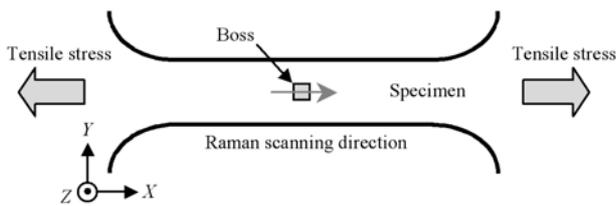


Fig. 5 A schematic of Raman Spectroscopic measurement line on a SCS boss.

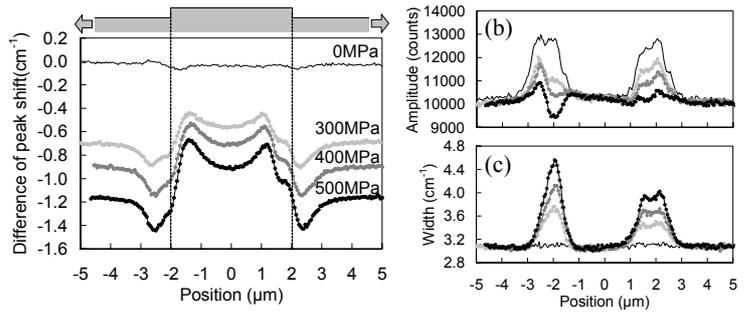


Fig. 6 Peak shift, amplitude, and width at a SCS boss when various tensile stress were applied.

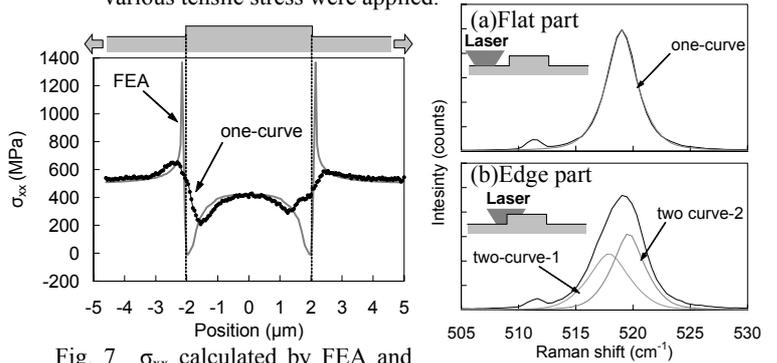


Fig. 7 σ_{xx} calculated by FEA and estimated with one-curve fitting.

Fig. 8 Two curve fitting at the edge.

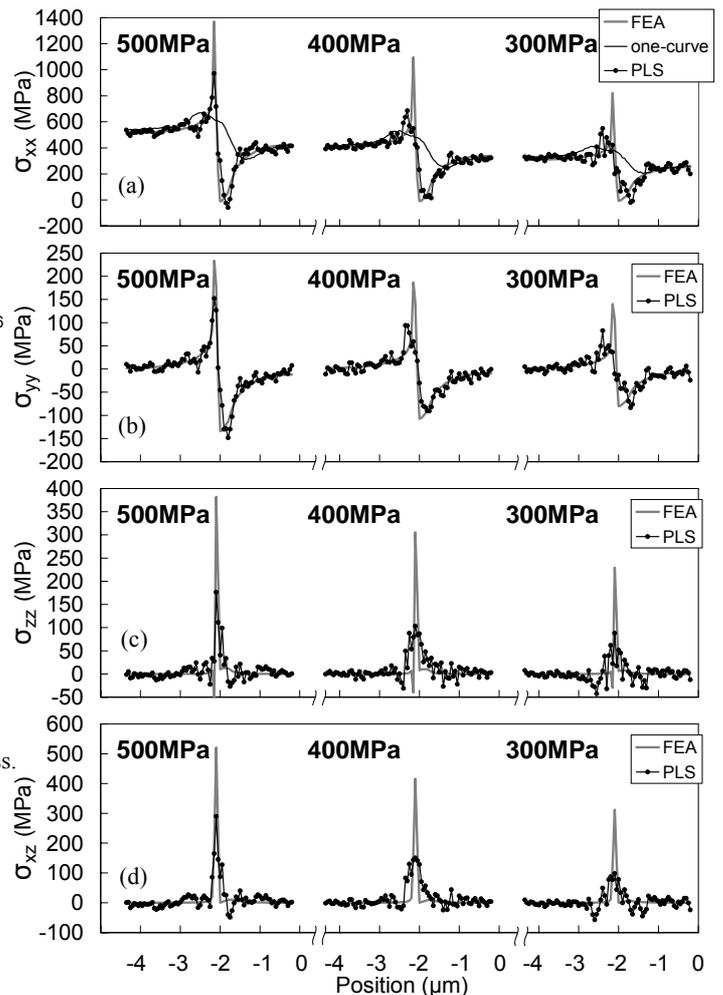


Fig. 9 PLS calculation results of Raman spectra at a SCS boss when the tensile stress of 500, 400, 300MPa applied.