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Structural Characterization of Strained Silicon Substrates by X-Ray Diffraction and Reflectivity

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1. Introduction

The benefits of strained Si for CMOS-based devices, namely increased chip speed and decreased power consumption, can be extended through the use of SiGe-free strained silicon-on-insulator (SSOI) substrates. Yet the development of bulk strained Si and SSOI presents unique materials challenges that must be considered: both contain a large (~1%) amount of strain in the strained Si layer, and in the case of SSOI, when formed by layer transfer, extra tilt and twist are imposed upon the strained Si layer.

Raman spectroscopy is widely used to characterize strained Si films, but it is only sensitive to parallel strain. X-ray diffraction, on the other hand, is capable of measuring both parallel and perpendicular strain, tilt, twist, and thickness. However, due to the small thickness (10–50 nm) of strained Si layers, previous x-ray diffraction studies have resorted to using synchrotron sources due to their extremely brilliant beam intensities.[1] The ability to perform routine characterization of strained Si layers with readily available, commercial x-ray sources is critical for throughput and ease of measurement considerations.

In this study, four different types of substrates were investigated by x-ray diffraction and reflectivity: strained Si layers on (i) ~30% Ge content bulk SiGe virtual substrates and (ii) SiGe-free SSOI substrates,[2] and, for comparison, bulk SOI substrates formed by (iii) wafer bonding and (iv) separation by the implantation of oxygen (SIMOX). The substrates were characterized for strain, tilt, twist, and thickness; the strain measurements were correlated with Raman spectroscopy.

2. Experimental Set-Up

All measurements were performed on a Philips X'Pert Pro Materials Research Diffractometer with a standard Cu anode x-ray tube source. High-resolution reciprocal space maps were collected with a four-bounce channel cut Ge x-ray monochromator and a three-bounce Ge analyzer crystal. Grazing incidence reflectivity spectra were collected with a narrow slit in place of the analyzer crystal.

3. Results and Discussion

Parallel and Perpendicular Strain

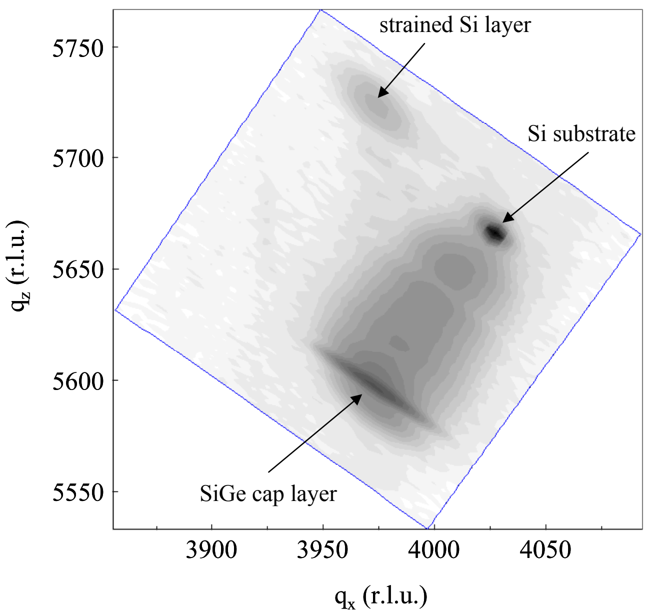

Fig. 1. A {224} reciprocal space map of a bulk strained Si substrate. The Si substrate, SiGe cap layer, and strained Si peaks are all clearly resolved.

The parallel and perpendicular lattice strain are determined independently with asymmetric {224} reciprocal space maps (RSMs). To eliminate the effects of tilt, four {224} RSMs were taken at 90° intervals with respect to the azimuthal rotation of the wafer. Fig. 1 contains an RSM of a bulk strained Si wafer clearly showing the peaks from the Si substrate, SiGe cap layer, and the strained Si layer, as well as intensity from the SiGe relaxed graded buffer layer. Based on the positions of the peaks, the parallel and perpendicular lattice constants of a layer can be determined, which give information on composition and parallel and perpendicular strain.

Table I. The structural parameters of the four types of substrates measured by x-ray diffraction and reflectivity.

Sample	Ge content in original SiGe cap layer (%)	Mismatch of original SiGe cap layer (%)	ε_{xx}, strained Si layer (%)	ε_{zz}, strained Si layer (%)	Tilt of Si layer *wrt* Si substrate (degrees)	Twist of Si layer *wrt* Si substrate (degrees)	Strained Si thickness, reflectivity (Å)	Strained Si thickness, rocking curve (Å)
Bulk Strained Si	32.7	1.26	1.28	-0.99	0.02	—	530	512
SSOI	32.8	1.26	1.27	-0.98	0.22	-0.68	455	—
Bonded SOI	—	—	0.00	0.00	0.12	-0.19	—	—
SIMOX SOI	—	—	0.00	0.00	< 0.01	< 0.01	—	—

The parallel (ε_{xx}) and perpendicular (ε_{zz}) strain for the four types of substrates are given in Table I. Although determined independently, the parallel and perpendicular strain obey the Poisson relationship, $\varepsilon_{zz} = -[\nu/(1-\nu)](\varepsilon_{xx}+\varepsilon_{yy})$, to within a 2% error (assuming $\varepsilon_{xx} = \varepsilon_{yy}$). The parallel strain of both strained Si wafers closely matches the mismatch of the SiGe cap layer—or for the case of SSOI, the SiGe cap layer of the donor wafer—showing that the strained Si layer is fully strained. Also, the parallel strain of the SSOI strained Si nearly matches that of the bulk strained Si, indicating that strain is fully preserved during the layer transfer process (the donor wafer for the SSOI substrate is the same as the bulk strained Si substrate.) Furthermore, no strain is detected in either SOI substrate, as expected.

The parallel strain measured by x-ray diffraction can be directly compared with that measured by Raman spectroscopy. To calculate strain with Raman, one must apply the formula $\varepsilon_{xx} = c\Delta\omega$, where c is a constant and $\Delta\omega$ is the separation of the substrate and layer peaks. Thus the value of the constant is critical to calculating strain. Previously, the value of c was determined to be 0.123.[3]

Fig. 2 graphs the results of ten different SSOI substrates with varying levels of strain; each sample was measured by both x-ray diffraction and Raman. A linear fit of the data reveals a slope of 0.134, thus the value of the constant c is 0.134. This value is believed to be more accurate since it was deduced through a *direct* measurement of strain in the strained Si layer.

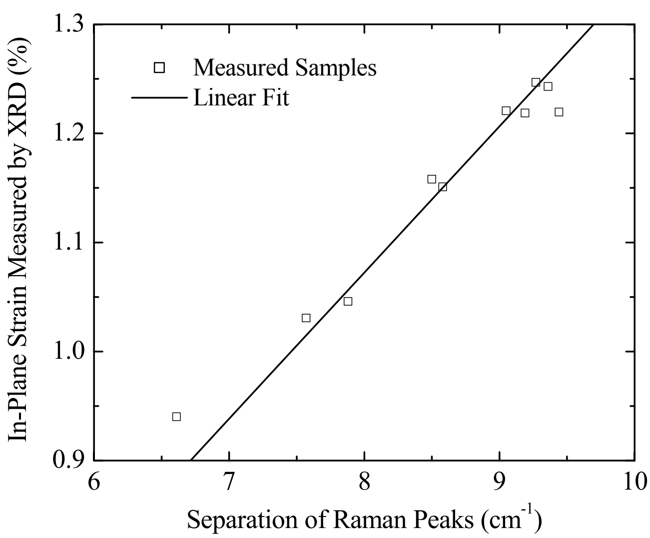

Fig. 2. The comparison of strain measurements by x-ray diffraction (XRD) and Raman spectroscopy.

Tilt

To determine tilt, four {224} RSMs were taken at 90° intervals with respect to the azimuthal rotation of the wafer, as in the case of strain measurement. The expressed tilt changes sinusoidally as the wafer is rotated around the azimuth.[4] The amplitude of the sinusoidal curve gives the absolute tilt. To determine the tilt of the layer with respect to the Si substrate, the sinusoidal curve of the layer is subtracted from that of the substrate, which results in a new sinusoidal curve.

The tilt results are given in Table I. Both bonded substrates have appreciable tilt, since the tilts of the two original wafers are random to one another, while the bulk strained Si and SIMOX SOI substrates have negligible tilt, since the layer and substrate in each are formed from the identical crystal lattice.

Twist

Twist is the rotational offset of the whole crystal lattice with respect to the wafer flat. It was determined by finding the angles of azimuthal rotation where the maximum intensity of the substrate and layer occurs. The {224} asymmetric geometry was used since the diffracted intensity varies strongly with rotation, whereas it is independent of rotation in a symmetric geometry.

The twist results are presented in Table I. Just as the case with tilt, the twist is non-zero for the bonded substrates since the original substrates have random twists to one another. The twist of the SIMOX SOI substrate is negligible, as anticipated.

Thickness

Layer thickness can be measured by using rocking curves or grazing incidence reflectivity.[5] Reflectivity is preferred since it is much more sensitive to thin layers, which allows for more rapid measurements. The bulk strained Si substrate was measured by both techniques, and a difference of ~3% is seen between the two. The value obtained by reflectivity is believed to be more accurate since the reflectivity fringe peaks are much stronger than those observed with the rocking curve. Also, the thickness of the SSOI strained Si is ~75 Å lower than that of the bulk strained Si, indicating that some of the strained Si was removed during the SiGe removal process.

4. Conclusions

Bulk strained Si and SSOI substrates have been characterized by x-ray diffraction and reflectivity for parallel and perpendicular strain, tilt, twist, and thickness. A direct comparison was established between strain measurements made by x-ray diffraction and Raman spectroscopy. The results of this study show that an x-ray diffractometer with a commercial source is fully capable of determining the complete structural parameters of strained Si substrates, which makes its use in a production environment feasible.

References

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