Nonlinear optical characterization of the surface of silicon wafers: In-situ detection of external stress

J. Reif\textsuperscript{a,}\textsuperscript{*}, R. Schmid\textsuperscript{b}, Th Schneider\textsuperscript{a}, D. Wolframm\textsuperscript{a}

\textsuperscript{a}Lehrstuhl Experimentalphysik II, Brandenburgische Technische Universität Cottbus, D-03044, Cottbus, Germany

\textsuperscript{b}Lehrstuhl Physikalische Chemie und Analytik, Brandenburgische Technische Universität Cottbus, D-03044, Cottbus, Germany

Abstract

The potential of nonlinear optical techniques for a rapid on-line and non-destructive inspection and characterization of silicon wafers is discussed. As an example, the in-situ detection of external stress on the wafer is reported, resulting from specific mounting conditions. As an outlook, the problem of radially non-uniform growth of the silicon crystal when utilizing the Czochralski-growth method is addressed. A simple technique is proposed to discriminate those sections of the wafer which are ready for use in further applications from those which are not useable for proper device fabrication, thus enabling the selection of appropriate material from as-grown crystals.

Keywords: Optical characterization of semiconductor surface; Nonlinear optics at surfaces; In-situ detection of external stress; Czochralski-grown silicon

1. Introduction

As a consequence of ever-increasing integration of semiconductor devices, an increase at the same pace is observed of the requirements of quality of the substrate wafer, the gate oxide layers, and the metallic contacts. Most desirable are methods for preselecting appropriate substrates as well as on-line growth-monitoring and non-destructive characterization of subsequent layers. This is a genuine field for optical techniques, which are per se non-destructive and in-situ-applicable wherever light has access.

A typical problem, encountered in this context, is the observation that Czochralski-grown silicon wafers are not uniform across their diameter [1]. This shows up, in particular, by the quality of gate oxide grown on this type of wafers. Two concentric regions are found with markedly different breakdown stability of the oxide. These regions, the width of which depends on the growth speed, are separated by a small ring, several millimeters wide, where practically no useable oxide can be grown at all (for more details see Refs. in [1]). Up to the present, several methods have been developed [1,2] to analyze this situation, all of which lack, however, the problem that the analyzed wafer is no longer usable for device fabrication.

An accepted explanation for the different oxidation behavior of the three zones postulates different composition during growth [1]. According to this picture, the inner zone consists of vacancy-rich silicon crystal, the outer one is oversaturated interstitial-rich. In the separ-
ating ring, no long-range regular crystalline structure is developed, as can be seen from the fact that additional oxidation reveals an agglomeration of stacking faults (cf Fig. 1). Bearing this in mind, it appears promising to devise a spatially resolved check of crystal symmetry to probe the wafer quality or, at least, to determine the position of the separating ring.

Unfortunately, conventional tests of crystal symmetry such as X-ray diffraction, are not very well adapted to rapid in-situ control of larger wafers. On the other hand, there are only very few cases where conventional optics yields information about crystal symmetry properties, such as dichroism or birefringence. The reason for this lack of sensitivity lies in the fact that in most cases the optical susceptibility (i.e., in principle, the dielectric constant) is only a scalar, relating input and output optical fields linearly to each other.

In nonlinear optics, however, such as second harmonic generation (SHG), the output optical field is the result of more than one input field. Consequently, the nonlinear susceptibility \( \chi^{NL} \) is highly symmetry sensitive, since it has tensor character, as is shown in Eq. (1):

\[
E_{o}^{out} = \chi^{NL}_{ijkl}(\omega_1, \omega_2)E_{i}^{in}(\omega_1)E_{j}^{in}(\omega_2)
\]

Unfortunately, this second-order susceptibility vanishes under inversion symmetry. At the surface of a cubic crystal, however, this symmetry is broken, and the nonlinear optical process becomes allowed. This matches well with the fact that, for visible light, we can only use reflection signals, anyway, and it may yield, in an easy way, the required information on the crystal symmetry [4,5].

In the present contribution, we demonstrate the sensitivity of surface SHG by detecting reversible stress in the sample, exerted by the mounting procedure. This enables a reliable in-situ and on-line control before further processing. At the end, we propose a simple technique, based on surface SHG, to discriminate the various growth zones in the silicon wafer.

2. Experimental

In our experiment, we want to apply the SHG technique to check an as-grown six-inch silicon wafer. It is well known [6], that the reflected SH-intensity strongly depends on the azimuthal orientation of the surface with respect to the light polarizations. So, Tom et al. [6] found a four-fold symmetry for the silicon (100) surface when they rotated their sample about the surface normal, relative to the light polarizations. Usually, this effect should only be observable, if the polarization of one of the three \( E \)-fields involved has a component perpendicular to the surface, because otherwise (all \( E \)-fields oscillating in the surface plane) the problem would, again, be of full inversion symmetry. If, however, unidirectional external stress is deforming the bonds between the surface atoms, this inversion symmetry is broken: surface SHG under pure \( s \)-polarization should become observable, exhibiting the direction of this external stress. Consequently, we first investigated the azimuthal dependence of surface SHG under this condition. The experimental set-up is shown schematically in Fig. 2.

In order not to charge the sample thermally, we use a femtosecond Titanium:Sapphire laser (800 nm, 100 fs, 1 mJ/pulse, 1 kHz) as the source for our experiments. The \( s \) - or \( p \)-polarized output is reflected from the wafer surface, and we detect the dependence of the reflected \( s \)-polarized second harmonic on the azimuthal orientation of the sample which may be rotated about its normal.

A typical result is shown in Fig. 3. For both input

![Fig. 1. Carrier recombination lifetime [3], revealing the three sectors in a wafer of Czochralski-grown silicon.](image1)

![Fig. 2. Experimental set-up: the \( s \)-polarized output of a femtosecond laser is directed under 45° to the surface of a silicon (100) wafer. The \( s \)-polarized reflected second harmonic light is detected by a photomultiplier. To obtain the SHG azimuthal dependence, the sample is rotated about its normal.](image2)
Fig. 3. Polar plot of the azimuthal dependence of second harmonic generation of a silicon wafer in (100) orientation: (a) $s$-polarized fundamental; (b) $p$-polarized fundamental.
polarizations, we observe a strong \( m \)-symmetry along the (in our plot) 30–210° axis, overlaid to the fourfold symmetry corresponding to the (100) surface. (The rotation with respect to each other of the two patterns in panels (a) and (b) is due to the different input polarizations.) We attribute this additional symmetry component to unidirectional stress, deforming the bonds in the sample and thus the nonlinear polarizability in the same direction. Assuming that the nonlinear response is largest when the electrons are forced to oscillate along the (011) surface diagonals, the result of panel (a) confirms this picture, with the mirror plane being along one (001) direction. In this configuration, the maxima of panel (b) correspond to the situation where the exciting field oscillates along the (001) direction and the second harmonic along (010).

In principle, it is not obvious that the observation of Fig. 3 is the result of external crystal deformation. A similar result would be obtained in the case of a vicinal cut of the wafer. That we, however, observe indeed the influence of external stress is demonstrated in Fig. 4; a new, slightly different mounting of our wafer leads to a different direction of the stress or strain, resulting in a completely different deformation of the azimuthal pattern.

3. Proposed scheme for the in-situ detection of growth zones

As can be seen directly from the results described above, for a given orientation of the sample with respect to the beam geometry, the expected second harmonic signal is different whether \( p \)-polarized light or \( s \)-polarized light is used as the fundamental [cf. direction 30–210° in Fig. 3(a) and (b)]. Consequently, a change in the ratio of \( p \)- to \( s \)-polarized excitation is the signature of a change in symmetry which is expected for the transitions between the three growth zones in Fig. 1.

This is the basis for our proposed experimental set-up, as shown in Fig. 5. In this case, the output of our laser is split into two beams, one of which is delayed and rotated in polarization, before both beams are recombined at the sample. The reflected second harmonic light is polarization-analyzed and then detected. The temporally separated signals from both exciting beams are further processed, to obtain their ratio. The sample may be scanned by translation along its diameter.

4. Conclusion

By monitoring the effect of external stress, we have demonstrated the potential of surface second harmonic generation to probe in-situ the symmetry of as grown silicon wafers. We propose to exploit this technique for the non-destructive analysis and control of wafer quality before and during the growth of gate oxide layers.
Acknowledgements

We thank H. Richter, IHP Frankfurt/Oder, for bringing this subject to our attention and for providing us with the sample wafer.

References


