Strain Modulations in Si Underneath Patterned Oxide Stripes

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We present a characterization method for lateral strain modulations in Si substrates underneath laterally patterned periodic SiO_2 stripes. For the investigations, the x-ray grazing incidence diffraction (GID) technique was applied to enhance the sensitivity to the interface near regions. Apart from a tensilely strained part below the oxide lines, we find two compressively strained regions close to the edges of the stripes. Furthermore, the experimental GID results clearly show the depth dependent in-plane strain distribution. These data are relevant for electronic transport, particularly in short channel structures.

1. Introduction

With the continuing miniaturization of electronic device structures, inhomogeneous strain distributions of various origins become more and more important for the electronic transport. Consequently, information on these surface-near strain distributions in nanostructures has to be obtained with sufficiently high resolution. Among the x-ray diffraction techniques, grazing incidence diffraction (GID) is particularly well suited for such investigations. Several groups [1] – [3] have employed this technique for the study of heterostructures and of buried nanostructures. However, the quantitative analysis of GID data requires the use of either the fully dynamical diffraction theory, which is barely treatable, or as an simpler approach, the distorted wave Born approximation (DWBA) [4] – [5]. As a suitable model system we have chosen a laterally periodic SiO_2 layer on a Si substrate, for the following reasons: (i) Silicon dioxide is widely used for the fabrication of high-density semiconductor integrated circuit devices. In particular, with their shrinking dimensions, the structure and the quality of the interface between the oxide and the Si substrate are crucial for the performance and reliability of the devices. Additionally, the evolution of internal stresses during the conversion of Si into SiO_2 becomes more and more important in these miniaturized structures. These stresses mainly originate from the thermal expansion mismatch created by the oxidation process. (ii) Due to the amorphous nature of the oxide, the scattered intensity distribution in an x-ray diffraction experiment results only from the strain distribution in the single crystalline Si substrate. This clear-cut situation allows to include not only transmission and specular reflection into the undisturbed wave fields in the DWBA-simulations, as it was done previously [2], but also diffraction. Coplanar high angle diffraction technique yields only information on the average strain in the Si substrate, whereas GID provides a depth sensitivity due to incidence and exit angles close to the critical angle of total external reflection [6].

2. Experiment

We started from a Si (001) wafer with a 100 nm thermal SiO_2. In order to estimate the value of the effective linear mismatch $\chi = (\langle a \rangle_{SiO2} - a_{Si})/a_{Si}$ the curvature of the sample was measured using x-ray diffraction in transmission geometry. $\langle a \rangle_{SiO2}$ is the mean distance of the Si atoms in the amorphous SiO_2, and a_{Si} the bulk lattice parameter of silicon. From the curvature we obtain a range of $3.4\times10^{-3} \leq \chi \leq 5.7\times10^{-3}$. The error of the curvature measurements is quite large and does not allow for an accurate determination of χ. After the curvature measurement, the oxide was structured into laterally periodic stripes by holographic lithography and an etching step. The stripes were oriented along the [-110] direction and had a period of about 800 nm. The height of the stripes, examined by atomic force microscopy, was about 100 nm, and the width of the stripes was 350 nm.

Quantitative strain calculations based on the finite element method were performed to obtain the strain distribution in the Si substrate. Since the effective mismatch χ depends sensitively on the particular growth parameters and can only be determined with some uncertainty from the curvature measurements, we use it as a fit parameter. We finally obtained the best correspondence with the x-ray measurements using a value of $\chi = 4.3\times10^{-3}$. Figure 1 shows the resulting contour plots for different components of the strain tensor $\boldsymbol{\varepsilon}$. Directly underneath the SiO_2, a tensile force is exerted in the Si substrate which leads to a larger in-plane lattice constant compared to unstrained bulk Si. In between the SiO_2 stripes the Si in-plane lattice constant becomes smaller than that of unstrained bulk Si, corresponding to a compressed strain state.

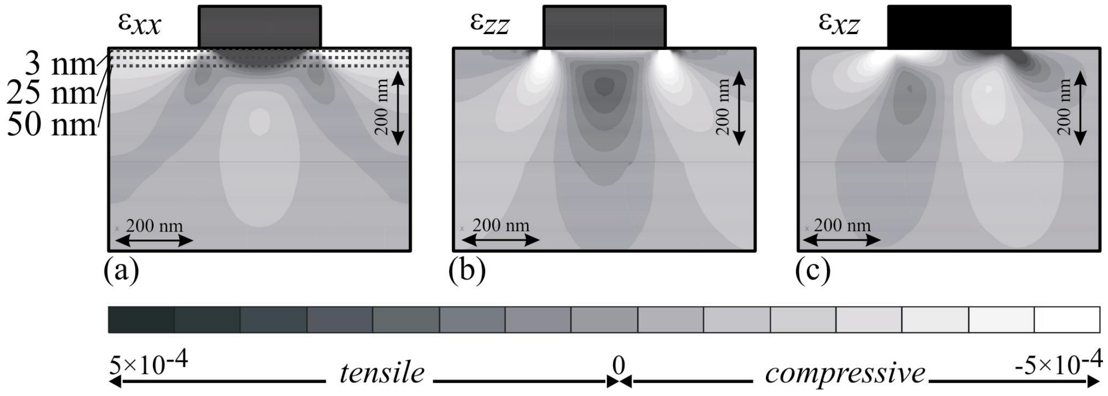

Fig. 1: Contour plots of the strain components (a) ε_{xx}, (b) ε_{zz} and (c) ε_{xz} based on finite element calculations for SiO_2 shadow mask and Si substrate.

Additionally, a compressively strained region appears in a larger depth > 100 nm below the center of the SiO_2 stripes. In the coplanar x-ray diffraction experiments, the whole region contributes to the detected signal, impeding a distinction between regions near and far from the Si–SiO_2 interface. In Fig. 2, ε_{xx} values for different depths in the Si substrate are shown, as indicated in Fig. 1(a).

For obtaining experimental information on such strain gradients in the Si substrate, GID experiments have been performed. In GID, the scattering plane is nearly parallel to the sample surface. If the angles of incidence α_i and exit α_f are close to the critical angle of the total external reflection α_c, the penetration depth of the x-ray beam depends very sensitively on α_i and α_f. It changes typically from 5 nm for $\alpha_i < \alpha_c$ to several µm for $\alpha_i > \alpha_c$. Moreover, it is possible to choose the diffraction vector **h** either parallel (2-20) or perpendicular (220) to the stripes. In the first case the diffracted intensity depends only on the shape of the stripes.

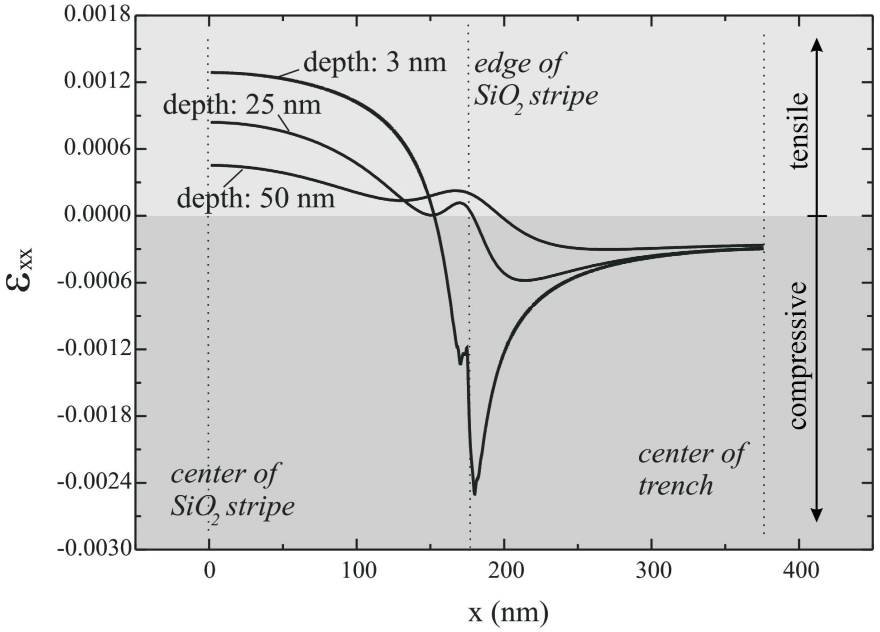

Fig. 2: Dependence of the strain tensor component ε_{xx} on lateral position in Si for three different depths below the interface.

In our case, the stripes are amorphous and thus in this geometry only a central peak at the position determined by the bulk Si lattice constant and no lateral peaks appear. This fact proves that the etching indeed stopped at the Si/SiO$_2$ interface and the Si substrate remains unpatterned.

In the second case, with the diffraction vector (220) perpendicular to the stripes, the intensity distribution depends both on shape and strain. However, in our case only the strain distribution in the crystalline Si accounts for the diffracted intensity distribution, reflecting both compressively ($q_x>0$) and tensilely ($q_x<0$) strained regions. Figure 3(a) shows longitudinal line scans measured around the (220) reciprocal lattice point for several angles α_i, keeping $\alpha_f = 0.20°$. The appearance of the satellite peaks proves the presence of the lateral periodic strain modulation in the Si substrate with a period of 765 nm. The envelope of the intensity distributions exhibits a slight dependence on the incidence angle α_i. For the simulation of the measured data we have to solve the problem of GID from a periodically strained semi-infinite crystal with a flat surface, since the SiO$_2$ stripes act only as stressors and they do not contribute to the diffraction process.

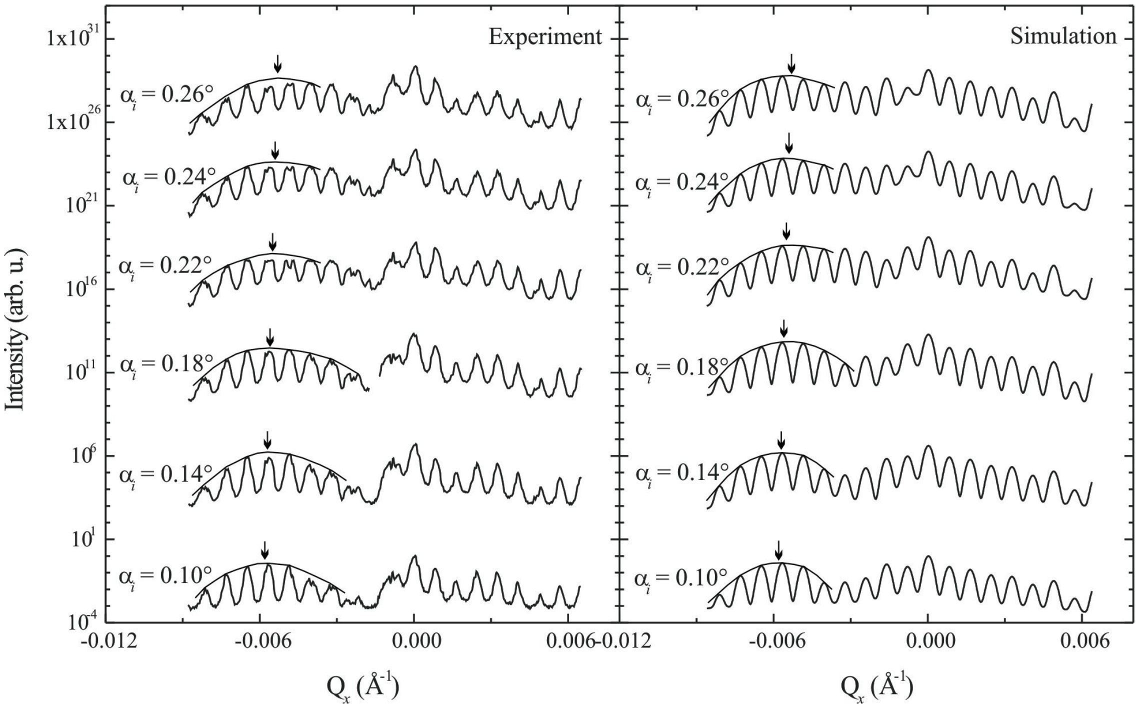

Fig. 3: Longitudinal line scans around the (220) reciprocal lattice point. (a) Experimental data, (b) simulations. For the tensilely strained regions, the envelope curve is indicated.

3. Results and Discussion

We calculated the dependence of the scattered intensity I on q_x using DWBA. A detailed description of the simulation model is given in Ref. [7]. The most significant influence of the effective mismatch χ on the simulations is found for values of $q_x < 0$ corresponding to the tensilely strained Si. Changing χ shifts the envelope curve and the best correspondence was found for $\chi = (4.3\pm0.2)\times10^{-3}$ (see Fig. 3(b)). Furthermore, the experimental data demonstrate clearly the presence of compressively strained regions in Si near the interface to the stripes. While for the tensilely strained regions beneath the stripes the lateral period is the same as for the stripes, two compressively strained regions exist near the surface at each edge of the SiO_2 stripes. Thus the lateral peaks for $q_x > 0$ exhibit an additional modulation. This is qualitatively well reproduced by the simulations.

4. Summary

A periodic array of SiO_2 stripes on the Si surface exerts a periodic stress field on the surface that results in a deformation field periodic in the direction perpendicular to the stripes. We have investigated this deformation field by grazing-incidence x-ray diffraction. The deformation field in the plane perpendicular to the stripes has been calculated by the finite element method. Using this result, the x-ray diffraction patterns were successfully simulated. These simulations have been performed by means of the distorted-wave Born approximation assuming a perfect crystalline substrate as an undisturbed system.

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