Annealing of praseodymia films on Si(111) in UHV

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Rare earth oxides have been studied intensively in the past decades and are of continued interest for industrial applications and scientific research. Apart from their use in electro-optics, sensor technology and catalysis, they have been discussed and investigated in the context of microelectronics, where they are researched as buffer material between the mature Si platform and alternative semiconductors[1, 2, 3, 4].

Pr_2O_3 deposited by MBE on Si(111) substrates crystallizes in hexagonal structure with (0001) orientation [5]. These films can be transformed to cubic Pr_2O_3 by annealing in low pressure oxygen [6] and to cubic PrO_2 by annealing in higher pressure oxygen [7].

Here we report on hexagonal Pr_2O_3 films of 5 nm thickness were grown on clean Si(111) surfaces by MBE with substrate temperatures of 625°C. Afterwards, the samples were annealed in 1 bar oxygen at 700°C in order to further oxidize the films to cubic PrO_2.

These films were analyzed at beamline W1 at HASYLAB using 10 keV synchrotron radiation and the MYTHEN detector. Before measurements, which were all performed at room temperature and under ambient conditions, the films were stored at room temperature. Four out of the five films were also annealed at temperatures ranging from 100 to 300°C in UHV for 30 minutes each.

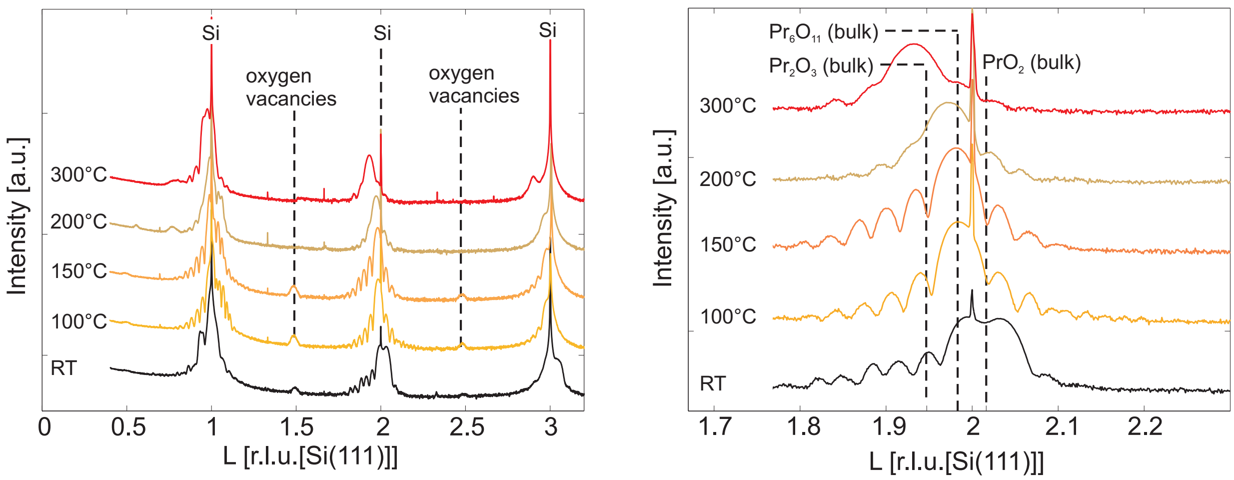

Figure 1: θ-2θ XRD scans of PrO_2 samples annealed at different temperatures at UHV. Even at a temperature of only 100°C, the oxide film is reduced, as can be seen from the shift of the broad praseodymia Bragg peak at $L \approx 2$. At higher temperatures, the film is reduced further.

GIXRD measurements (not shown here) confirm that all investigated samples keep their cubic or pseudocubic structure. The results of XRD θ-2θ scans are shown in Fig. 1. All investigated samples show broad praseodymia Bragg peaks close to the sharp Si substrate peaks at $L = 1, 2$ and 3. Additional peaks at half integer positions occur due to partially ordered oxygen vacancies in the oxide film. These additional peaks become stronger for samples annealed at higher temperatures until 150°C and vanish for samples post deposition annealed at higher temperatures.

Because the Bragg peak at $L = 1$ is difficult to analyze due to the interference between the diffraction signals originating from film and substrate, a more detailed analysis is performed at $L = 2$. The praseodymia peaks tend to consist of two subpeaks originating from laterally coexisting species [8, 9]. These subpeaks move to smaller scattering vectors for samples annealed at higher temperatures, pointing to an increased vertical lattice constant due to more oxygen vacancies in the (pseudo)cubic structures. This means that a *reduction* of the oxide film in UHV already

takes place at rather low temperatures of 100°C. This is remarkable because *oxidation* of hexagonal praseodymia films on Si(111) only takes place at significantly higher temperatures of 200 - 300°C and above [8].
Further experiments to quantify the amount of oxygen in the oxide film are in progress. Because the investigated films are strained, it is essential to determine the Poisson factor of praseodymia films. Also, an in situ study of the phase transitions and interface formations of the films is planned as these are expected to play a major role for the final properties of praseodymia films which act as a buffer material between Si and alternative semiconductors [10]. Here, a new (GI)XRD analysis method, which was developed in the context of the current project [11], will be used.

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