ESRF	**Experiment title: Time and temperature resolved surface x-ray diffraction study of the oxidation of the CoGa(100) surface**	**Experiment number**: SI582
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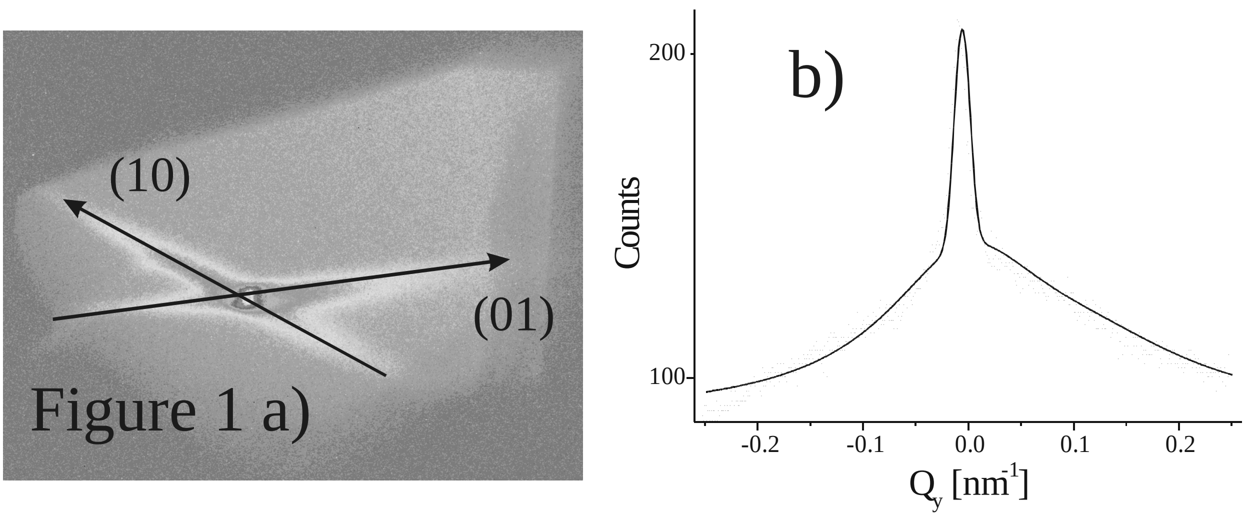
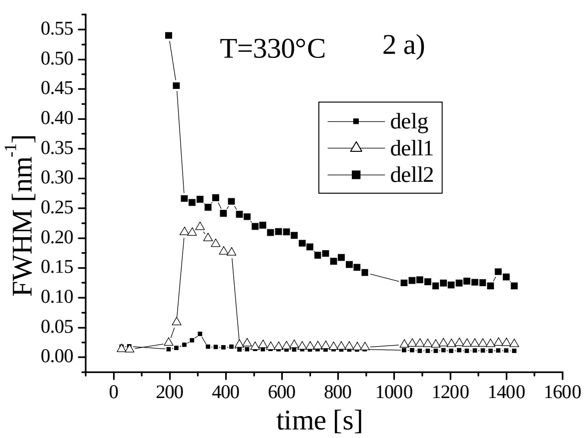
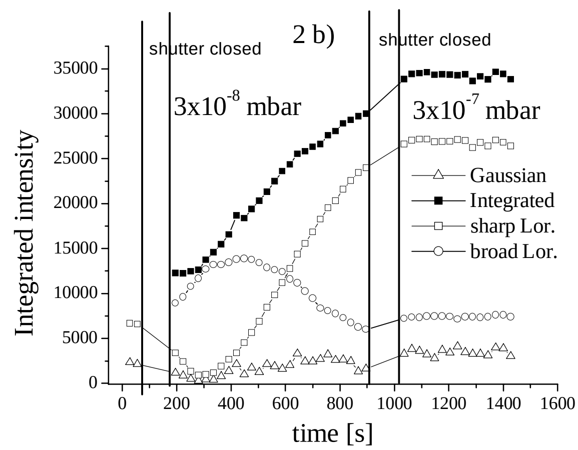
Report:



The goal of our experiment was the temperature and time dependent study of the initial oxidation of CoGa(100) surfaces. In addition, it turned out during the experiment, that also the oxygen partial pressure plays a crucial role. To study in-situ the oxidation reaction we used surface sensitive x-ray diffraction in combination with a 2D detector to image the cross-section of the CoGa crystal truncation rod (CTR) with the Ewald sphere. In contrast to our previous experiments during which we used a Photometrics CCD camera with a readout time of 8 s per image, we employed this time a 2D gas filled wired detector (HISTAR / BROKER) from our home lab. The detector has a sub-second readout time of the 1024 x 1024 channels of the 100 mm diameter image field. The detector was calibrated using an amorphous Ge containing scatterer provided by the ESRF detector group. The drawback of this detector is its lower sensitivity at higher energies, as compared to the CCD camera. For this reason the experiment was performed at 10.25 keV. During the experiment temperature range from room temperature up to 520°C was covered and an oxygen pressure range form $3x10^{-8}$ mbar to $3x10^{-6}$ mbar. In Figure 1 a) a typical image is given taken after oxidation at 330°C at (1,1,1.4), the anti-Bragg condition of the commensurate oxide layer ontop of the CoGa(100) substrate together with the linescan and fits (Figure 1 b)). The lineshape is composed of a sharp component consisting out of one Lorentzian and one Gaussian line. In addition a broad Lorentzian component is included. The double lineshape sharp component is also found on the clean surface; it originates from the stepped surface, representing an infinte staircase. According to diffraction theory from stepped surfaces [1], this infinte staircase gives rise to a Lorentzian broadening of the diffaction peak. The Gaussian component arises from a resolution limited component of large, flat terraces on the surface. In contrast, the broad Lorentzian component originates from the growing oxide islands with a uniform height. For this ideal 2 level system ontop of the flat terraces also a Lorentzian peak broadening is predicted [1]. Its main physical meaing is, that





an exponential terrace length distribution is present.

In Fig 2 the evolution of the FWHM of the different components (a)) and the integrated intensities (b)) are plotted. The total integrated intensity (black squares in Fig. 2 b)) serves as a calibration of the coveridge, since the oxidation stops after the formation of a complete 0.8 nm thick layer. As a consequence, the total integrated intensity saturates also. The FWHM of the broad Lorentzian decreases from 0.5 nm^{-1} at the beginning of the oxidation to 0.15 nm^{-1} at the end. Taking into account the anisotropy of the diffuse scattering one can conclude, that the oxide grows initially in very narrow stripes (only 3 unit cells in width), until it reaches a saturation value of about 11 unit cells, when the surface is completey oxide covered. The increase of the FWHM dell1 of the sharp Lorentzain may be an artefact of the automatic fitting routines that have to be employed for the handling of such data quantities. For the whole data series we obtained recently, a new image analysis program had to be written, which allows automatic linescan handeling and processing. From the analysis of the whole set of data we will get the evolution of all lineshapes as a function of oxidation temperature, time and oxygen pressure, giving the possibility to draw a very detailed scheme of the onset of CoGa oxidation.

[1] P. R. Pukite, C. S. Lent, P. I. Cohen, Surf. Sci. 161, 39 (1985).