ESRF

Experiment title:

The determination of substrate surface structures with x-ray standing waves

Experiment number:

SI 127

Beamline:

ID32-BL13

Date of Experiment:

from: 6. Dec. 95 to: 11. Dec. 95

Date of Report:

17. 6. 96

Received at ESRF :

20 JUN 1996

Shifts:

15

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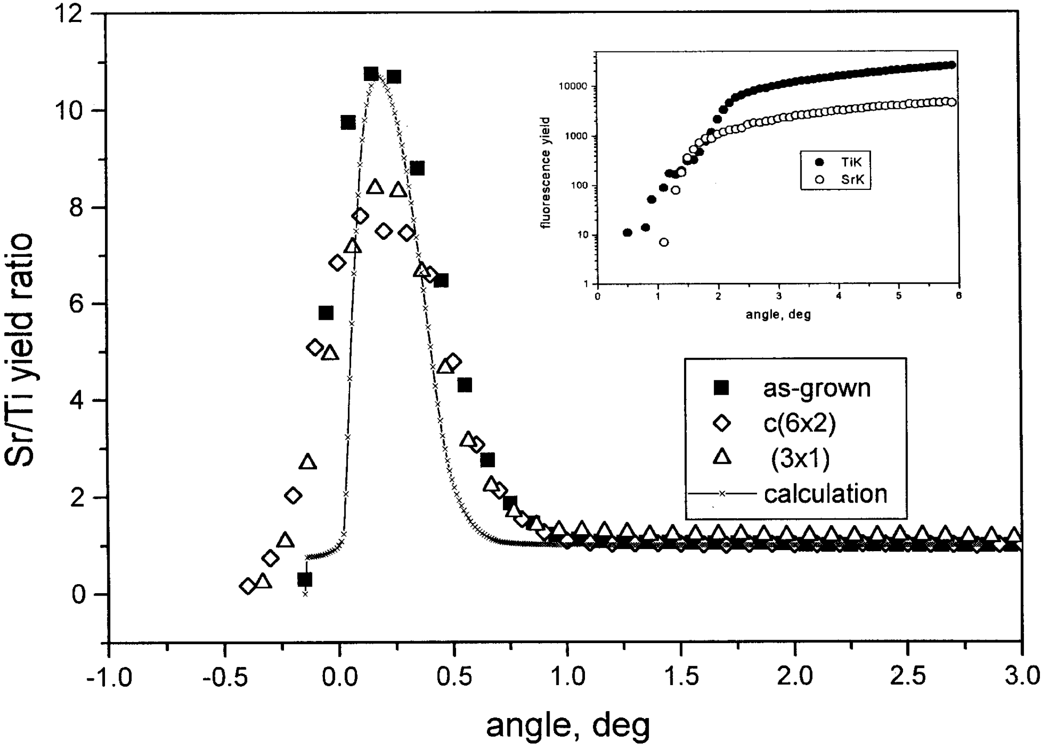
Report:

The x-ray standing wave (XSW) technique is a powerful tool for analyzing the structure of interfaces, thin films and adsorbates. Inherently an interferometric method, it employs x-ray diffraction for generating an x-ray interference field, the nodes and antinodes of which are scanned to selectively photo-excite atoms, the scattering of which in terms of photoelectrons, Auger electrons or fluorescence as a result of the photoabsorption process is recorded. While a large number of adsorbate systems have meanwhile been analysed by the XSW technique, reports about structural studies of clean surfaces are scarce. The reason for this is that it is not trivial to discriminate the scattering signal from the surface layer from the strong scattering from the bulk of the crystal since the penetration depth of the x-rays is of the order of μm. One way to circumvent this problem, is to record x-ray fluorescence from the sample within a very narrow glancing exit angle. In analogy to the total external reflection of x-rays from a crystal surface a certain angle a., the reciprocity theorem of wave propagation predicts, that x-ray ***refraction*** away from the surface with an angle α_c occurs for x-rays originating from the bulk of the crystal. This means that within the narrow angular range O to α_c with respect to the surface fluorescence from the bulk is suppressed and the detected fluorescence must originate from the surface.



We intended to study the surface structure of $SrTiO_3(001)$ crystals in this way by employing a $SrTiO_3(005)$ reflection in backscattering geometry. Because of technical problems with the hardware of the newly commissioned beamline, XSW scans could not be carried out. However, using a solid state detector with a 1 mm pinhole at a distance of 170 mm from the sample, we analysed the grazing exit fluorescence behavior of three different $SrTi0_3(00l)$ samples. Shown in Fig. 1 in the inset is the Ti K-fluorescence (4.5 keV) and Sr K-fluorescence (14.2 keV) as a function of escape angle. The zero of the angular scale in this plot is arbitrary. Also shown is the ratio of the Sr to the Ti fluorescence yield as a function of take-off angle α for three different samples. The curve is calculated for an undistorted, stoichiometric $SrTi0_3(00l)$ crystal. It is a particular feature of $SrTiO_3$ that it exhibits reconstructions stable under ambient conditions. The plot shows that at small angles the Sr/Ti yield ratio for a $c(6 \times 2)$ reconstruction crystal is smaller than for a (3x1) reconstructed tryst al which in turn is significantly smaller than for an as-grown tryst al. This means, that the reconstructed surfaces are Ti rich and depleted of Sr.