ESRF	**Experiment title:** **Study of the $(3\sqrt{3} \times 3\sqrt{3})R30°$ reconstruction of the α-$Al_2O_3(0001)$ surface**	**Experiment number:** SI-310
Beamline: ID3	**Date of experiment:** from: 05Sep-97 to: 12-Sep-97	**Date of report:** **22-02-98**
shifts: 18	**Local contact(s):** E. Lundgren	*Received at **ESRF**:* 06 MAR. 1998

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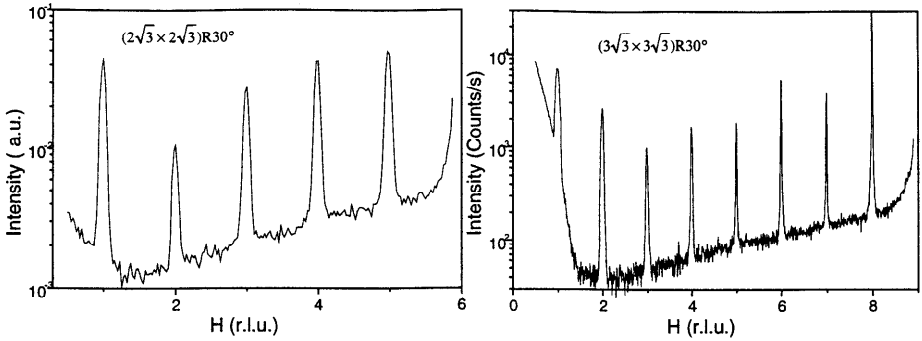
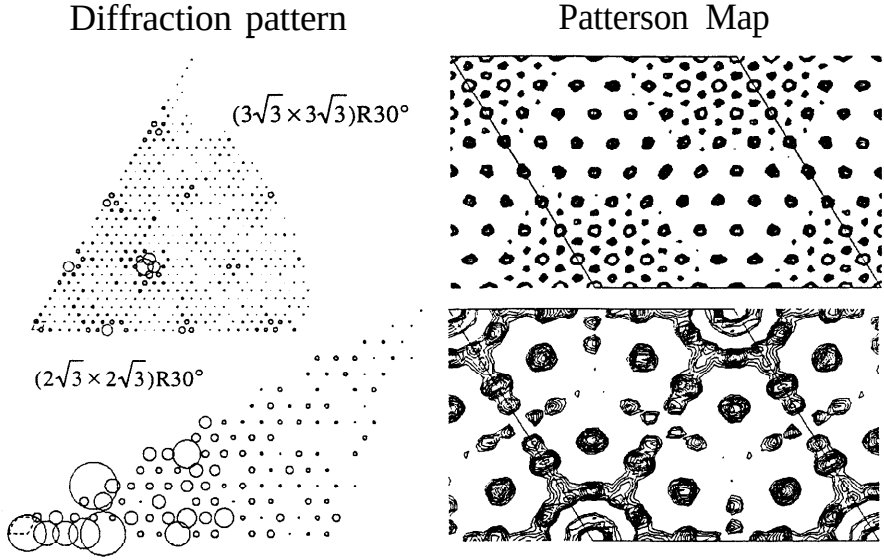
Report:

The α-$Al_2O_3(0001)$ surface is involved in many technological processes, for instance as a catalyst support, for electronic packaging, or as a substrate for the growth of metals, semiconductors and high-?;. superconductors. Its initial state is known to play a dominant role on the overlayer properties. The present proposal is part of a long-term research project including experimental and theoretical work on the atomic structures of the different phases of the α-Al_2O_3 (0001) surface. When annealed at different temperatures under ultra-high vacuum (UHV), four structures are successively obtained: the unreconstructed (1x1) surface, followed by three reconstructions: $(2\sqrt{3} \times 2\sqrt{3})R30°$, $(3\sqrt{3} \times 3\sqrt{3})R30°$ and finally $(\sqrt{31} \times \sqrt{31})R \pm 9°$. We have recently solved the first [1] and the last [2] surface structures by Grazing Incidence x-ray Diffraction (GIXD). The aim of the present experiment was to elucidate the atomic mechanisms involved in the transformation between these two surface states, by solving the atomic structure of the intermediate $(2\sqrt{3} \times 2\sqrt{3})R30°$ and $(3\sqrt{3} \times 3\sqrt{3})R30°$ reconstructions.

Two samples with the $(2\sqrt{3} \times 2\sqrt{3})R30°$ and $(3\sqrt{3} \times 3\sqrt{3})R30°$ reconstructions were prepared *ex situ* and regenerated *in situ* by annealing around 1000°C. Both displayed very nice reconstructions, as illustrated by the radial scans performed along the (h00) direction, shown in the figure below for each reconstruction.
All accessible in-plane reflections at the energy of 14.5 keV were measured over 360" in the case of the $(2\sqrt{3} \times 2\sqrt{3})R30°$ reconstruction, and over 120° in the case of the $(3\sqrt{3} \times 3\sqrt{3})R30°$ reconstruction. The in-plane diffraction pattern and Patterson maps are shown in the other figure. The incident angle was fixed at the critical angle for total external reflection. Both diffraction pattern show p6mm symmetry, corresponding to either p3m1, or p3lm, or p6mm symmetry of the real structure. The reproducibility between the numerous equivalent reflections is 5%.



There is a strong similarity between the $(3\sqrt{3} \times 3\sqrt{3})R30°$ reconstruction and the $(\sqrt{31} \times \sqrt{31})R9°$ we investigated previously, except that no rotation of the overlayer, and hence no discommensuration defect, is found for the $(3\sqrt{3} \times 3\sqrt{3})R30°$ reconstruction. Several out-off plane rods were also measured for both reconstructions. Further analysis hopefully leading to a structural model for each reconstruction is in progress, but it is too early to assert a model.



We hope to be able to propose a model of surface reduction, that is oxygen evaporation, leading to the different phases observed by removal of the successive 0 planes below the surface during heating in UHV. We also hope to describe precisely the transition from non-rotated to rotated reconstruction by use of a generalized theory of rotational epitaxy. A group of theoreticians (I. Vilfan, J. Villain and F. Lançon) is working on the structures of these reconstructions, their energy, how they are linked to each other, and on the process leading to them.

[I] P. Guénard, G. Renaud, A. Barbier and M. Gautier, Mat. Res. Soc. Symp. Proc. Vol. 437, p 15-20, 1996
[2] G.Renaud, B.Villette, I.Vilfan and A.Bourret, Phys. Rev. Lett. 73[131, 1824-28