ESRF	**Experiment title:** Determination of the a-A1203(0001) surface relaxation and termination by measurements of crystal truncation rods.	**Experiment number:** SI-99
Beamline: **ID3-BL7**	**Date of experiment:** from: 21/09/1995 to: 30/09/1995	**Date of report:** 28/2/1996
Shifts : **18**	**Local contact(s):** Salvador Ferrer	*Received at ESRF:*

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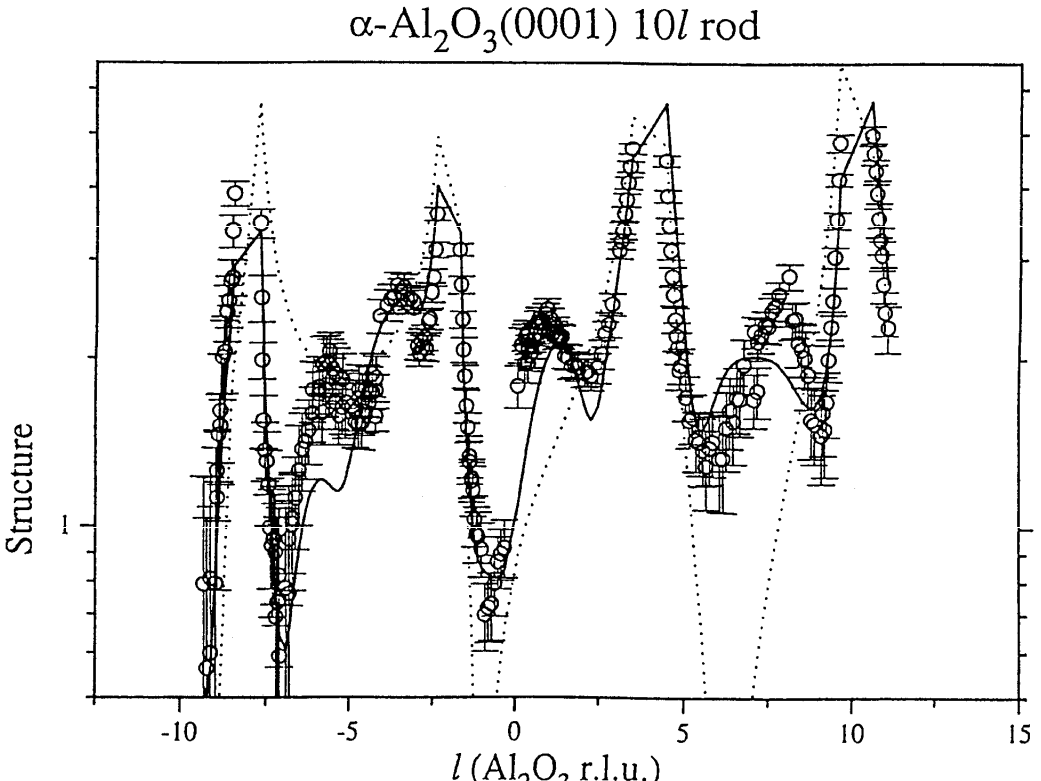
Report:

The structure, composition and morphology of ceramic surfaces directly influence their chemical, mechanical and electrical properties, and thus have a dominant contribution in many important processes such as corrosion, catalysis and sintering. They also affect the nature and strength of bonding at metal/ceramic interfaces used in composites or in electronic packaging. The (0001) surface of sapphire is of major importance, especially as a substrate for epitaxy, and its initial state is known to play a dominant rôle on the overlayer properties.

However little is known about the structure and energetic of oxide surfaces. In particular, the nature (Al or O) of the terminating plane of the a-A1203 (0001)(1x 1) surface is still an open topic because of the lack of experimental result. Moreover, the numerous theoretical calculations that concentrate on the unreconstructed surface structure relaxation and enegy yield different answers. The Al terminated surface is favoured by electrostatic considerations as well as surface energy calculations. However the (lx 1) structure can be observed on surfaces heated in oxygen-rich atmosphere, which are expected to be O-terminated. In addition theoretical calculations predict a very large negative relaxation of the last atomic plane ranging from -40% to -80% depending on the method used.

We investigated the structure of the (1X1) surface by measuring the crystal truncation rods (CTRs). *The* sample was heated in air for 3 hours at 1500°C and then annealed in the UHV chamber at 900°C with an oxygen pressure of -10-5 Torr. Preliminary measurements have been made at LURE but we only measured the two most intense rods because of the lack of intensity. On the ID3 beamline we were able to measure these rods and other ones up to (almost) the largest possible out-of-plane momentum transfer with a much better signal to noise ratio. This is because we could use very small slits (- 10 μm) before the sample and thus reduce the background coming from bulk defects while having a strong signal from the surface because of the brightness of the beam. The sample was kept aligned at ± 2 μm within the slits, at the small critical angle of 0.10.

We measured 8 non-equivalent CTRs on this surface. The first results show that the most likely termination is a single aluminium layer and that relaxations of the first four atomic plane distances are -47%, - 1%,-25% and +7%. These results compare qualitatively well with the most recent theoretical calculations.



Experimental and calculated (101) rod. The best fit line is obtained by fitting all the rods together. The bulk-like terminated surface is shown for comparison (dashed line).

[1] T.J. Godin and J.P. LaFemina, *Atomic and electronic structure of the corundum (α-alumina)* (0001) *surface,* Phys. Rev. B49, 7691-7696 (1994).