ESRF	**Experiment title:** Determining the structure of ZnO(0001)-O using surface X-ray diffraction	**Experiment number:** SI-446
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Report:

In this experiment we investigated the surface relaxation of the clean 1x1 surface of ZnO(0001)-O using surface X-ray diffraction (SXRD). This work forms part of a larger research programme of the applicants which studies the structure/property relations of well-defined metal oxide surfaces. This is a frontier area of surface science which has enormous fundamental and technological potential.

While the main instrumentation worked very well, at the time of the allocated experimental period the RHEED equipment was not available. For this reason we used hkl scans to evaluate the state of the surface, for which surface preparation is relatively straightforward. No additional peaks between those corresponding to the 1x1 surface structure could be detected, whereby the 1x1 surface structure was established. The surface relaxation of this surface of ZnO(0001)-O was studied at room temperature by measuring crystal truncation rods (CTR). The latter were selected on the basis of computer modelling using the code of Vlieg et al [1]. Auger data allowed us to confirm that we had a nominally clean surface.

The diffraction data were collected using conventional rocking scans which enabled a set of CTRs [2] to be compiled. Some rods measured from the ZnO(0001)-O surface are shown in Fig. 1. After subtracting the background intensity, the diffraction peaks were corrected for effective sample area, polarisation of the X-ray beam and Lorentz factor, such that $I_{hk} = |F_{hk}|^2$. Reference reflections were regularly measured throughout the data acquisition period as a method of monitoring surface contamination, none being apparent.

Full quantitative analysis of each dataset should yield a complete structural determination of the surface. The data analysis is still in progress where the perpendicular displacement of Zn and O atoms near the surface are expected to be resolved.

References

1. E. Vlieg *et al*, Surf. Sci. 209 (1989) 100.
2. R. Feidenhans'l, Surf. Sci. Rep. 10 (1989)105 .