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. 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.

The data, which were recorded at room temperature, has been analysed using the code of Vlieg et al [1]. The best fits to the five CTRs are shown in Fig. 1. The errors on the data points were calculated by taking the square root of the sum of the squares of the statistical uncertainty of the measured I_{hk} and an estimate of the systematic error, which was taken to be 10%. The error bars close to the Bragg peaks were enlarged to account for uncertainty in *l*-slit resolution. A schematic of the ZnO(0001)-O surface structure is shown in Fig. 2. The atomic displacements derived from our best fit are listed in Table 1. The main point to note is that the top oxygen (O2) layer is displaced towards the bulk by about 0.2 Å. This is in exellent agreement with recent *ab initio* calculations by Wander and Harrison [3]. The lower layers (Zn2, O1, and Zn1) are in essentially their bulk terminated positions. This is also consistent with ref [3]. We plan to jointly submit these results for publication in Physical Review Letters.

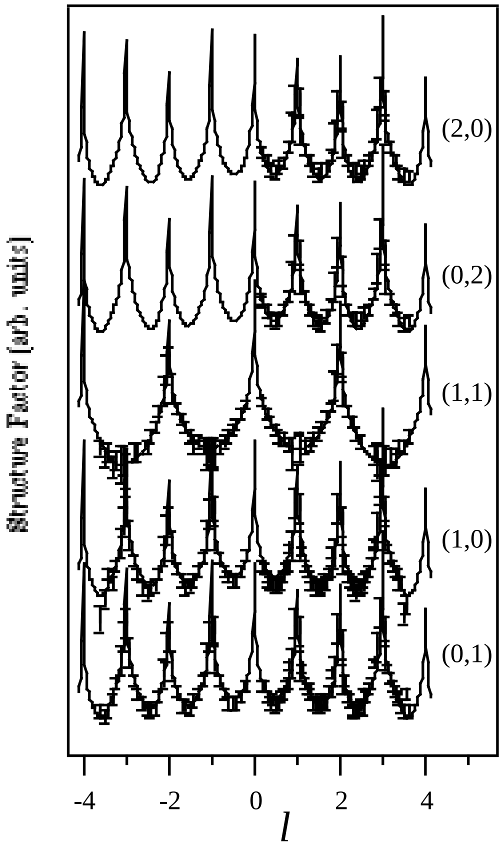

Figure 1. Experimental CTR datapoints displayed on a logarithmic scale. The fitted CTR profiles are shown as solid curves through the datapoints.

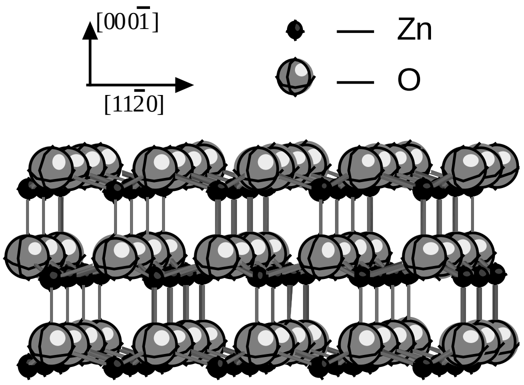

Figure2. Schematic diagram of the ZnO(0001)-O surface.

Atom type	Displacement (Å)
Zn1	0.010 ± 0.004
O1	-0.027 ± 0.024
Zn2	0.004 ± 0.005
O2	-0.217 ± 0.029

Table 1. The atomic displacements of the ZnO(0001)-O surface derived from SXRD data. The numbering corresponds to the top surface layer being O2 and following layers in order Zn2, O1, Zn1. A negative value indicates displacement towards the bulk.

References

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

3. A. Wander, and N. M. Harrison, private communication.