ESRF	**Experiment title:** Vicinal ZnO(10-14): surface structure and stability under H_2O adsorption	**Experiment number**: CH-4766
Beamline: ID03	**Date of experiment**: from: 15 Sep 2016 to: 20 Sep 2016	**Date of report**: 1.3.2017
Shifts: 15	**Local contact(s)**: Raja Znaiguia	*Received at ESRF:*

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Report:

Zinc oxide (ZnO) plays an active role in many catalytic reactions, such as methanol synthesis and the water gas shift. [1]. Determination of the stable ZnO surface structure and studies of how it interacts with the gases is essential for understanding these catalytic processes, where the detailed reaction mechanisms are under current discussion [2]. The non-polar, vicinal, ZnO(10-14) surface has recently been suggested to be a stable facet of ZnO(0001) and (000-1) [3,4]. During the beamtime we for the first time studied a vicinal ZnO(10-14) single crystal with the aim to determine the structure of the vicinal surface, as well as its stability and structure after water exposure.

Initially the ZnO(10-14) crystal was cleaned by cycles of Ar^+ sputtering and annealing to 550°C, according to a recipe pre-determined in our home laboratory. Thereafter we characterised the clean surface through CTR measurements using a photon energy of 18 keV. These measurements confirm that the (10-14) facet of ZnO is a stable facet also as a single crystal surface. We determined the unit cell of the (10-14) surface to be 12.4×2.3×40.3 $Å^3$, with the step periodicity being 12.4 Å. This is in excellent agreement with the the 12.5 Å step periodicity given in the STM based model suggested by Zheng et al. [4] (see figure 1). We aquired a large set of CTRs of the clean surface, a few examples are displayed in figure 2 (black squares). From this data we expect to be able to determine the atomic structure of ZnO(10-14) after further detailed analysis.

After characterising the clean ZnO(10-14) surface we exposed the surface to 20 L of water at room temperature and once again characterised the surface. Through analysing the differences to the data aquired on the clean crystal (see figure 2, blue dots) we expect to be able to determine the water induced changes to the ZnO(10-14) surface.

Currently we are preparing a manuscript on the structure of the vicinal ZnO(10-14) surface and its behaviour upon water exposure containing structural information obtained at this beamtime together with scanning tunneling microscopy and x-ray photoelectron spectroscopy of the same surface.

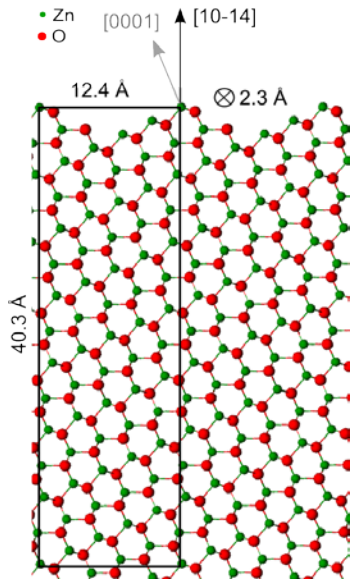

Figure 1: Model of ZnO(10-14) as proposed by Zheng et al. [3].

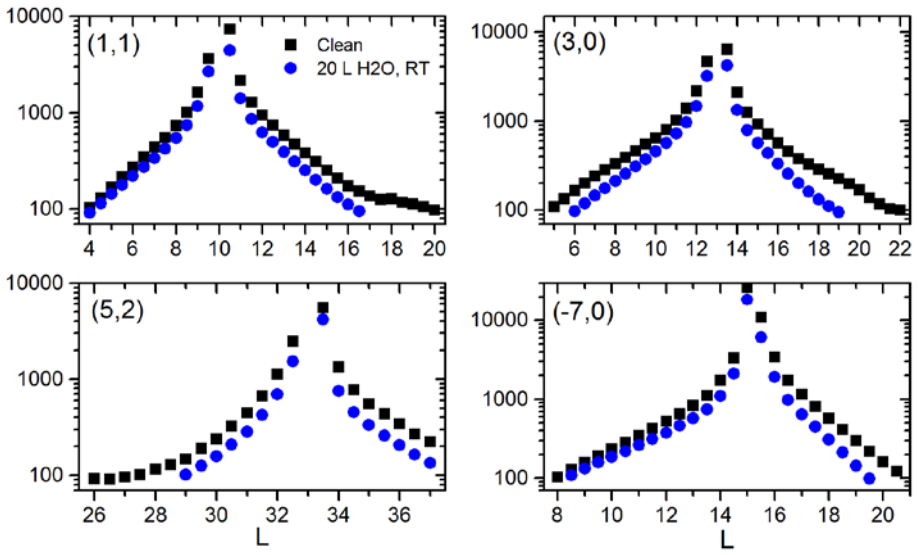

Figure 2: Some of the measured CTRs of the clean [black] and water exposed [blue] ZnO(10-14) surface.

[1] C. Wöll, *Progress in Surface Science* 82, 55 (2007)
[2] M. Behrens, F. Studt, I Kasatkin *et al.*, *Science* 336, 893 (2012)
[3] H. Zheng, M. Gruyters, E. Pehlke, R. Berndt. *Phys. Rev. Lett.* 111, 086101 (2013)
[4] H. Wang, H. Zhan, Y. Zhou *et al.*, *Nanoscale* 8, 4381 (2016)