Structure and stability of vicinal ZnO

E. Grånäs[1], B. Arndt[1,2], M. Creutzburg[1,2], G. Dalla Lana Semione[1,2], A. Schaefer[3], J. Gustafson[3], H. Noei[1], V. Vonk[1], A. Stierle[1,2]

[1]*Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*
[2]*Department of Physics, University of Hamburg, Hamburg, Germany*
[3]*Synchrotron Radiation Research, Department of Physics, Lund University, Lund, Sweden*
elin.granaes@desy.de

Many of the industrial catalysts used today for chemical reactions such as methanol synthesis ($CO + 2H_2 \leftrightarrows CH_3OH$), low temperature water-gas shift ($CO + H_2O \leftrightarrows CO_2 + H_2$) and methanol steam reforming ($CH_3OH + H_2O \leftrightarrows CO_2 + 3H_2O$) [1] contain zinc oxide (ZnO) as an active component together with metal nanoparticles. The ZnO plays not only the role as nanoparticle support; instead it is much actively involved in many reactions, with detailed reaction mechanisms under discussion [2]. For a deeper understanding of the catalytic process it is essential to determine the stable ZnO surface structures and how they interact with the relevant gases.

The low-index surfaces of wurtzite ZnO are polar resulting in surface instability. Instead a higher-index surface, (10-14), has been suggested to be the most stable ZnO surface [3]. The proposed model for this surface consist of Zn-terminated (0001) terraces and O-terminated steps, resulting in a charge neutral, high step-density, vicinal surface. However there are hitherto no studies of the single crystal ZnO(10-14) surface structure or stability. In general, the interaction between steps on vicinal surfaces plays a crucial role for the equilibrium structure and very little is still known about the equilibrium structure of vicinal oxide surfaces. Here first studies performed on vicinal ZnO(10-14) single crystals will be presented. We have characterized the ZnO(10-14) surface using techniques such as scanning probe microscopy, surface x-ray diffraction, and x-ray photoelectron spectroscopy.

Another aspect of uttermost importance for catalytic applications is the stability of such vicinal oxide surfaces under gas exposures. Water plays a key role in many of the relevant catalytic reactions and as a first step we have studied chemical and structural changes of the vicinal ZnO surface upon exposure.

References:
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