Structure and stability of vicinal ZnO

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Many of the industrial catalysts used today for chemical reactions such as methanol synthesis (\(CO + 2H_2 \rightleftharpoons CH_3OH\)), low temperature water-gas shift (\(CO + H_2O \rightleftharpoons CO_2 + H_2\)) and methanol steam reforming (\(CH_3OH + H_2O \rightleftharpoons CO_2 + 3H_2\)) [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: