

A New Stabilization Mechanism for the Polar ZnO(0001)-(2×2) Through Hydrogen Trapping on Zn-vacancies

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Zinc oxide (ZnO) is a wide-band gap semiconductor with great technological applications such as UV-LEDs, photocatalysts, and solar cells [1]. The ZnO(0001) surface displays a (2×2) reconstruction which was poorly understood until now. Here we present an X-ray photoelectron diffraction (XPD) and density-functional theory (DFT) calculation study that unambiguously determines the ZnO(0001)-(2×2) surface as well as unravels its stabilization mechanism [2]. Comparing the XPD measurements with multiple-scattering simulations, the single Zn vacancy per (2×2) surface unit cell model is confirmed, and structures with O adatoms are ruled out. Furthermore, the analysis indicates an outward relaxation of the topmost Zn layer, in contrast to the usually reported results by DFT calculations [3]. Based on our DFT, we describe a new stabilizing mechanism of the polar ZnO surface through surface reconstruction where three hydrogens atoms occupy the Zn vacancies. The DFT surface relaxation of the proposed model is in excellent agreement with the XPD findings. Our DFT simulations also strongly indicate that the migration of hydrogens atoms to the surface, coming from the bulk, plays a central role in the desorption of the surface Zn atom to create the vacancy.

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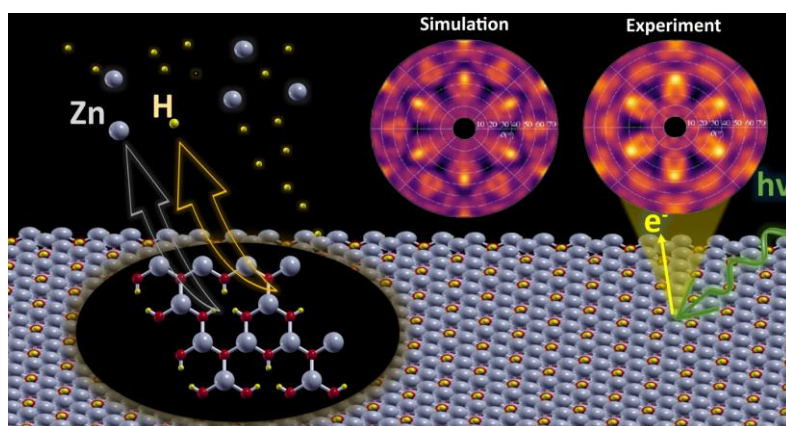


Fig. 1. Representation of the ZnO(0001)-(2×2) with Zn-vacancies trapping hydrogen atoms. Comparison of the Photoelectron diffraction experiment and multiple scattering simulation.

[1] A. Tsukazaki, *et al.*, Jpn. J. Appl. Phys, 44, L643–L645 (2005).

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