

The Interaction of Hydrogen Atom with ZnO: A Comparative Study of Two Polar Surfaces

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The interaction of hydrogen with ZnO single crystal surfaces, ZnO(0001) and ZnO(000-1), has been investigated using a temperature programmed desorption (TPD) technique. Both surfaces do not interact with molecular hydrogen. When the ZnO(0001) is exposed to atomic hydrogen at 370 K, hydrogen is adsorbed in the surface and desorption takes place at around 460 K and 700 K. In ZnO(000-1), the desorption peaks are observed at around 440 K and 540 K. In both surfaces, as the atomic hydrogen exposure is further increased, the intensity of the low-temperature peak reaches maximum but the intensity of the high-temperature peak keeps increasing. In ZnO(000-1), the existence of hydrogen bonding to the surface O atoms and the bulk hydrogen has been confirmed by using X-ray photoelectron spectroscopy (XPS). When the Zn(0001) surface is exposed to atomic hydrogen at around 200 K, a new H₂ desorption peak has been observed at around 250 K. The intensity of the desorption feature at 250 K is much greater than that of the desorption feature at 460 K. This low-temperature desorption feature indicates hydrogen is bonded to surface Zn atoms. We will report the effect of the ZnO structure on the adsorption and bulk diffusion of hydrogen.

Keywords: Hydrogen, ZnO, Bulk diffusion