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Adsorption and absorption of hydrogen in Titanium dioxide

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Titanium dioxide (TiO_2) surfaces are of interest and importance in both physical and chemical aspects including photocatalytic H_2 generation, hydrogen sensors, and two-dimensional electron gas formation. Titanium dioxide reveals polymorphism of rutile and anatase. Upon interaction with TiO_2 surfaces, hydrogen might adsorb on the surface and diffuse into the interior of TiO_2 , which significantly affects the electronic structure of TiO_2 . In these regards, interaction of hydrogen with TiO_2 surfaces is of particular importance. We have studied the hydrogen adsorption and absorption in the rutile $\text{TiO}_2(110)$ and anatase $\text{TiO}_2(101)$ surfaces with nuclear reaction analysis (NRA) and ultraviolet photoemission (UPS). Whereas the former allows us to quantify hydrogen in the sample in a depth-resolved manner [1], the latter provides us with the information on the electronic occupied and unoccupied states.

When the nearly stoichiometric surfaces of rutile $\text{TiO}_2(110)$ and anatase $\text{TiO}_2(101)$ are exposed to atomic hydrogen, NRA shows adsorption of hydrogen with a coverage of about 0.5 monolayer [2]. Concomitantly, a decrease in the work function and downward band-bending are observed by UPS suggesting electron transfer from adsorbed hydrogen to the substrates. Upon annealing the samples, the hydrogen amount near the surface is reduced without desorption indicating that hydrogen undergoes diffusion into bulk. When the rutile $\text{TiO}_2(110)$ surface is exposed to a hydrogen ion beam at 500 eV, an enhanced hydrogen concentration within 10 nm from the surface is detected as compared to the exposure to atomic hydrogen along with an enhanced band-bending. UPS using ultraviolet laser reveals hydrogen-induced features in the unoccupied states, which could be related to photocatalytic activity.

References

- [1] M. Wilde, K. Fukutani, Surf. Sci. Rep. 69, 196 (2014).
- [2] K. Fukada et al., J. Phys. Soc. Jpn. 84, 064716 (2015).

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