Operando analysis of hydrogen in solids and on surfaces

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Metal hydrides are an interesting class of materials not only for hydrogen storage but also for catalyzing hydrogenation reactions. Exemplary for these processes is the activity of early transition metal hydrides towards the ammonia synthesis reaction.¹ At first glance, the presence of large amounts of hydrogen in/on the catalysts should be beneficial to the catalytic process. Upon closer inspection, it was found that the catalytic activity of metal hydrides compared to metals is decisively influenced by electronic changes induced by hydrogen uptake.² The conceptual difficulty arises from the interrelation of bulk and surface hydrogen concentration. To determine the bulk hydrogen concentration of a large number of materials we have developed a combinatorial high throughput method for neutron imaging.

The analysis of hydrogen on surfaces is based on in situ membrane hydrogenation of thin films in combination with reflecting electron energy loss spectroscopy (REELS).³ This method enables time resolved surface hydrogen concentration measurements as a function of the applied hydrogen pressure. The combination of a high throughput method for bulk hydrogen concentration determination with careful analysis of pristine surfaces will enable fast screening of hydride forming compounds for hydrogenation catalysis.



Figure 1. a) Bulk hydrogen concentration measurement by neutron imaging. b) Schematic representation of REELS measurements on TiH₂ surfaces.

References

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