

Molybdenum disulfide as new catalyst for electrolyzers

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There is a growing interest in alternative catalysts as a cost efficient alternative to noble metals for heterogeneous catalysis applications. Particularly for PEM fuel cells and electrolyzers for hydrogen production the catalyst costs are a decisive factor for a broader use. Recently, inorganic materials, like MoS₂ and mixed Fe-oxides, came into focus again. While most bulk minerals are rather inert, strongly increased reactivity is found for nanopowders or nanostructured materials. This effect arises from a complex interplay of structural, electronic and dynamical effects of material and support, and is not fully understood, yet.

Using a combination analytical techniques directly or indirectly sensitive to hydrogen (neutron spin-echo (NSE), neutron diffraction (ND), low energy electron diffraction (LEED), nuclear reaction analysis (NRA), X-ray photoelectron spectroscopy (XPS)) the reactivities of two types of samples, natural crystals (SPI) and commercially available nanopowder (Sigma-Aldrich), towards hydrogen have been investigated.

Diffraction experiments with neutrons and electrons reveal that both types of samples (single crystal and nanopowder) are well defined and show activity also in crystalline form, which allows drawing fundamental mechanical conclusions. There is a striking similarity of the single crystal and nanopowder signals, both showing a diffraction peak around $Q = 1 \text{ \AA}^{-1}$ and, in addition, the nanopowder showing stronger small angle scattering.

By nuclear reaction analysis (NRA) using the reaction $^1\text{H}(^{15}\text{N},\alpha\gamma)^{12}\text{C}$ on single crystals we could show that a considerable percentage of hydrogen is absorbed into the bulk. The time dependence of the NRA curves reveals diffusion of surface hydrogen into the bulk. The powder is considerably more reactive towards H₂, as can be concluded from neutron spin-echo spectroscopy evidencing fast conversion of ortho- to para-H₂ (several minutes) at low temperatures and reinstating hydrogen uptake above room temperature. With the same technique, over the whole accessible temperature range between 20 and 500 K unusually fast incoherent hydrogen motion was found. The observed dynamical processes also show a strong dependence on crystal direction.

On single crystals, which have been loaded with hydrogen electrochemically and heated afterwards, a cycle of surface reduction and oxidation is observed by photoelectron spectroscopy. This temperature dependence, however, is not reflected in the diffusional or vibrational dynamics.

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