X-rays to Elucidate the Structure of Catalysts: Probing the Local and the Crystalline Structure by XAS and XRD

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Both X-ray diffraction and X-ray absorption spectroscopy are widely used in heterogeneous catalysis, since the synthesis of heterogeneous catalysts often aims at high surface area materials. Hence, the materials are often at least partly X-ray amorphous and X-ray absorption spectroscopy is an ideal complementary tool to XRD to monitor the local structure. Recent examples in the field of heterogeneous catalysis and the field of nanomaterials are discussed, where novel synthesis methods, such as flame spray pyrolysis, were used to produce high surface area materials.

An important advantage of the use of X-rays is that the solid catalysts can be studied in situ. Recently, we studied the formation of MoO_3 nanorods from $MoO_3 \cdot 2H_2O$ by XAS, monitoring both the liquid phase and the solid phase. XAS uncovered the formation of soluble species as soon as the transformation to MoO_3 started. No evidence for an intermediate product was found, which is supported by in situ XRD results. Another key field is the identification of the active species under reaction conditions [2-4]. Also here X-ray based techniques are powerful, as will be illustrated using recent examples.

[1] Michailovski A., Grunwaldt J.-D., Baiker A., Kiebach R., Bensch W., Patzke G.R., **submitted.** [2] Clausen B. S., Topsøe H., Frahm R., *Adv. in Catal.,* 1998, **42**, 315. [3] Sankar G., Thomas J. M., Catlow C. R. A., *Topics Catal*., 2000, **10**, 255. [4] Grunwaldt J.-D., Clausen B. S., **Topics Catal.**, 2002, **18**, 37.

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