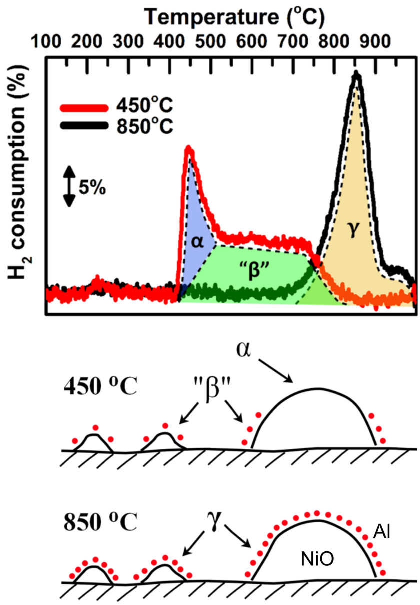

Figure 1. TPR results on Ni/MgAl2O4 catalysts calcined at 450°C (red curve) and 850°C (black curve). The mechanism resulting in the different contributions (α, "β" and γ) is proposed below.

Keywords: NiO reduction, Al migration, in situ XRD

MS36-O5 *In situ* diffraction studies during transition metal catalysis

Claudia Weidenthaler[1], JoChi Tseng[1]

1. Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr

email: cweiden@gwdg.de

Transition metal compounds are nowadays tested as substituents for noble metal catalysts. Ammonia is an excellent hydrogen carrier and the decomposition of ammonia would be an elegant way to generate hydrogen for fuel cell applications without formation of CO_x. The most active catalyst so far is Ru on carbon nanotubes, but bimetallic compounds or metal nitrides are also under investigation as potential catalysts for ammonia decomposition. Noble metals are rather expensive and limited in availability. In contrast, metal nitrides are much cheaper and easy to prepare by the nitridation of metal oxides. In this work we study different transition metal catalysts during the decomposition of ammonia. Starting from transition metal oxides, the catalyst formation was studied by *in situ* X-ray diffraction under reaction conditions. Crystallographic studies with respect to phase changes, crystal structure variations, and microstructure properties have been performed [1,2]. The behavior under reaction conditions and the catalytic activity can significantly differ for each catalyst system: while some transition metal oxides reduce during the reaction with ammonia to the metals, others form nitrides after reduction. Changes of the chemical composition associated with structure changes as well as alterations of the microstructure properties of the catalyst in terms of domains size or defect variations may influence the catalytic activity. So far, iron oxides and cobalt alumina spinels were investigated as precursors for ammonia decomposition. In case of iron oxides nitrides are formed during the reaction with ammonia while for cobalt oxides metals form after activation [3,4]. Molybdenum-based catalysts are a very good example that various factors govern activity. Structure changes as well as changes of specific surface areas, and defect concentrations have to be considered [1,2]. In this work we also present studies on the use of bimetallic catalysts (Fe-Co, Fe-Ni) for ammonia decomposition. The formation of metal nitrides, metals and/or alloys during the reactions is monitored by *in situ* XRD using in-house laboratory instruments. The structural changes and detailed reaction pathways were studied by the evaluation of the diffraction data.

[1] Tagliazucca et al., J. Catal. 2013, 305, 277. [2] Tagliazucca et al., Phys. Chem. Chem. Phys. 2014, 16(13), 6182.[3] Feyen et al., Chem.-Eur. J. 2011, 17, 598. [4] Gu et al. J. Phys. Chem. C. 2015, 30, 17102.

Keywords: transition metal catalysts, ammonia decomposition, in situ diffraction