



MAX-PLANCK-GESELLSCHAFT



15. Conference of GDCh Division for Solid State Chemistry and Material Research
Berlin (Germany), 20.09.-22.09.2010

In situ Neutron Diffraction Study of a Methanol Synthesis Catalyst under Working Conditions

Timur Kandemir,^[a] Dirk Wallacher,^[b]
Michael Tovar,^[b] and Malte Behrens^{*,[a]}

Keywords: Neutron diffraction; Heterogenous catalysis

A reactor setup for the *in situ* study of methanol synthesis catalysts using neutron diffraction (ND) was designed, which allows investigation of structural and microstructural features of Cu-based catalysts [1] under demanding reaction conditions like elevated pressure and temperature (up to 250 °C and 60 bars). The evolution of phase composition, crystallite size, lattice strain and defect density during the catalytic reaction is probed *in situ* with ND data (Fig. 1) acquired using the Fine Resolution Powder Diffractometer (FIREPOD) at the BER2 research reactor of the Helmholtz Centre Berlin [2].

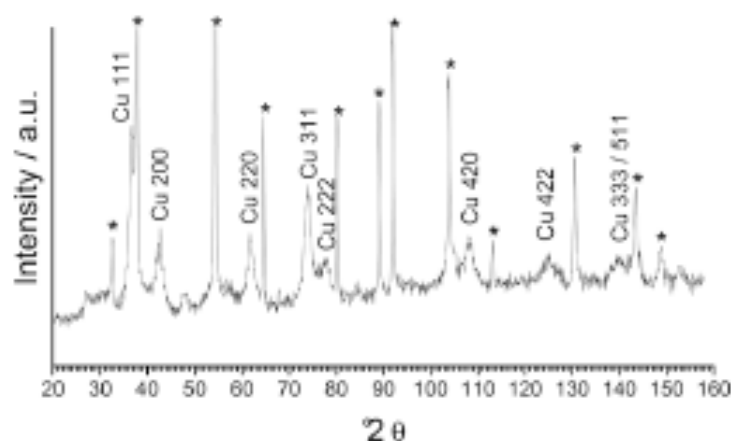


Figure 1. ND pattern of a Cu/ZnO/Al₂O₃ catalyst in 50 bar D₂ at 250 °C. Sharp reflections "*" are due to Al reactor.

[1] I. Kasatkin, P. Kurr, B. Kniep, A. Trunschke, R. Schlögl, *Angew. Chem. Int. Ed.*, 2007, 467324-7327.

[2] R. Michaelsen, *Neutron News* 2001, 127-9.