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Continuous flow experiments at high-pressure for characterization of catalysts in working state using neutron diffraction

T. Kandemir[1], *D. Wallacher*[2], *T. Hansen*[3], *K.D Liss*[4], *R. Schloegl*[1], *M. Behrens*[1]
[1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin
[2]Helmholtz-Zentrum Berlin, Berlin
[3]Institut Laue-Langevin, Grenoble
[4]ANSTO, Lucas Heights

The present contribution describes a reaction cell, which allows in-situ neutron diffraction of solid catalysts in the working state under high pressures close to industrial relevant reaction conditions.
Conventional catalyst characterization from the range of UHV to ambient pressures does often not allow extrapolating catalytic properties into the high-pressure regime, which makes in-situ characterization necessary.
A new approach to bridge this so called pressure gap is a continuous flow-reactor for in situ neutron diffraction, which is suitable for reaction temperatures up to 330°C and pressures up to 60 bar. Changing the reduction potential of the gas atmosphere in the steady state experiment (e.g. from pure D_2 to a mixture of D_2, CO, CO_2), allows determination of effects of feed composition on catalyst structure.
The temperature-dependent formation of the catalytic active material was studied using high-intensity neutron diffraction on D1B at ILL. Merging this data with complementary high-resolution experiments carried out on ECHIDNA at ANSTO allow a comparison of the active and inactive state of the catalyst. On-site gas phase analysis with mass-spectroscopy makes it possible to track the progress of reduction of the catalyst and proof catalytic activity. Additional laboratory experiments like gas chromatography and surface area determination allow conclusions to be drawn on the structure-activity correlation.
Email of the presenting author: kandemir@fhi-berlin.mpg.de