

## Report for Proposal Code CH 5785; Operando X-ray diffraction of zeolite catalysts

This experiment was carried out as a remote experiment with mail-in samples. Nevertheless, we would characterize this as a very successful session. Thanks to the excellent help of the ESRF staff, we were able to record data for a large amount of samples in pre-sealed capillaries and some single crystals. More importantly, the bulk of the experiment was dedicated to temperature programmed oxidation of deactivated zeolite catalyst samples. By heating in open ended capillaries exposed to laboratory air, we were able to follow the coke oxidation and thus regeneration of both ZSM-5 and H-beta zeolite catalysts by high energy time resolved operando X-ray diffraction. The data for H-beta were particularly valuable, and were used to develop a DIFFAX stacking fault model comprising up to 100 unit cells. As the H-beta zeolite is disordered, quantitative analysis of XRD data is challenging, but the development of this model amounts to a major breakthrough.

This experiment will result in 2 publications (in preparation) and contributed significantly to one PhD:

“A new XRD model for deactivated Beta zeolites” Nico König, Nicolai Haaber Junge, Dmitry Chernyshov, Georgios Kalantzopoulos, Evgeniy Redekop, Pablo Beato, Stian Svelle, David Wragg, Lars Fahl Lundegaard, in preparation (2021).

“An XRD based descriptor to monitor the degree of coking of H-beta zeolite catalysts” Nicolai Haaber Junge, Nico König, Dmitry Chernyshov, Georgios Kalantzopoulos, Evgeniy Redekop, Pablo Beato, David Wragg, Lars Fahl Lundegaard, Stian Svelle, in preparation (2021).