In-situ Synchrotron XRD Studies of Combustion Processes

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Synchrotron based diffraction techniques are powerful tools for the characterization of the crystal phases involved in fast chemical reactions. The flexibility of the instrumental setup and the brilliance of the source allow for optimal selection of the experimental parameters, so that reliable structural information can be obtained even on metastable or transient species.

Two in situ experiments were selected, related to the high temperature combustion processes on catalytic materials. In both cases the full-profile analysis of the diffraction data, including cell parameters, phase abundance, peak width, and Rietveld-type structure refinement yield a wealth of information on the reaction mechanisms and kinetics.

In the first case, the burning of the organic template within the cavities of a high-silica MFI zeolites has been followed in situ using the ESRF BM-8 translating image plate [1]. The structural refinements allow quantification of the template occupancy in the channels, and the dimensionality of the diffusion kinetics of the reaction products [2]. In the second case, the combustion of methane over iron oxide catalysts has been followed by coupled XRD and gas MS, gaining insight on the changes taking place in the solid state catalysts during the production of hydrogen [3].

[1] Meneghini C., et al., *Journ. Synch. Rad.,* 2001, **8**, 1162. [2] Milanesio M., et al., *J. Am. Chem. Soc.,* 2003, **125**, 14549. [3] a) Gemmi M., et al., *Journ. Appl. Cryst.,* 2005, *in press*; b) Ghisletti et al., *this conference*.

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