catalytic material under operative conditions. To recreate actual conditions in a catalytic reactor, and to be able to study many catalytic processes, require a robust and flexible system. We have developed a facility at the Swiss-Norwegian beam lines (SNBL) at the European Synchrotron radiation Facility (ESRF), where operating (flow) conditions up to 20 atm. and 900C in variable and switchable gas mixtures may be achieved. The system will be used for in situ powder diffraction as well as for XAS studies. A mass spectrometer is available for analysis of exhaust gases and a Raman spectrometer has been installed for combined in situ experiments. Results from studies of catalytic materials at operating conditions will be given.

Keywords: *in situ*, catalysis, operating conditions

MS.18.4

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In situ simultaneous Raman/XRPD study of solid-state reactions at non-ambient conditions

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Materials containing disordered moieties and/or amorphous or liquid-like phases or showing surface- or defect-related phenomena constitute a problem for their characterization using X-ray powder diffraction (XRPD), and in many cases Raman spectroscopy can provide useful complementary information. We have designed and realized a novel experimental set-up for simultaneous in situ Raman/High-resolution XRPD experiments to take full advantage of the complementarities of the two techniques in investigating solid-state transformations at non-ambient conditions. The invaluable added value of the proposed experiment is the perfect synchronization of the two probes with the reaction coordinate and the elimination of possible bias caused by different sample holders and conditioning modes used in *in-situ* but separate approaches. A gas blower allows studies from RT to 700K and 100K can be reached using a nitrogen cryostream. The experimental setup flexibility allows the addition of ancillary devices, such as a UV-lamp used to study photoreactivity or DAC to study high pressure regime. The set-up was tested on three solid-state transformations: i) the kinetics of the fluorene:TCNQ solid-state synthesis, ii) the thermal swelling and degradation of stearate-hydrotalcite nanocomposites, iii) the photoinduced 2+2 cyclization of (E)-furylidenoxindole. The reported experiments demonstrated that, even though the simultaneous Raman/XRPD experiment is more challenging than the separated ones, high resolution XRPD and Raman data can be collected. Concerning the obtained results, Raman gave information on surface reactivity and on flexible and disordered organic moieties hydration states while XRPD gave information on bulk properties and on stiff inorganic moieties.

Keywords: *in-situ* time-resolved powder diffraction, reaction mechanisms, raman spectroscopy

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Application of a high-pressure CO_2 cell to time-resolved studies with a lab powder diffractometer

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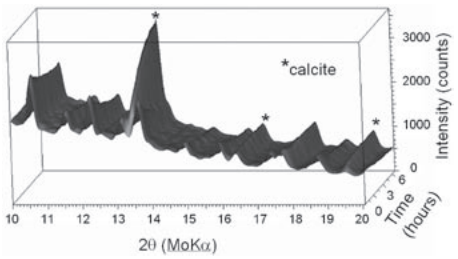
A gas-cell design for laboratory diffractometers rated to 12.4 MPa and 200 ℃ has been certified and constructed to the latest pressure vessel design codes [1]. The gas of interest in this case is CO_2 which is supercritical above 7.4 MPa and 31℃. The temperature/pressure behaviour of CO_2 adds significant complications to the experimental application. The cell has been coupled with MoKα radiation and the Bruker Vantec PSD to enable time resolved studies to be conducted on a laboratory diffractometer. The snap-shot mode of the detector has been used to study the crystallization of poly-lactic acid (PLA) and PLA-clay composites under CO_2 pressure. Additionally, the carbonation of wollastonite has been studied as an initial model system for potential application to CO_2 sequestration studies. Given the sluggish kinetics of many sequestration reactions under milder conditions, restricted beamtime allocations at synchrotrons could be seen as a practical disadvantage for comprehensive studies versus a laboratory diffractometer.



[1] Whitfield, P.S., Nawaby, A.V., Blak, B., & Ross, J., J.Appl.Cryst, v41 (2008), 350-355

Keywords: gas-solid reactions, *in-situ* powder diffraction, time-resolved powder diffraction

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Evolutionary crystal structure prediction and its applications to materials at extreme conditions

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Crystal structure prediction on the basis of just the chemical formula has long been considered a formidable or even insoluble problem. Several methods have recently been proposed to tackle this problem, among which the evolutionary algorithm USPEX (Universal Structure Predictor: Evolutionary Xtallography [1-3]) proved to be particularly efficient and reliable. Key ingredients of this method (selection, variation operators, redundancy control and constraint techniques) and its current developments will be discussed. Applications of this methods so far are quite numerous and include several technologically important systems and many materials of mainly fundamental interest (high-pressure phases of hydrogen,