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Phase Determination using a Wide-band Parallel Synchrotron Radiation Beam
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New diffraction system has been constructed at the Synchrotron Radiation Center at Ritsumeikan University, in which a wide-band parallel X-ray beam is produced by reflection from the depth-graded multilayer monochro –mator [1]. The band width is 600eV and the monochro -mator is useful in the photon energy range from 6000eV to 8000eV.

In diffraction patterns of an oscillating single crystal recorded using this system, Bragg reflections appear in an elongated form on an imaging plate and, if the absorption edge of an atom in the sample crystal is included in the band, a characteristic intensity profile is seen due to anomalous dispersion. As an application of this system, we determined the phase of the structure factor of a ferrocene derivative crystal, $C_{36}H_{32}O_7Fe$, choosing the Fe atoms as anomalous scatterers, based on a newly developed method of phase determination [2].

[1] Koganezawa T., Uno K., Iwasaki H., Nakamura N., Yoshimura Y., Shoji T., *J. Appl. Cryst*., 2004, **37**, 136-142. [2] Iwasaki H., Yurugi T., Yoshimura Y., *Acta Cryst. A*, 1999, **55**,864-870.
Keywords: synchrotron radiation, anomalous dispersion, wide-band beam

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Simultaneous XRPD-MS Study on Iron Oxides Supported on Spinel-like Aluminate
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Iron oxides are suitable oxygen exchangers in redox cycles, to be employed in an innovative process of hydrogen production from natural gas [1]. Infact, these oxides, once reduced with hydrocarbons, are capable to re-oxidize by splitting [O] from water, thus producing a pure stream of H_2.

In-situ time-resolved synchrotron X-ray powder diffraction (XRPD) experiments coupled with mass spectrometry (MS) were performed on iron oxides supported on spinel-like aluminate [2], both during high temperature reduction with methane and oxidation with air.

The reactive gases were fed directly through a capillary quartz reactor containing the sample and the evolved products analyzed by an on-line connected mass spectrometer

By means of the Translating Image Plate (TIP) installed on the GILDA beamline (ESRF- Grenoble, France), the photons diffracted from the sample were collected step by step during the reaction, the translating speed determining the time resolution. The Rietveld refinement of the diffraction spectra gave the quantitative sample composition at each step of the reaction and information about the interaction of the active species with the support.

[1] EP 1134187 (19/09/2001) to Snamprogetti. [2] United States Patent Application 20040152790.
Keywords: synchrotron, in-situ time-resolved powder diffraction, iron oxides

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Automation of MX Data Collection and Processing
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We present the DNA project, a collaboration with the aim of fully automating the collection and processing of macro-molecular X-ray crystallography data including rapid crystal screening. The DNA system takes strategic decisions about the data collection based on information provided by the data processing software and some basic parameters relating to the project which will be supplied by the user. The modular nature of the system simplifies installation on different beamlines and allows the use of different data collection and data processing software.

The DNA system forms a major part of the fully automated sample screening pipeline being but in place at many European synchrotron radiation facilities. Version 1.0 of the software is now working successfully at both the ESRF (Grenoble, France) and SRS (Daresbury, UK) and will be transferred to beamlines of other synchrotrons in the near future. We are also working on an off-line version that will be used at laboratory sources.
Keywords: automation, automatic data collection, data processing

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Still Bad Crystals, but Good Data and Results from Synchrotron Facilities
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In many cases it is simply not possible to transform bad crystals into good ones, but a crystal structure is still required. The use of high-intensity synchrotron radiation can overcome some of the problems, particularly weak diffraction, whether this be a result of small crystal size or of structural faults such as disorder or twinning.

For real success, dedicated single-crystal facilities are needed, optimized for this application and using good quality X-ray optics, state-of-the-art diffractometer and detector systems, and usually low-temperature equipment. The "small-molecule" diffraction station at Daresbury SRS, constructed about 10 years ago, has been a spectacular success with great productivity and a high level of oversubscription by users, and a second station is now available.

More recently the facility has been used for a national crystallography service for UK chemistry research groups, providing rapid access and expert staffing. As many as 12 data sets per day have been measured from samples that are known to be beyond the capabilities of the most powerful rotating-anode area-detector chemical crystallography system in the country (perhaps in the world) and have been brought to us as a last resort. Although some samples really are beyond hope (including those that simply aren't crystalline at all), the majority have yielded their inner secrets, though the effort involved is often considerable when twinning, disorder, pseudosymmetry and other challenges have to be faced.
Keywords: synchrotron X-ray diffraction, structure determination, service crystallography

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Recent Developments and Diffuse Scattering Studies at Beamline F1 (Hasylab/DESY)
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In order to enhance data collection possibilities at beamline F1 a new marresearch CCD-detector with an active area of 165 mm in