line positions. Here we present a comprehensive study of these effects by means of Monte Carlo simulations followed by data evaluation. Results of an optimization that includes intensity, resolution and line precision are presented. These findings have been used for the design of the new diffractometer ODIN at the JEEP II reactor at IFE in Norway. It will be a flexible, high-resolution instrument. Take-off angle, collimation, monochromator radius and illuminated monochromator area can be varied to adapt the instrument to the needs for the measurement in terms of intensity, resolution and line precision.

MS36 P04

Pseudo-merohedral twinning : how to treat a six-fold twin Leo Straver and Rob Hooft, *Bruker AXS, Oostsingel 209, NL 2612 HL Delft, The Netherlands*
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Keywords: multiple domains, twins, data reduction

The introduction of two dimensional detectors for single crystal diffraction has made it possible to easily collect data of pseodo-merohedral twins, incommensurate structures and structures including diffuse scatter. Many programs exist, e.g. GEMINI [1], CELL_NOW[2] and DIRAX[3], with which these more complex matrices can be indexed. A common problem with pseudo-merohedral twinning is cell refinement due to closely overlapping spots. Careful selection of trusted areas to refine the cell in, will improve the reliability of the cell parameters. Recent versions of integration programs, such as SAINT [4] and EvalCC [5] utilize the different orientation matrices and can integrate the entire intensity of every reflection labeling them as overlapping or not. One of the pitfalls during integration of data from pseudo-merohedral twins is that the spot shape changes continuously due to the systematic overlap of areas of adjacent spots. Special care has to be taken when setting up the integration parameters. Most semi-empirical scaling and absorption correction programs are not able to handle datasets of such complexity. The program TWINABS was developed [6] specifically to carry out absorption correction and scaling on datasets which contain reflections from different domains. Resultant data files distinguish between non-overlapping and overlapping reflections [7] and can be seamlessly used for structure refinement. The approach is illustrated using a six-fold twin that shows a reversible transition to single crystal state.

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MS36 P05

Non-Conventional Scattering Studies of Materials using a Laboratory Image Plate Diffractometer Lynne H. Thomas[a], Sylvia E. McLain[b], Andrew Parkin[a], and Chick C. Wilson[a]. *a. Department of Chemistry and WestCHEM Research School, University of Glasgow, Glasgow, G12 8QQ, U.K. b. ISIS Facility, Rutherford Appleton Laboratory,* ***Chilton, Didcot, Oxon, OX11 0QX, U.K.***

Keywords: Image plate; diffuse scattering; liquid scattering

Recent trends in the development of X-ray diffractometers have been towards fast readout detectors such as CCDs. Image plate detectors, however, have the advantage that long exposure times are possible due to their high dynamic range, allowing weaker scattering to be observed without suffering from detector overloads or from dark current accumulation. Experiments involving measurements such as liquid scattering and diffuse scattering which have previously required the use of high flux synchrotron radiation have been demonstrated to be possible on a laboratory diffractometer using a curved image plate detector. Diffuse scattering has been observed to arise from a wide range of different materials and its presence is often unexpected. The mechanism behind such scattering is often complex, however insights can be gained from consideration of the average structure of the material and the comparison to similar features in systems where the disorder has been characterised using modeling techniques such as Monte Carlo and Reverse Monte Carlo. The feasibility of collecting liquid diffraction patterns with the aim of studying the early stages of molecular arrangement within solution prior to crystallisation has also been investigated and preliminary results arising from this will be presented.

MS36 P06

The Present and the Future of Protein Microcrystallography at SPring-8 M. Kawamoto[a], N. Shimizu[a], K. Hasegawa[a], A. Nisawa[b], G. Ueno[b], K. Hirata[b], T. Kumasaka[a] and M. Yamamoto[a,b], [a]*SPring-8/JASRI,* [b]*RIKEN SPring-8 Center*
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Keywords: microcrystals, microbeam, synchrotron radiation

BL41XU is an undulator beamline at Japanese third-generation synchrotron facility SPring-8. This beamline has been improved for obtaining high quality data from protein micro crystals (~ 25 μm) using a micro beam (~ 25 μm). The new K/B mirror system was installed at the autumn of 2006, and the monochromatized beam is focused to V70 × H100 μm (F.W.H.M.) at sample position. The final beam size at sample position is defined from 25 × 25 to 70 × 100 μm^2 (F.W.H.M.) by using two set of quadrant slits. Photon flux and flux density of the 25 × 25 μm^2 beam at 1 Å are 3.0×10^{11} photons/sec and 4.8×10^{14} photons/sec/mm^2, respectively.
It is essential for the data collection to control the radiation dose since micro crystals will be received remarkable radiation damage. The data collection software installed to BL41XU can change the beam irradiation position automatically to suppress the effect of radiation damage by using multiple positions on a crystal and multiple crystals. SAD measurements of Se-methionine samples with the crystal size from 15 to 50 μm were performed by using this tool, and we successfully obtain the initial phase at the resolution from 2.7 to 3.9 Å.
A new micro focus beamline in order to utilize the real micro beam; target beam size is 1 × 1 μm^2, is planned at SPring-8. We present the present status of protein