micro- and nanofocusing, in imaging in absorption and phase contrast. They are excellently suited in crystallography to match the beam size to the size of the sample and to control the divergence of the beam.

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Keywords: X-ray optics, microtomography, X-ray microscopy

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Solid State Detectors for Present and Future X-ray Sources
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At the Paul Scherrer Institut, solid state detector development for the Swiss Light Source SLS is successfully done since several years. Results of these efforts are two large area detector systems: The MYTHEN detector is an array of microstrip detectors installed at the powder diffraction station of the material science (MS) beamline X04SA. It covers an angle of 60° and has a resolution of 0.005°. Powder patterns can be recorded in a fraction of a second, which opens a new field of experiments. The PILATUS 1M detector is a large area pixel detector with more than 10^6 pixels. Experiments benefit from the properties of the single photon counting detectors: No background from dark current, no read-out noise, very good efficiency in the energy range of 6-15 keV and readout-times below 10ms. Examples of some experiments are given.

In order to improve the pixel detector, a new read-out chip was designed, with much improved performance. It has a 20-bit dynamic range, a count rate capability per pixel of 1MHz and a pixel size of 0.172 x 0.172 mm^2. Based on these components, the new PILATUS 6M detector for the protein crystallography beamline will be built.

For future applications, we have started a development program for a high speed digital X-ray imaging system. The system operates in single photon counting mode and should work at frame-rates of up to 1 KHz. The pixel-size will be approximately 50 x 50 um^2, the system should have about 1000 x 1000 pixels.

Keywords: pixel detectors, powder diffraction, protein crystallography

MS12 DISORDER DIFFUSE SCATTERING

Chairpersons: Reinhard Neder, Thomas Proffen

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Diffuse Scattering and Monte Carlo Studies of Relaxor Ferroelectrics
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A renewed interest in the field of ferroelectricity has taken place in recent years since the finding of exceptional piezoelectric properties in the lead-oxide class of relaxor ferroelectric (RF) materials typified by the disordered perovskites $PbMg_{1/3}Nb_{2/3}O_3$ (PMN) and $PbZn_{1/3}Nb_{2/3}O_3$ (PZN) [1-5].

Although PMN, PZN and numerous related materials have been extensively studied over a long period a detailed understanding of the exact nature of their polar nanostructure has still not emerged. In this paper we describe experiments in which full three-dimensional diffuse neutron scattering data have been recorded from a single crystal of PZN using the time-of-flight (tof) Laue technique on the SXD single crystal instrument at ISIS.

Monte Carlo simulation has been used to demonstrate that the observed diffuse patterns are due to planar nano-domains oriented normal to the six ⟨110⟩ directions. A simple model has been developed which explains the observed scattering. This is based on the fact that Pb atom possesses a lone-pair of electrons, which gives it directionality.

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Keywords: diffuse scattering, monte carlo treatment, ferroelectric materials

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Order and Disorder in Lysozyme Crystals Caused by the Phase Transition
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Some lysozyme crystals transform to low-solvent crystals by dehydration-induced phase transition [1], [2]. The transition took several hours and the change of X-ray diffraction was recorded to monitor the process [2]. Strong diffuse streaks were observed in the intermediate state where the crystal contains two types of micro-crystals, one with the native lattice and the other with the transformed lattice. At the end of the transition, the transformed micro-crystals were re-ordered as indicated by disappearance of the diffuse streaks. However, the relatively large mosaicity and distinct diffuse scattering indicated that the order of the micro-crystal as well as the crystal packing was not fully recovered.

The structures of native and transformed crystals were determined at resolution 1.13-1.16 Å. They shared essentially the same backbone structure between native and transformed crystals. In the triclinic crystal, however, a conformational change in the main chain was observed in the large loop region of Ser60-Leu75, where a sodium ion was bound in the transformed crystal in place of water molecules in the native crystal. The peptide plane linking Arg73 and Asn74 was rotated 180° in the transformed crystal. In contrast, a sodium ion bound in the monoclinic crystal was removed in the transformed crystal where the corresponding loop region showed a water-bound structure.

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Keywords: phase transition, lysozyme crystal, dehydration

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X-ray and Neutron Diffuse Scattering by Cation and Anion Deficient Zirconia
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Zirconia, ZrO_2 doped with cations (e.g. Y^{3+}, Sc^{3+}, Ca^{2+}), is a technologically important material, e.g. with respect to its high ionic conductivity based on oxygen vacancies. An alternative route to create the vacancies is the doping with anions (e.g. nitrogen). To understand the properties of these materials it is necessary to know both long-range and short-range ordering effects of cations, anions and vacancies as well as relaxations of atoms surrounding the defects. The diffuse scattering of zirconia with different types of cation dopants with or without co-doping with nitrogen has been investigated by neutron and X-ray scattering. The typical neutron diffuse scattering of cubic stabilized zirconia shows diffuse maxima being part of global features, such as diffuse bands perpendicular ⟨111⟩, whose distance corresponds to the smallest Zr-O distance. This can be described by a defect model based on statistically distributed vacancies surrounded by radially displaced ions [1], ascribed to rhombohedral short-range order. The parameters of this model, i.e. the various amounts of the displacements of the ions, are obtained by fitting them to the experimental data and are compared to theoretical (ab initio) predictions.

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Keywords: zirconia, diffuse scattering, defect structures