will be open for general user access. TOPAZ will be a time-of-flight Laue diffractometer using a polychromatic incident beam to collect a full data set of Bragg peaks in a matter of tens of minutes rather than hours. The instrument will be optimized for high through-put small molecule crystallography of moderately sized and complex unit cells (up to around (50 Å)^3). To achieve this goal, custom designed focusing optics are employed for incident beam transport to the sample. Highly pixilated Anger detectors have been developed, and a novel sample positioning and loading scheme will be presented. The combination of innovative development in all areas of the instrument will enable TOPAZ to measure data from standard X-ray size crystals with an order of magnitude decrease in measurement time compared to current instruments. Various sample environments will be available including cryogenic cooling, heating, and magnetic fields. The magnetic field environment coupled with the planned polarized neutron option will allow for future experiments investigating magnetic structure and phase transitions in materials. This research is supported by UT Battelle, LLC under Contract No. DE-AC05-00OR22725 for the U.S. Department of Energy, Office of Science.

Keywords: ToF Laue diffractometer, neutron single crystal diffraction, high throughput crystallography

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First results from the KOALA neutron Laue instrument

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The KOALA instrument is a single-crystal Laue diffractometer optimised for small molecule structural studies and based on a cylindrical image-plate detector. Compared to monochromatic instruments, much smaller samples (0.1 - 1 mm) can be used due to the high beam flux and the large coverage of the detector. The instrument is well suited to studies performed at multiple temperatures. The typical sample environment is a CCR with a hot-stage that provides sample temperatures from 4 to 800K. Electric-field and gas charging/discharging experiments are also possible, and a high-pressure capability will be available in the near future. The KOALA instrument has been installed and awaits the scheduled restart in May 2008 of OPAL, the new Australian research reactor. Commissioning will extend over a three month period from the reactor startup. Early results from the instrument will be presented. In particular, a comparison will be made between KOALA and the VIVALDI instrument at the ILL, on which KOALA was based. Access to KOALA is typically via a 6-monthly peer review of proposals. No access charges are made for non-proprietary research. International users are encouraged to apply.

Keywords: neutron instrumentation, single-crystal diffraction, small molecular crystallography

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Mismatch cobaltite lattices investigated by white beam neutron diffraction

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The majority of all single crystal diffraction data is collected using monochromatic sources as this eases the step from measured intensities to corrected intensities. Synchrotrons have continuously pushed the limit for what can be considered a single crystal, recently a nano-porous crystal of a few micron was investigated using a microfocused X-ray beam of 1 mu m.[1] The advances in X-ray single crystal diffraction at synchrotrons have been aided by the abundant flux and improvements of optical elements. Reactor based neutron sources have only seen minor improvements in flux compared to synchrotrons and the nature of the neutrons makes it difficult to construct optical devices. However, advances in area detectors systems and white beam diffraction methods have allow a considerable reduction of crystal size need for a neutron diffraction experiment. The size has been reduced by about two orders of magnitude from about 1 mm^3 to 0.01 mm^3. This is by no means comparable to the improvements of synchrotrons, but it allows neutron investigation of single crystals suitable for laboratory X-rays. The possibility of using relative small crystals allow exploiting the complementarities between X-rays and neutrons, without going through the effort of growing large single crystals for the neutron experiment. We present data from Laue diffraction instruments: Vivaldi, ILL and KOALA, at the new reactor source OPAL, Australia. The white beam Laue technique has been employed to elucidate the oxygen positions in layer misfit cobaltite of small single crystals V of about 0.01 mm^3. The high intensity of the white beam and the large coverage by the cylindrical area detector are crucial for reasonable data collection times.
[1] C. Volkringer et al. Nat. Mat. (2007), 6, 760-764

Keywords: Laue diffraction, neutron diffraction techniques, mixed layer compounds

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Unconventional single crystal diffraction studies with hot neutrons on HEiDi at FRM II

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The instrument HEiDi at the neutron source Heinz Maier-Leibnitz (FRM II) uses hot neutrons for single crystal diffraction analysis of structural and magnetic properties of samples for which other methods are not applicable. Multiferroic compounds like $REMnO_3$ (RE=Dy, Gd) whose highly absorbing and heavy rare earth elements make it normally extremely difficult to get accurate structural and magnetic diffraction data are good examples for the unique capabilities of this instrument using both large penetration depth and large q range [1]. This contribution shows an overview of the instrument (like gain factor from hot source, see figure and [2]) and its applications in different fields of solid state physics, chemistry and crystallography concerning structural details (highly accurate atomic positions, anisotropic mean square displacements, phase transitions, local disorder, magnetism, etc.).
References:
[1] *Magnetic Structure of $GdMnO_3$*. A. Möchel; J. Voigt; M. Meven, J.-W. Kim; and T. Brückel; Verhandlungen der Deutschen Physikalischen Gesellschaft, R. 6, Bd. 43, MA 29.2 (2008).
[2] *HEiDi:...*; Meven M., Hutanu, V.; Heger, G.; Neutron News 18,

19-21 (2007).

Keywords: multiferroics, neutron diffraction, high resolution

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New design for D16 at the ILL

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D16 is one of ILL's cold neutron diffractometer. It is a 2-axis small-momentum transfer diffractometer with variable vertical focussing, for the study of partially ordered structures such as stacked membranes or clays. The scattering geometry obtained with large, vertically oriented samples, profits the most from the large vertical cross section of the beam at the sample position. A high-resolution SANS setup is used routinely in experiments requiring the 1% wavelength band width and the high angular resolution of the instrument. Because of its special characteristics, D16 remains unequaled for the study of a wide range of systems in biology, physics and material science. In the last decade D16 has undergone several major upgrades: in 1999 with a completely new design, in 2007, in the frame of the ILL millennium program the instrument has been re-sitted and the design revisited. In 2008 D16 will have a new high resolution, high count rate detector (MILAND). The poster will present the new design, the major characteristics and performances of the instrument, as well as recent examples of experiments performed on D16.

Keywords: neutron diffraction, SANS, instrumentation

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CG2 general-purpose high-flux SANS instrument at HFIR at Oak Ridge National Laboratory

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Within the past year, the High Flux Isotope Reactor (HFIR) has resumed routine operation and service to the scientific user community with a number of significant upgrades. Among the most important of these is a new supercritical hydrogen moderator (T ~ 20 K) that is the brightest cold source currently available. While this will eventually provide neutrons to a whole suite of scattering instruments through four cold neutron guides, the two flagship instruments, new small-angle neutron scattering (SANS) instruments on CG2 and CG3 have been installed and commissioned. The CG2 SANS (General Purpose SANS, also known as SANS1, funded by the Department of Energy (DOE) Office of Basic Energy Sciences) is a 40m maximum total flight path pinhole SANS instrument variable wavelength and a large area (1m^2 squared) high count-rate, (more than 100 counts/pixel/s) high-resolution (5mm^2 pixels) detector that can translate from 0 to 45 cm off-axis to increase the dynamic Q-range (~0.001-1 A^{-1} overall). With a measured flux on sample of 10^7/sec/cm^2 and beyond in high-throughput configurations, this instrument is comparable to the best worldwide. This dramatically improves both the quantity and quality of data that we can collect from samples from a variety of systems, enabling us to better serve the neutron scattering community. At the time of this abstract the instrument has successfully operated for 7 reactor cycles, including 3 in which it was fully available to users through an open, peer-reviewed proposal system.

Keywords: instrumentation, SANS, neutron scattering techniques

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Neutron transmission strain tomography

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In many respects, strain mapping by neutron and synchrotron X-ray diffraction can be regarded as imaging techniques in 2D or 3D, i.e. the spatially resolved determination of a material property within the interior of an object. However, whereas in the conventional sense 3D imaging is normally concerned with the spatial variation of attenuation coefficient, in the case of strain mapping it is the spatial variation of elastic strain which is being imaged. The aim of the study here is to present the concept of strain tomography using Bragg edge neutron transmission measurements. The principle of this novel approach is to analyze residual strain fields by de-convolution of unknown distributions of residual elastic strains from redundant sets of data collected from gauge volumes representing sections through the region of interest. The setup of Bragg edge neutron transmission measurement is such that the gauge volume represents the complete trace of the incident beam through the sample. As a result, each individual measurement can be thought to represent an average strain within the sampling volume. Thus, the strain variation within the gauge volume may be significant. On the other hand, a data set collected over a range of positions and rotations allow the possibility of reconstructing the entire strain distribution within the interior of an object. This study illustrates the application of the principle using neutron transmission Bragg edge measurements on a well characterized VAMAS round robin shrink fitted Al ring and plug sample. The large strain discontinuity present within the sample was successfully resolved and the prediction of hoop and radial strain showed very good agreement with the known strain field within the sample.

Keywords: neutron transmission, Bragg edge, residual stress

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BioRef - a time-of-flight reflectometer at Hahn-Meitner Institute Berlin

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