

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 throughput small molecule crystallography of moderately sized and complex unit cells (up to around $(50 \text{ \AA})^3$). 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 μm . [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 GdMnO₃*. 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,