P.01.02.12
Acta Cryst. (2005). A**61**, C138

Time-resolved and Charge-density Studies at ChemMatCARS

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ChemMatCARS, a synchrotron-based national facility for Chemistry and Materials Science located at the Advanced Photon Source, is developing strong programs in time-resolved, charge-density, and micro (~10 μm) crystallography. This presentation will focus on the time-resolved and charge-density capabilities at the sector.

In small-molecule time-resolved studies, monochromatic x-rays are used to probe optically pumped molecular excited states. Experiments are performed using a rotating chopper wheel to gate the x-ray source and trigger the laser. Results show significant changes in molecular structure after laser excitation[1].

Recently, several experimental runs were devoted to assessing whether or not the beamline/instrument quality was sufficient for precision charge-density measurements[2]. For these high-resolution studies, a relatively short wavelength is used (λ=0.42 Å) typically yielding an instrument resolution of 1.34 $Å^{-1}$. These experiments produced R internal values as low as R_{int}~0.02.

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Keywords: time-resolved, charge-density, synchrotron

P.01.02.13
Acta Cryst. (2005). A**61**, C138

A Comprehensive Environment for Doing Macromolecular Crystallography at SSRL

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The Macromolecular Crystallography (MC) group at Stanford Synchrotron Radiation Laboratory is currently developing, maintaining and providing support at 5 experimental stations, with 2 more under construction. A considerable effort is put into designing an efficient and intuitive environment that makes the experiment as productive as possible for the visiting scientists.

All MC beam lines now provide automated mounting and screening of samples, a feature, largely driven by the high throughput crystallography and structural genomics projects, that is now made available to all users. New tools for accessing resources at SSRL remotely have been added recently. A Linux based terminal server, NX by NoMachine, allows for secure and responsive remote graphical sessions in which the data collection and processing environment is nearly identical to that locally on the beam line. Several new and improved web based applications for diffraction image viewing, analysis, auto-indexing and strategy calculation are provided under the umbrella of the WebIce project. Many enhancements have been made to the beam line control software, BluIce, to make screening and sample robot operation easy and safe to use. More data backup options and tools make it easier for each user to find the best option.

The combination of advanced automation at the beam lines and remote access to all data collection resources provide users with the choice of just sending a cassette with samples to SSRL and conduct the experiment entirely from their home lab.

Keywords: remote access crystallography, synchrotron beam line, experiment control

P.01.02.14
Acta Cryst. (2005). A**61**, C138

Development of Protein Crystallography Beamlines at the Photon Factory for Automated Experiment

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We have completed the construction of two ID beam lines (AR-NW12 and BL-5) for protein crystallography at the Photon Factory, both of which were designed for efficient MAD experiments. In addition, a new beamline BL17, dedecated to the measurement for crystals of micron size, is under construction while refurbishing existing beamlines. The newly developed beam lines have the following features: (1) high-speed data acquisition using CCD detectors, (2) fast and reliable tuneability of X-ray energy with DCM, (3) extremely precise samle rotation axes, and (4) motorized stages in the experimental stations. To operate all the beamlines efficiently, a network-based beam line control system has been developed, which provides not only a common user interface but also a function to enable remote experiments through secure TCP/IP communication. As part of the system, software using relational database has also been developed to keep all the necessary information related to PX experiments. Together with the sample exchange robots installed on the ID beamlines, fully automated experiments will become available.

Keywords: protein crystallography with synchrotron radiation, automated data collection, remote control

P.01.02.15
Acta Cryst. (2005). A**61**, C138

New Optical Design and Performance of the NSLS X21 X-ray Wiggler Beamline

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For 10 years, the X21 x-ray beamline at NSLS, whose radiation source is a hybrid wiggler, was dedicated to inelastic x-ray scattering studies of electronic excitations in condensed matter. Its optical design consisted of a dispersive four-reflection Si(220) monochromator followed by a bent cylindrical mirror, that delivered an energy resolution of 0.2 eV at 8 keV.

The two X21 experimental stations were rebuilt to accommodate new experimental programs that address elastic x-ray scattering studies of materials under high magnetic fields, thin films grown in-situ, and materials studied with small angle x-ray scattering, with appropriate setups permanently installed in the stations. To meet the needs of these programs, the beamline optics have been re-designed. The first component is a new non-dispersive double silicon crystal or multilayer monochromator, which contains selectable pairs of silicon crystals or multilayer elements that can be chosen in-situ to suit the experiment at hand. The first silicon crystal and multilayer element are mounted side-by-side on a helium-gas-cooled cryogenic support, that serves to suppress thermal distortions of the crystal or multilayer when subjected to the 500 W wiggler beam. The monochromatic beam that emanates can be used as is, or further conditioned by the existing four-reflection Si(220) monochromator which remains, if high energy resolution is desired. Finally, the beam is then focused and delivered to the appropriate experimental setup by one of two bent cylindrical mirrors, each of which is shaped to focus the beam into one or the other station.

Performance results and experimental highlights from the first year of operation of this beamline, in its new configuration, will be presented.

Research carried out at NSLS, Brookhaven National Laboratory, which is supported by the US Dept. of Energy, Office of Basic Energy Sciences under Contract No. DE-AC02-98CH10886.

Keywords: synchrotron radiation optics, synchrotron X-ray diffraction, synchrotron X-ray instrumentation