P.01.15.2
Acta Cryst. (2005). A**61**, C149
Symmetrisation of Powder Diffraction Peak Profiles by a Fourier Method
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Powder diffraction intensity data with asymmetric peak profiles measured with a conventional Bragg-Brentano diffractometer and a high-resolution synchrotron diffractometer are treated with a fast Fourier transformation method [1, 2] to obtain intensity data with symmetric peak profiles. The method is based on deconvolution of analytical expressions of the optical aberrations of the diffractometers [3-6]. The symmetrised peak profiles enable simplified analytical procedures for individual peak profile fitting, whole pattern decomposition and Rietveld refinement.

The symmetrised diffraction data of fine SiC powder (JFCC, RP-2) measured with a conventional powder diffractometer has revealed a "super-Lorentzian" character of intrinsic diffraction peak profiles, which is reasonably explained by a theory for diffraction from small spherical crystallites with broad log-normal size distribution [7]. The results of a least-squares refinement applied to integrated intensity values of 42 reflections extracted from symmetrised high-resolution diffraction data of standard ZnO powder (NIST, SRM674) measured at Photon Factory in Tsukuba has been coincidence factor of R = 0.45% with reasonable structure parameters.

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Keywords: powder diffraction, profile analysis, Fourier methods

P.01.15.3
Acta Cryst. (2005). A**61**, C149
The Role of *e*-Science in Service Crystallography: The UK National Crystallography Service on the Grid
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The The EPSRC funded UK National Crystallography Service (NCS) facility has been exploring the use of Web/Grid services in e-Science applications. The NCS approach [1], [2] combines aspects of software and instrument automation to produce a service that increases user interaction and provides sample submission and data acquisition, processing and analysis services on the Grid.

A prospective user of the NCS applies for an allocation by filling in an electronic form and uploading a case for support, initiating the metadata capture process. Following successful peer review, the user and is provided with digital keys that enable secure access to the NCS Grid Facility. The user may now submit samples to the NCS through an electronic interface, which gathers all the chemical metadata concerning the sample, e.g. synthetic pathway, proposed formula 2D structure, sensitivity, COSHH safety information, etc.

A sample status database is used to monitor the progress of sample(s) in the queuing system. When a sample is scheduled for examination the user may initiate a secure, Web services based, interactive experiment from the sample status database. The crystal is mounted on the diffractometer by the sample changing robot or by a service operator. The user is then involved in a series of decision making stages, either automatically or with the service operator, which control the outcome of the unit cell determination and data collection procedures. At the conclusion of the experiment the data is automatically processed and made available to the user for download.

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Keywords: e-science, service crystallography, grid computing

P.01.15.4
Acta Cryst. (2005). A**61**, C149
Automated Data Collection at the IMCA-CAT Advanced Photon Source User Facility
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The Industrial Macromolecular Crystallography Association Collaborative Access Team operates a data collection facility for protein crystallography at the Advanced Photon Source. The IMCA-CAT insertion device beam line is the only facility for protein crystallography at APS currently offering fully functional robotics for routine use. A Rigaku/MSC ACTOR robot provides automated mounting, centering and retrieval of protein samples. Integrated with user-friendly software, robotics enables high-throughput sample screening and unattended data acquisition according to user–programmed schedules, thus significantly reducing both the time necessary for crystal screening and the need for direct operator interaction.

While targeting the needs of drug discovery research for IMCA member pharmaceutical companies, the automation capabilities at IMCA-CAT are also ideally suited for structural genomics and other research efforts requiring high-throughput experiments. IMCA-CAT facilities are available to interested researchers through the APS General User Program.
Keywords: synchrotron beamline, automation, robotics

P.01.15.5
Acta Cryst. (2005). A**61**, C149
An Ultra-fast Mechanical Shutter for Sub-microsecond Time-resolved Experiments
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A new high speed, high rep-rate X-ray beam shutter for time-resolved photo crystallography [1] at synchrotron sources has been developed and tested. The new design is based on a commercially existing DC servomotor and a frequency-lock control capable Linear Amplifier. Accurate speed control combined with an air bearing results in extremely low jitter in the motor rotation. Measured jitter at rotation speeds of 200 Hz to 500 Hz is less than 2 ns at a 6σ level confidence. The chopper disk is interchangeable, allowing maximum flexibility. The current chopper disc with 45 radial slots allows synchronizing with the APS storage ring from the 12th to the 24th subfrequencies, corresponding to X-ray pulse frequencies of 11.3 to 22.6 kHz. At 30000 RPM the opening time for 350 μm slots is 1.65 μs, i.e. less than half the orbit time at the APS source. Results demonstrate that low cost components can be used to build an exceptionally precise instrument. The shutter provides high accuracy and efficient use of X-rays at a modest cost.

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Keywords: photo-crystallography, synchrotron, ultra-fast shutter

P.01.15.6
Acta Cryst. (2005). A**61**, C149-C150
High-throughput Protein Crystallization
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For high-throughput protein crystallography, we are developing a fully automated X-ray structural analysis system that consists of several subsystems for protein crystallization, harvesting and freezing