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G-ROB, a 6-Axis Robotic Arm Based AUTOMATED System for Crystallography. Franck Borel[a], Xavier Vernede[a], Jacques Joly[a], Phillipe Charrault[a], Michel Pirocchi[a], Florian Bouis[a], Julie Quilez[a], Gael Pages[a], Jean-Luc Ferrer[a]. [a]*Institut de Biologie Structurale J.-P. Ebel, Grenoble, France.*
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The G-Rob system was developed on beamline FIP-BM30A at the ESRF, as a continuation of the CATS system [1], a successful sample changer (~11 units currently installed on various synchrotrons, such as SLS, BESSY, Diamond, APS, Alba ...). G-Rob, a 6-axis robotic arm based system, is a fully integrated device that provides unique technical performances for crystallography beamlines as well as laboratories.
G-Rob is an "all in one" system, since it integrates the following functions:
- sample changer (transfer of the frozen sample from the Dewar to the beam)
- goniometer for frozen samples, capillaries, ...[2]
- plate/µ-chip screening for in situ analysis of diffraction condition and data collection [3]
- goniometer for non-classical sample environments (high pressure cells, ...)
G-Rob provides unique features:
- it is automated: thanks to its tool changer, it switches automatically from one application to another
- it is highly flexible:
1. if a new application or a new sample format emerges in the community, it's just a new tool to be designed, and G-Rob can work with that new application or sample;
1. G-Rob's hardware interface and software are open, so anyone can develop new tools and bring them on any G-Rob platform.
- it is highly reliable: G-Rob is based on well-known, industrial quality equipments with reduced maintenance.
G-Rob is commercialized via a partnership between IRELEC (commercializes the CATS systems), and NatX-ray, the start-up in charge of the industrialization of the G-Rob developments made on the FIP-BM30A beamline (www.natx-ray.com). G-Rob is the generic name for a full range of modular robotized systems, going from the robotized part alone specifically designed for beamlines, to more complete systems that include an X-ray source and a detector. The version designed for beamlines is currently in use on FIP-BM30A. It was made available to the research community in 2007 and up to now, users have expressed an unprecedented high degree of satisfaction. Several results obtained on FIP-BM30A will be presented, such as in situ screening of membrane proteins, ribosome, high pressure protein diffraction, etc...).

[1]. Ohana et al., *J. Applied. Cryst.*, 37, **2004**, 72-77. [2]. Jacquamet et al., *Acta Cryst.* D60, **2004**, 888-894. [3]. Jacquamet et al., *Structure* 12, **2004**, 1219-1225.

FA5-MS03-P02

X06DA, A Versatile Protein Crystallography Beamline at the Swiss Light Source. Vincent Olieric[a], Meitian Wang[a], Rouven Bingel-Erlenmeyer[a], Roman Schneider[a], Claude Pradervand[a], Wayne Glettig[a], Takashi Tomizaki[a], Ezequiel Panepucci[a], Vincent Thominet[a], Jose Gabadinho[a], Elke Zimoch[a], Andreas Isenegger[a], Clemens Schulze-Briese[a]. [a]*Swiss Light Source, PSI, 5232 Villigen PSI, Switzerland.*
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X06DA is the third macromolecular crystallography beamline at the Swiss Light Source. It receives light from a 2.9 T superbend magnet and has been designed to fulfill the requirements of both academic and industrial users. To achieve maximum efficiency, high degree of automation was implemented from the optics to the experimental environment. X06DA is equipped of a Bartels dual channel cut monochromator (DCCM) that ensures rapid energy changes with a true fixed position. The resulting beam size is of 90 x 70 microns at the sample position with a total photon flux 5E11 photons/sec, *i.e.*, comparable to an undulator beamline. The experimental station offers both rapid manual mounting with a mini-hutch design and automatic robotic sample mounting (CATS from IRELEC). In addition, a crystallization facility is currently being integrated next to the experimental mini-hutch and will allow automated transfer of crystallization plates for *in-situ* diffraction screening. Current status and future development of this new beamline will be described. Recent crystallographic results collected at X06DA such as the first successful phasing by P-SAD of a medium-size RNA molecule (27 nucleotides) will be presented as well.

Keywords: crystallography instrumentation; automation; phasing

FA5-MS03-P03

Compact Multi-Crystal Analyzer and Its Applications to Crystal Structure Analysis. Hisashi Konaka[a], Akito Sasaki[a], Hideo Toraya[a]. [a]*X-ray Research Laboratory, Rigaku Corporation, Japan.*
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It is important to obtain a high angular-resolution data for all powder x-ray diffraction profile analysis, such as qualitative and quantitative phase analysis, powder pattern indexing, *ab initio* structure determination, structure refinement, etc. However, it is unavoidable to trade intensity in return for high resolution.
We have been developed a new compact multi-crystal analyzer called CALSA consisting of ten pieces of Ge crystals coupled with a 1D-SSD (Si strip detector). Using the analyzer attached to a laboratory diffractometer system (SmartLab), the diffraction data of some powder samples were measured with considerably high angular-resolution (0.018 degree in FWHM for the 110 reflection from NIST SRM 660a LaB_6). The features of this multi-crystal analyzer are the capabilities to apply to parallel beam optics

for obtaining ten times higher intensity than that of the ordinary-type single crystal analyzer with equal resolution. Experimental details and applications to structure analysis such as Rietveld refinement will be reported.

Keywords: multi-crystal analyzer; high angular-resolution; crystal structure analysis

FA5-MS03-P04

The Precision of XRD Apparatus Can Be Assessed by Accounting for Secondary Extinction of a Single Reflection.

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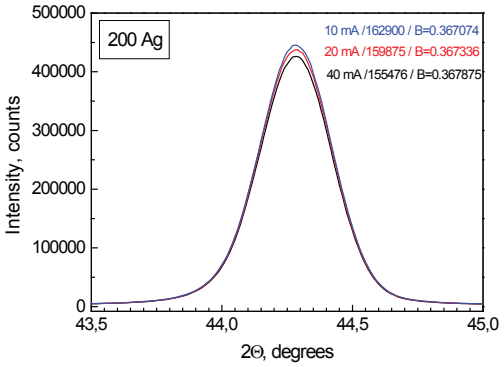
The purpose of this study is to gain insight into the operative capabilities of XRD apparatus to supply measurement data informative for its precision. One can assess apparatus precision using parameterized criteria bounded inextricably by a measurement procedure that insists particularly on a change of the incident X-ray beam intensity I_0. Quantifying kinematical intensity I_{kin} [$=PI_0QS/2\mu$] and secondary extinction (SE) coefficient g [$=kPI_0S/2\mu$], the intensity I_0 defines the level of interaction between X-radiation and crystal media. Here P is the texture factor (pole density): it represents the relative volume fraction of crystallites whose <*hkl*>-poles contribute to reflection [1], k is the empirical extinction coefficient, and other symbols have their usual meaning (see [2] as well). The second equation above read that decrease of the level of interaction of *the diffraction process* is controlled by g in terms of I_0 under otherwise equal conditions. Hence, the intensity measured at a level of interaction is affected by SE as strongly as higher I_0 is. This is illustrated by the figure below showing profiles of 200 reflection corresponding to the main <100> component of a textured sample of silver measured at three different levels of interaction under the same time(τ)-generator current(i)-factor as defined: $\tau i = \tau^* i^* = \tau^{**} i^{**}$. The legend inside the figure represents i-values used to cause discrete changes in the I_0-intensities that reflect in the areas under profiles and integral breadths B due to respective SE effects. Whereas these measurements show a simple qualifying of the SE effects, the single reflection method [2] is a proper tool for quantification of the same data.



[1] Bunge. H. J. **1997**. *Textures and Microstructures*. 29, 1-26. [2] I.Tomov, **2007**. *Z. Kristallog*. Suppl. 26, 131-136.

Keywords: precision; X-ray diffraction apparatus; secondary extinction