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Metrological Assurance of the Substance and Materials Investigations by Diffraction Methods
B.N. Kodess, S.A. Kononogov, *Crystals Metrology Dept. CMD, of VNIIMS, Russia.* E-mail: bnkodess-vm@vniims.ru

Volume and reliability of information about the properties of crystalline substances and materials are frequently determined by the optimum experiment planning and application of the corresponding equipment. However, solving of reverse type problem on the obtaining the characteristics of crystals from the diffraction pattern is determined by the level of the development of data processing methods and by the quality of the chosen starting model. The latter component is connected to some extent with intuition and researcher confidence in the admissibility of the model used.

Crystals Metrology Dept. (CMD) develops metrological assurance for the diffraction measuring instruments. For practical Crystals Metrology this assurance includes the system of the Certified Standard Reference Materials (SRM) diffraction properties of materials, Procedures of Measurements, Databases, Sequence of test steps and other normative documents for the tests according to declared functions (designations) of diffraction equipment (for Type Approval and conformity tests). CMD organizes and processes the data of interlaboratory experiments of round-robin type, carries out its own experiments of high and the highest accuracy for some poly- and single-crystals key materials of modern technologies, develops the methods for investigation and characterization of new complex substances, including certification of medications and determination of resources of materials and products made of these materials. The task of establishment of reproducible Mass Unit (both as the characteristic of a Substance Quantity and the characteristic of its inertness measure - gravitational constituent - namely the Kilogram Unit on the basis of high-clean certified Silicon) remains urgent among CMD basic tasks of fundamental Diffraction Crystals Metrology the same as the task of the interrelation of the basic units of SI.
Keywords: materials metrology, data accuracy, standard reference samples

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The EU BIOXHIT Standard Test Crystal
Ina Dix[a], Madhumati Sevvana[a], Gábor Bunkóczi[b], Judit É. Debreczeni[b], George M. Sheldrick[a], [a]*Dept. Structural Chemistry, University of Göttingen, Tammannstr. 4, 37077 Göttingen, Germany.* [b]*SGC, Botnar Reseach Centre, University of Oxford.* E-mail: inadix@shelx.uni-ac.gwdg.de

The standard test crystal is intended to provide an automated, fast and robust procedure for identifying potential problems in the complex hardware and software infrastructure of modern protein crystallographic (PX) synchrotron beamlines.

A quick test dataset should be collected whenever changes have been made to the hardware or problems are suspected. Indeed, for highly automated pipelines the first crystal in the dewar could be a test crystal in case the robot drops it! The test crystal should have high symmetry so that a short rotation about a single axis suffices to collect redundant data, the crystals should be easy to obtain and freeze reproducibly giving a small mosaic spread. The cubic form of insulin fulfils all these conditions and has been used in our tests so far, however we are also looking for possible inorganic test crystals for Se-MAD beamlines.

The diagnostics should be independent of the data integration software employed, so as a first step we have compared the processing of cubic insulin data using the widely used programs XDS, MOSFLM/SCALA and HKL2000. We will present our experiences with test crystal data collected on a number of the participating beamlines in the BIOXHIT consortium.

We are grateful to the EU for support (LHSG-CT-2003-503420) and to the other BIOXHIT partners for the fruitful collaboration.
Keywords: synchrotron structural biology research, diagnostics, test crystal

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Strain Analysis using High Energy X-ray White Beam Diffraction
Alexander Korsunsky[a], Jian Liu[b] , Mina Golshan[c], [a]*Department of Engineering,University of Oxford, OX1 3PJ, UK.* [b]*Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, UK.* [c]*Daresbury Laboratory, Warrington,Cheshire, WA4 4AD, UK.* E-mail: alexander.korsunsky@eng.ox.ac.uk

One of the principal advantages of energy-dispersive diffraction for the determination of macroscopic average lattice parameters (and hence strain) is the possibility of refinement of the large section of the diffraction pattern, leading to improved accuracy and stability of interpretation. Precise channel to energy conversion is very important in full-pattern refinement in energy-dispersive X-ray diffraction. The channel to energy conversion of most detectors is not entirely linear. This presents an obstacle to obtaining accurate quantitative data for lattice strains by pattern refinement. We present a procedure for precise energy calibration determination, and show how the new energy conversion function was used successfully to perform whole pattern fitting of energy-dispersive X-ray diffraction patterns of Ti64 samples. The strain across the Ti64 bar calculated from the fitting results was compared with the profile obtained by single wavelength X-ray diffraction utilising Laue monochromator, and showed excellent agreement.
Keywords: energy-dispersive diffraction, synchrotron radiation, titanium alloy

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Improving Data Quality – without having to grow new Crystals
Anita Coetzee[a], Bram Schierbeek[a], Gregor Witte[b], Ute Curth[b], Dietmar J. Manstein[b], Roman Fedorov[b], [a] *Bruker AXS B.V. Delft, The Netherlands.* [b] *Institute for Biophysical Chemistry, Hanover Medical School, Hanover, Germany.* E-mail: anita.coetzee@bruker-axs.nl

In order to obtain the best possible results for structure solution and refinement, it is imperative to collect the best quality data from a given crystal. This generally means measuring the highest possible resolution data. With recent advances in microfocus X-ray sources, such as the MicroStar, more brilliant sources are available to evaluate very small crystals in-house. Combining these sources with the latest developments in graded multilayer optics can result in excellent data being measured at home on samples that were previously only tractable at the synchrotron. Using a kappa-goniostat in combination with sophisticated data collection strategy software can ensure that a complete dataset is measured up to the diffraction limit of the crystal. The combination of high resolution, completeness and redundancy can improve the data quality significantly. In this study we will show examples of how data quality can be improved. It was possible to trace more residues in a dimeric single-stranded DNA binding protein, by collecting a dataset using the strategy program COSMO [1] in combination with the 4-circle goniometer on the X8 Proteum.

[1] COSMO, Data collection strategy program, Bruker AXS
Keywords: data collection, protein crystallography, detectors

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High Resolution Data Collection in the Home Lab
Matthew M. Benning, Cary B. Bauer, *Bruker AXS Inc.,5465 East Cheryl Parkway, Madison, WI 53711 USA.* E-mail: mbenning@bruker-axs.com

Data collection on protein crystals to very high resolution (> 1.3Å) typically requires a trip to the synchrotron. Due to advances in optics and the introduction of micro-focus rotating anode generators, there has been a remarkable increase in brightness and flux density available in home laboratory systems. When combined with ultra-sensitive detectors, these systems provide an alternative means of