collected with it at 8 keV. Within the argument favoring the hybrid pixel detectors, one is related to its point spread function which is nearly limited by the pixel size. Data have been collected on the Small Angle X ray Scattering camera of BM2/ESRF using the same setting with XPAD3 and the beamline CCD camera show that not only the hybrid pixel detector allow higher count rate but it allows to measure weaker signals.

1 Basolo S. et al., J. Synchrotron. Rad, 2007
2 Pangaud et al. NIM A, 2008, in press
3 Basolo S. et al. , NIM A 2008, in press

Keywords: detector development, CCD detectors, SAXS

P01.11.73

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More signal, less noise : Making good use of bright sources & fast detectors

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With the availability of in-house high-brilliance X-ray sources, highly reflective X-ray optics and low-noise, fast read-out detectors we have the tools available to screen protein crystals and often to collect complete data sets in the home laboratory. For CCD detectors the read out time is in the order of seconds. New types of high-speed detectors with zero dead-time are now on the horizon. For in-house use we have recently released the ÅXIOM 200, a gas-filled Microgap detector. This is a high speed photon-counting detector with no intrinsic noise. The zero read-time allows shutter-free data collection and infinitely fine slicing. The availability of these new properties opens avenues for new protocols for crystal screening and data collection, which exploit the benefits of this new detector. By using these new protocols it is possible to get much more accurate data then would be obtained with traditional detectors and data collection methods. The new data collection method can lead to a dramatic rise in signal to noise ratio, with the same amount of X-ray photons falling on the crystal. This increases the chances of a structure solution using SAD phasing, as the solution of the sub-structure will be more straightforward and solvent flattening will more rapidly converge.

Keywords: high speed detectors, accurate intensity data collection, SAD phasing

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DATAVIEW: A new post processing analysis tool

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CCD detectors have become the standard in modern X-ray laboratories. The use of 'black box' methodologies (integration) to convert diffraction images into discrete hkl's and intensities, has led to the possibility of systematic errors creeping into any given dataset. Multi-scan absorption techniques such as SADABS[1], given sufficient redundancy, smooth out random errors and can potentially highlight the more significant systematic errors, such as an incorrect masking of the primary beamstop. Potentially far more damaging are the possibilities of inaccurate detector corrections being applied to the data during the integration phase of data processing. These corrections, which are necessarily machine dependant, may require modification after initial instrument installation. Analysis of the effects of these corrections on real data can in principle be conducted relatively easily, although can be time consuming. Data will be presented demonstrating a new program (DATAVIEW[2]) that reads raw integrated diffraction data and presents graphical representations of the internal data integrity. The output will also provide a suggested improvement to the data treatment during integration, highlighting potential corrections that may not have been applied correctly. DATAVIEW currently operates on Bruker .raw data but could easily be converted to read multiple data formats.

1. SADABS, Multi-scan absorption correction, Sheldrick, G.M. (2003)
2. DATAVIEW, Post Processing Data Analysis Tool, Probert, M.R. (2008)

Keywords: accurate measurement, data processing optimization, X-ray diffraction data

P01.12.75

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A hyperquenching tool

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It has been clearly elucidated by Warkentin, M. et al that the removal of the cold gas layer above liquid nitrogen in a dewar dramatically increases the cooling rate of a protein crystal (Warkentin, M., Berejnov, V., Husseini, N. and Thorne, R. "Hyperquenching for protein cryocrystallography" J. Appl. Cryst. (2006). 39, 805-811) . By removing the cold gas layer, one can not only raise the success rate but also reduce concentrations of cryoprotectant therefore minimize damages to crystals caused by changes in osmotic pressure. Being stimulated with this eye-opening study, we created a dewar having a simple mechanism to remove the cold gas layer. It consists of a dewar and a fan and the cold gas layer is suck in to the sideway. We have done a simple measurement and observed rising temperature from -175 to 10 degs. ca. 5mm above the surface of liguid nitrogen. We will perform additional experiments to confirm the effect of the device by the conference.

Keywords: hyperquenching, cryo-crystallography, protein crystal

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In situ crystallizations of Cl and Br substituted anilines and its intermolecular interactions

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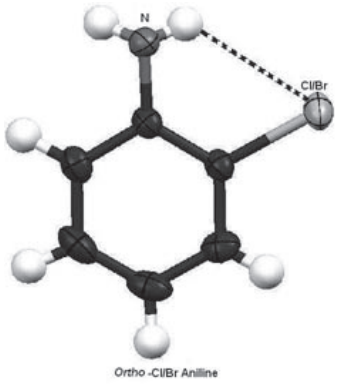
In situ cryocrystallization of a liquid, the subsequent structure determination and its study of intermolecular interactions has emerged as an area of contemporary interest. *In Situ* crystallization of fluoro substituted anilines and evaluation of the variability in halogenated trifluoroacetophenones [1] clearly bring out the importance of interactions generated by fluorine in crystalline

lattices and establishes that indeed fluorine has a directing influence in molecular assembly. In order to evaluate the propensity of interactions in halogens in general *ortho* chloro and *ortho* bromo anilines were crystallized from their respective liquids via *in situ* cryocrystallization method. The crystal structures are isostructural belonging to a trigonal system, space group $P\,3_1$. The crystal packing is due to intramolecular N-H…Cl or Br and intermolecular N-H...N hydrogen bonds. However, in the case of *ortho* bromo aninline short Br...Br contacts (3.64 Å) are observed suggesting that this interaction is a consequence of the size of Br atom.



Ortho -Cl/Br Aniline

1. Deepak Chopra and T. N. Guru Row,*Journal of the Indian Institute of Science*, 2007,**87**, 167

Keywords: cryocrystallography, *in-situ* structure determination, intermolecualr interactions

P01.15.77

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Relation of DLS distribution of protein samples with thermal stability

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With the rise of ultimate methods such as X-ray crystallography and NMR, the number of proteins, of which complete quaternary structure was confirmed, has rapidly increased. To be analyzed by X-ray spectroscopy, protein purification is very important to evaluate the detail of its structure. Sample separation is often used by gel permeation chromatography and it's been checked by poly acrylamide electrophoresis, such as SDS-PAGE, however it is required for crystallography to be purified as a level of quaternary structure of proteins. So we often use the system of dynamic light scattering (DLS). It is expected that protein quality is accepted by result of the DLS distribution below 20% for crystallography, but it's not always. Various kinds of proteins have various kinds of strutures and stiffness for thermal stability, and DLS distribution depends on the aspect ratio of particle or stiffness of the surface. In this study, we discuss relation of DLS distribution of proteins with thermal stability and other factors.

Keywords: dynamic light scattering, polydispersity, protein stability

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Microseed matrix screening: A modified version

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The crystallization of purified proteins has remained one of the bottlenecks for the determination of protein structures by X-ray diffraction methods. The crystallization process can be considered composed of two sequential processes. The first is an initial nucleation step and the second subsequent growth of crystal nuclei to well ordered crystals. A method that influences the first step of this process "Microseed Martix Screening" has recently been published. The method is further development of the work by Ireton and Stoddard [2] aims at influencing the nucleation event in crystallization screens. We report the implementation of and experience of with this method in our laboratory. The seed-bead method is used for preparation of the seed stocks. The protein, reservoir solution and seed stock are pipetted simultaneously using a three-bore dispensing tip mounted on the Oryx 8 robot (Douglas Instruments), setting up screening crystallization experiments with seed stock solution added. The authors of [1] used the method with 5 test proteins and observed that the number of crystals hits increase from 1-9 to 21-63. We have also observed an increased number of crystal hits, but that include both protein crystals ad nonobvious salt crystals. Salts crystals can lead the crystallization experiments astray and consume valuabe time and sample. We have therefore modified the method to inlude two control experiments: 1) Crystallization experiments with the Izit Dye for positive indentification of protin crystals and 2) Crystallization experiments with protein buffer for positive identification of salt crystals.

1. Allan D'Arcy, Frederic Villard and May March Acta Cryst. (2007) D63, p550-554
2. G.A., Ireton and Barry L. Stoddard Acta Cryst (2004) D60, 601-605.

Keywords: crystallization strategies, microseeding, protein crystallization

P01.12.79

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An open and flexible robotic system designed towards autonomous protein crystal harvesting

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Process automation with robotic mounting equipment has become an essential element of modern crystallography facilities, resulting in efficient utilization of valuable X-ray resources. However, serious rate-limiting manual operations persist in the crystal harvesting process. Based on experience gained during development of an operator-assisting universal micromanipulation robot (UMR) prototype, we discuss progress and challenges ahead for the design of a fully autonomous, integrated system capable of reliable harvesting of protein microcrystals. Harvesting of micron-sized objects requires a sophisticated mechanical system, and autonomy means that a capable real-time machine vision system embedded in powerful control software must be developed. The vision system and the mechanical system interact in a complex way, and the demands on the optical system pose additional and formidable design challenges. Real time image processing interfaced with mechanical control and