

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

Acta Cryst. (2008). A64, C193

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

P01.11.74

Acta Cryst. (2008). A64, C193

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

Acta Cryst. (2008). A64, C193

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., Hussein, 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 sideways. We have done a simple measurement and observed rising temperature from -175 to 10 degs. ca. 5mm above the surface of liquid nitrogen. We will perform additional experiments to confirm the effect of the device by the conference.

Keywords: hyperquenching, cryo-crystallography, protein crystal

P01.12.76

Acta Cryst. (2008). A64, C193-194

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