Xspress 3
Application Notes

Macromolecular Crystallography: Application Note

Multiwavelength Anomalous Dispersion (MAD) is a technique frequently used to solve protein crystal structures. With high intensity synchrotron beams it is easy to saturate the fluorescence detector, and as such an ample level of attenuation must be selected, usually through trial and error. This whole process often takes around 10 minutes, compared with 2 minutes for collection of a complete diffraction data set.

Xspress 3 features a unique adaptive filter, which ensures that the readout system very rarely saturates. This coupled with a very fast readout rate means that a typical fluorescence spectrum can be collected in around 1 minute. This short time scale means that is it possible to routinely collect fluorescence spectra from samples at the beginning of an experiment, thus providing insight in to the sample heavy atom content from the outset. Xspress 3 is in use on the micro-focus beamline I24 at Diamond Light Source.

Dr Gwyndaf Evans, Principle Beamline Scientist I24 Microfocus MX beamline, Image © Diamond Light Source

EXAFS: Application Note

EXAFS beamlines commonly make use of SDD and HPGe detectors to record their resultant spectra. Xspress 3 is an advanced readout system for such detectors with readout rates often10x faster than most existing systems. Key features for spectroscopists include Xspress 3's adaptive filter that reduces saturation whilst providing excellent resolution. Existing systems require the incoming beam to be attenuated when saturation occurs, thus lower flux results in slower readout rates. Xspress 3's adaptive filter coupled with fast readout rates means that resultant spectra can be collected significantly quicker, while retaining resolution. This makes it a perfect partner for the QEXAFS mode of operation.

Dr Giannantonio Cibin, Senior Beamline Scientist, B18 Core EXAFS beamline, Image © Diamond Light Source

Xspress 3 is able to show events arriving and being histogrammed in real time giving immediate feedback. The system can also show frames as they appear one by one as QEXAFS scans are run to ensure no time is wasted should a change of instrument or sample settings be required. Window or virtual scalar readout allows simplified data collection, and with Xspress 3 regions can be flexibly chosen such as one region of interest (ROI) of a Kß peak and one for the rest of the data.. Window readout enables the display of a subset of data, such as a predefined peak rather than the whole spectrum. In this case, the full MCA may also be saved so that if the ROI or Window should need expanding or moving, this is possible in post-process. Xspress 3 is currently in use on the Core EXAFS beamline B18 at Diamond Light Source.

Mapping: Application Note

On Stanford Synchrotron Radiation Lightsource beamline 2-3, microfocus fluorescence mapping is a popular technique. It enables users to scan surfaces to provide an elemental map. These maps can take up to 12 hours for large samples. With standard readout systems the shaping time is often set to 1µs so that acceptable resolution is collected at all points. This means that the beam has to be attenuated to ensure that the readout system doesn't become saturated, which would lead to artifacts and unphysical results.

A side effect of this lower flux is that too few photons may be detected from dilute elements in the sample, so the attenuation must be adjusted and dwell times altered. A second scan may also be used, one for high fluorescence samples, one for low. These can then be combined to give a higher dynamic range than was mapped in each individual scan.

However, due to Xspress 3's excellent resolution at low count rates and output rate limit above 3.4 Mcps, little attenuation needs to be used meaning minimal waste of photons and much faster scan speed. In addition, setup time is minimal and only a single scan is needed.

The following maps of the Cu channel of this sample show the impact of the effect noted in the section above: the standard readout system has saturated in the areas that can be seen as the highest intensity in the Xspress 3 map. Without using both systems, the first map may mislead the user into believing that the areas in question have lower concentrations than the surroundings, skewing results and masking correlations.
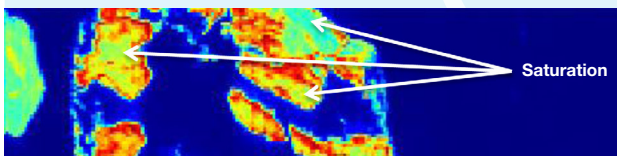
Cu channel Deadtime corrected standard readout system
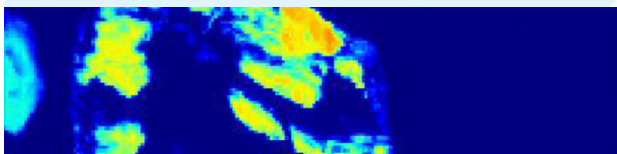

Cu channel Xspress 3

Experimental Setup:

- Beamline 2-3 at the SSRL

- Beam energy 10KeV

- Stream bed sediment mixed element sample from acid mine drainage basin high in Cu and Fe

- Data collected with 50 ms dwell time, 8 micron pixels

- Standard readout and Xspress 3 'T'ed to readout same events from Vortex EX

- Maximum user recorded readout rate: 3.4 Mcps

Mapping: Application Note 2

At GSECARS' 13-ID-D beamline at the APS, Mark Rivers, Matthew Newville and Tony Lanzirotti have collected a wide range of data using mapping and tomography. They have also made significant improvements to the EPICS and stand alone analysis software to aid analysis of the data streamed from Xspress 3.
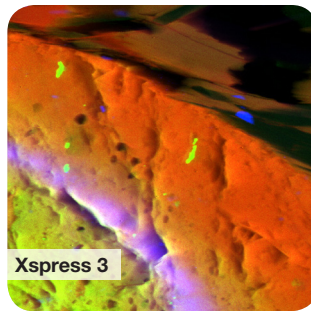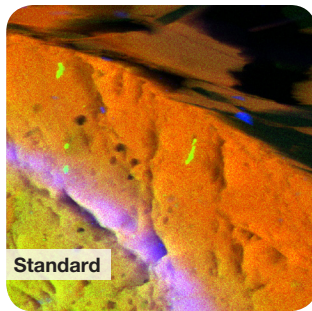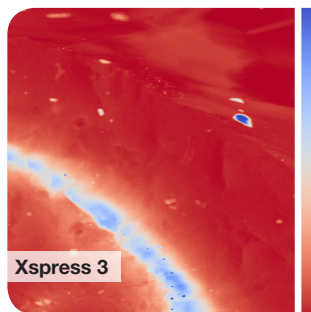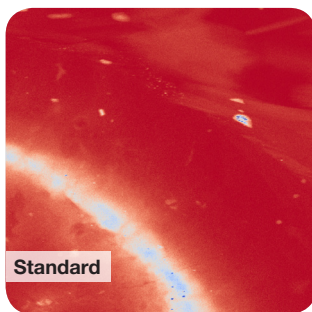

Standard

Xspress 3

Data collected at GSECARS, APS 13-ID-E with a Vortex ME4 and 2 x 2 micron X-ray beam at 18 keV.

1 x 1 mm area, 2 x 2 µm pixels, 10 ms per pixel (45 minute acquisition).

Using standard electronics (1 µs peaking time) and Xspress 3 electronics.

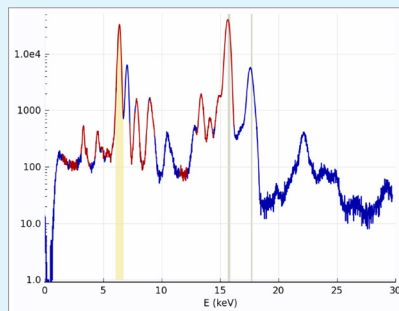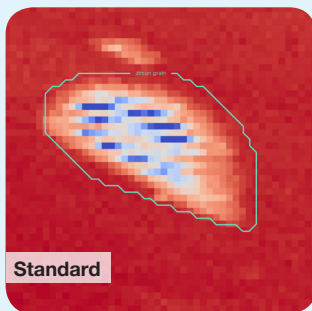Sample: polished thin section of garnet with zoning in yttrium (the purple band).

Fe / **Ca** / **Y**

Standard

Xspress 3

Sample–detector distance ~ 40 mm for Xspress3, 65 mm for a standard readout (to avoid saturation).
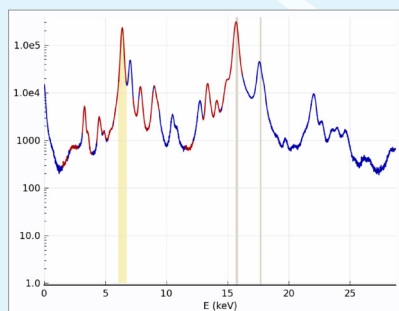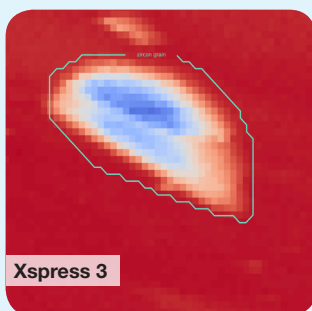
Y intensity map (blue = high intensity).

Signal-to-noise and image contrast are noticeably improved with Xspress3.

Standard

Xspress 3

XRF extracted from zircon grain (574 pixels, 5.7 sec). Count rates (sum of 4 elements, dead time corrected):

◀ **Standard Readout System**

0.456 MHz total,
0.106 MHz Fe Kα,
0.211 MHz Zr Kα.

◀ **Xspress 3**

5.538 MHz total,
1.083 MHz Fe Kα,
2.194 MHz Zr Kα.