The XPDF beamline at Diamond Light Source: An integrated hardware-software approach to X-ray PDF

Philip A. Chater[a], Dean S. Keeble[a], Matthew G. Tucker[a,b], John P. Sutter[a], Michael Hillman[a] & Heribert Wilhelm[a]

[a]Diamond Light Source, Harwell Campus, Didcot, Oxfordshire, OX11 0DE, UK, e-mail: xpdf@diamond.ac.uk

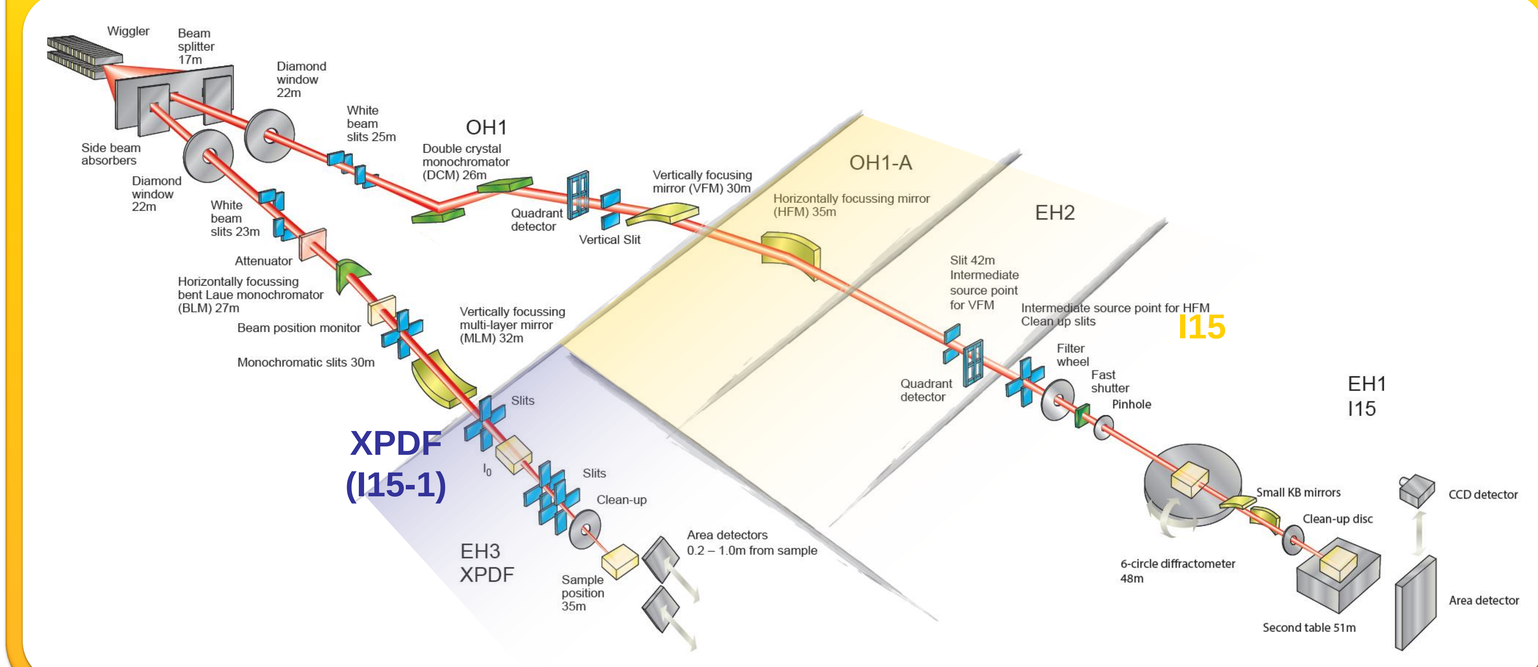
[b]ISIS Facility, Harwell Campus, Didcot, Oxfordshire, OX11 0QX, UK.

Introduction

The importance of understanding local structure is becoming increasingly apparent in diverse disciplines such as materials chemistry, solid-state physics, earth sciences and pharmaceuticals. The pair distribution function (PDF) technique provides a quantitative probe of the local correlations in materials, and as such can be used to drive the refinement of local structure models.[1]

XPDF will be a new, independent side-station to the Extreme Conditions beamline I15. It will be dedicated to the rapid and reliable production of PDF data. Processing software will deliver PDF data in real-time. XPDF is scheduled for First Users in June 2016.

I15 and XPDF Beamline Layout



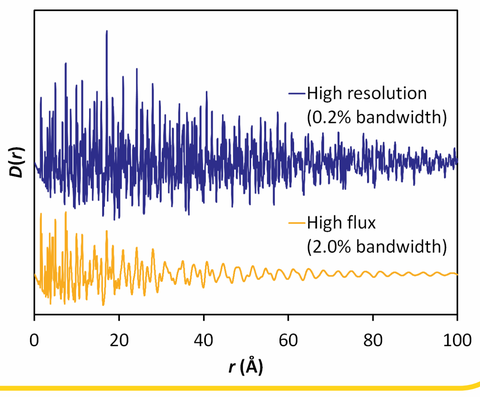
XPDF Hardware

XPDF will share the I15 superconducting wiggler X-ray source, which provides a large horizontal fan of X-rays in the energy range 20-80 keV. The new optics have been optimised to deliver high flux at the high X-ray energies required for PDF measurements.

Bent-Laue Monochromator

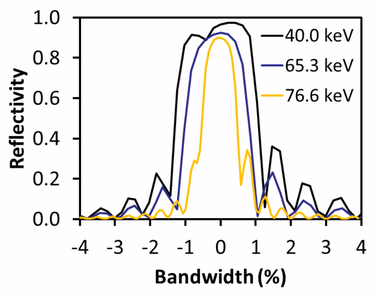
XPDF will use a Laue monochromator with three cryogenically cooled, bent silicon crystals to select X-rays at three energies. Meridional crystal bending will achieve focussing in the horizontal plane to a beam size of ~700 μm. The bandwidth and flux at the sample position will be tuneable to the requirements of the experiment.

Silicon crystal	(111)	(220)	(311)
Energy (keV)	40.0	65.4	76.6
Wavelength (Å)	0.310	0.190	0.162
Q_{max} (Å^{-1})	21.5	35.1	41.2
Bandwidth (%)	0.05 to 2.0		



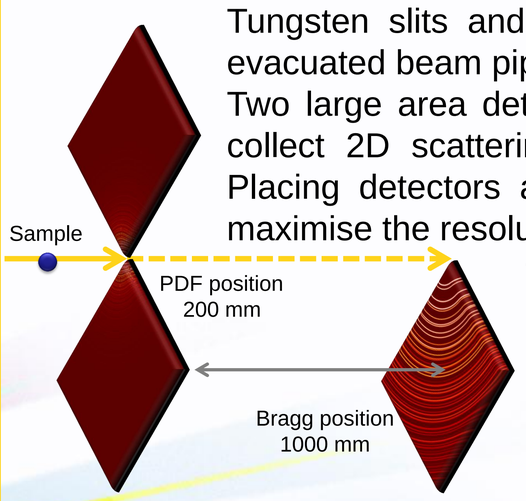
Multi-layer Mirror

A one meter long, elliptically-bent bimorph mirror provides focussing in the vertical plane down to a beam size of ~20 μm. Three stripes of laterally graded multi-layer coating will deliver high reflectivity and provide harmonic rejection.



Endstation

Tungsten slits and collimation, mounted inside an evacuated beam pipe, will provide a low background. Two large area detectors (430 mm × 430 mm) will collect 2D scattering data over a wide Q range. Placing detectors above and below the beam will maximise the resolution of the scattering data.



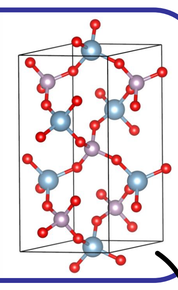
The two detectors will move independently along the beam direction, allowing simultaneous collection of PDF and higher resolution Bragg data.

XPDF Software

Processing of PDF data requires information about the composition of the sample being measured, as well as information on any containers that the sample may be in. XPDF will use a suite of software to deliver PDF data in real-time.

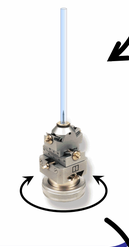
Sample data

Users will be able to enter sample information into a database before they arrive at Diamond. The database will store the essential information required for PDF processing, such as composition and density, as well as additional non-essential information, such as a crystal structure, which may be useful for data analysis.



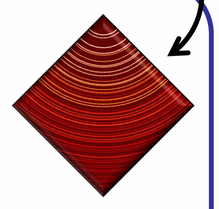
Experiment data

Planned data collections will be entered into the database. Users will be able select the energy, sample environment and type of measurement, such as “Rapid PDF” or “PDF + Bragg”. Data collections are then queued for measurement on the beamline. The database will also act as a log book for the experiment.



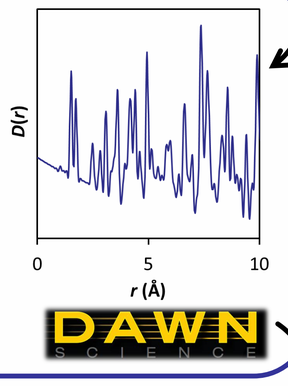
Data collection

Diamond uses the open source Generic Data Acquisition (GDA) framework to operate experiments on its beamlines. GDA will set-up the beamline for the desired measurement, and coordinate the collection of data from the area detectors and intensity monitor. The sample information from the database will be written with the measurement data into NeXus file format.



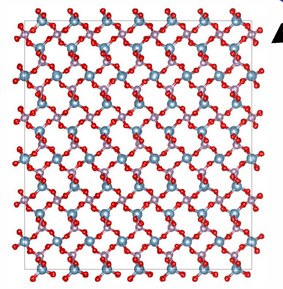
Data processing

PDF processing is being developed in the Data Analysis WorkbeNch (DAWN).[2] The data correction methods are akin to those of Gudrun[3], with additional features to handle 2D scattering data. The PDF processing will form part of the GDA data collection, allowing PDF data to be viewed in real-time. The same PDF processing will also be freely available to users within DAWN.



Data analysis

There is also potential to extend the software to run data analysis, utilising software packages such as RMCProfile[4] and Topas 6.[5] We are investigating ways to improve compatibility of XPDF data with existing PDF analysis software, and the potential of using the Diamond Cluster for large scale calculations.



[1] C. A. Young and A. L. Goodwin, *J. Mater. Chem.* 2011, **21**, 6464.
[2] M. Basham, J. Filik, M. T. Wharmby, P. C. Y. Chang, B. El Kassaby, M. Gerring, J. Aishima, K. Levik *et al.* J. Synchrotron Rad. 2015, **22**(3), 853.
[3] A. K. Soper and E. R. Barney, *J. Appl. Cryst.* 2011, **44**, 714.
[4] M. G. Tucker, D. A. Keen, M. T. Dove, A. L. Goodwin and Q. Hui, *J. Phys.: Condens. Matter.* 2007, **19**, 335218.
[5] A. A. Coelho, P. A. Chater and A. Kern, *J. Appl. Cryst.* 2015, **48**, 869.

For more information please visit www.diamond.ac.uk/Home/Beamlines/I15/xpdf.html, email xpdf@diamond.ac.uk or follow us on Twitter @xpdfdls