Diffraction

X-ray Pair Distribution

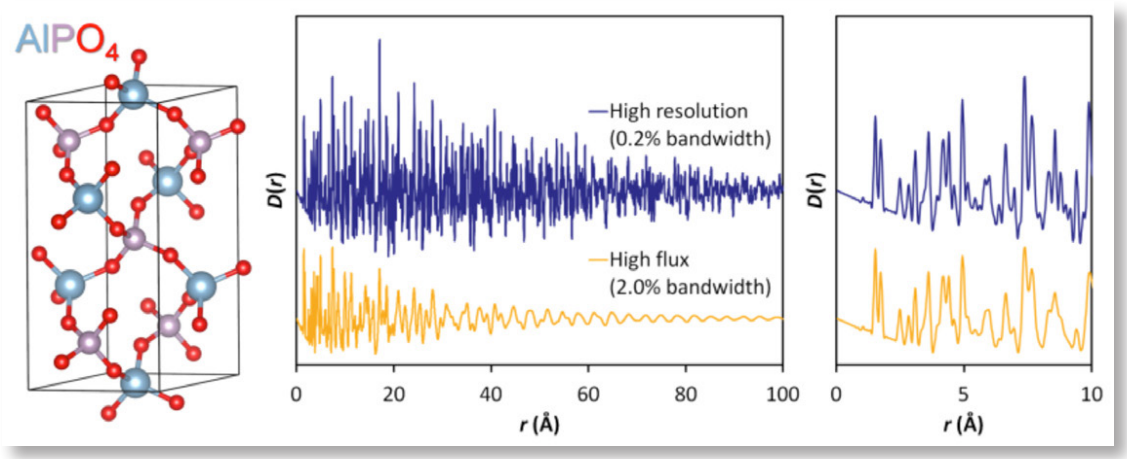
I15 -1 Technical Information

I15-1 X-ray Pair Distribution Function

I15-1 is the first dedicated X-ray PDF instrument of its kind in Europe. The XPDF method is applicable to crystalline, nanocrystalline, amorphous and fluid materials for probing local structure. XPDF measurements are the primary approach to understanding atomic structure for glasses and fluids, but they have the potential to provide a unique insight into the properties of crystalline materials as well. Many properties of crystalline materials are to a large extent determined by short-range fluctuations of the crystal structure, and the local structure seen by the atoms can differ from that suggested by the average periodic arrangement. In these cases, XPDF in conjunction with traditional crystallographic approaches can give entirely new insights crucial for the understanding of the physical and chemical properties of these materials.

Across fields as diverse as pharmaceuticals, optoelectronics and shape memory alloys, XPDF can be used to understand chemical and physical interactions that occur on the atomic scale - be it, for example, to watch and control catalytic mechanisms, to investigate adsorption in porous materials, or to characterise the structural rearrangements that accompany electron flow in battery materials. All these processes are affected by the local environments of individual atoms.

As the pair distribution function (PDF) is quantitative, it is unique among experimental local structure probes in its ability to drive the refinement of structural models. Moreover the models obtained are inherently consistent over different length scales and other experimental and theoretical information can be readily included in the refinement process.



Beamline Specification

Energy (keV)	40.0	65.3	76.6
Wavelength (Å)	0.310	0.190	0.160
Q_{max} ($Å^{-1}$)	21.5	35.1	41.2
Beam size H x V (µm x µm)	~700 x ~20	~700 x ~20	~700 x ~20

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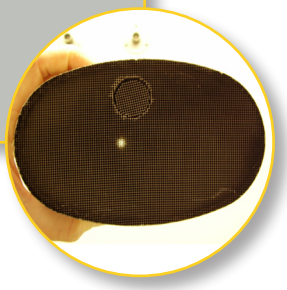
I15-1 Applications

Pharmaceuticals & Biomaterials

- Structural finger-printing of amorphous active pharmaceutical ingredients;
- Characterisation of local packing in amorphous and nanocrystalline drugs to control, monitor and eventually design new non-crystalline molecular materials;
- Studies of biomaterials and bio-mineralisation.

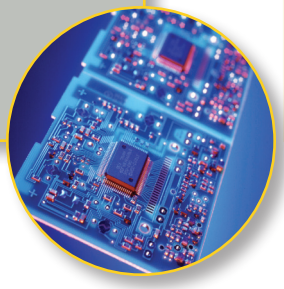
Chemistry & Catalysis

- Characterisation of functional porous compounds, nanoparticles, functionalised zeolites, thin films and layered materials;
- Direct information about host-guest interactions;
- *In situ* nucleation and growth studies of catalytic materials at the local level;
- Study of structural phenomena such as liquidliquid phase transitions and amorphisation processes.



Electronics

- Elucidate structural details of amorphous transparent conducting oxides to help understand their transport properties;
- Local structure characterisation of thin films for use in microwave circuits and photovoltaics;
- Investigation of optoelectronics and electrically or magnetically ordered materials.



Energy

- Aid in the development of new battery technologies;
- Characterisation at the local scale of ion transport through disordered materials as a function of time;
- Measurements of structural degradation through radioactive decay for damage prediction modelling of nuclear waste storage materials;
- Atomic scale models for fuel cell processes.

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