XPDF

X-ray pair distribution function beamline

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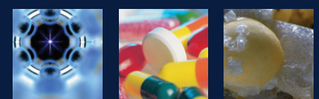
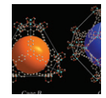
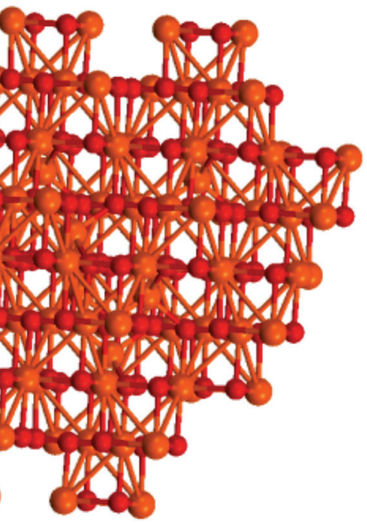



A dedicated X-ray Pair Distribution Function Beamline



Local structure determination is essential for a wide range of condensed matter and materials science. Examples include pharmaceutical, optoelectronic, electrically or magnetically ordered materials and materials with unusual properties such as negative thermal expansion, amorphisation and shape memory alloys.

The XPDF beamline will be a dedicated facility for local structure measurements, which will be ready for first users in 2016. It will be built as a side station in the footprint of the existing I15 beamline, but operated independently.

Why have a PDF beamline at Diamond?

Understanding local structure is fundamentally important for basic and applied science alike.
Across fields as diverse as bio-mineralisation and condensed matter physics, in industrial applications and in basic research, the science of interest involves understanding 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.

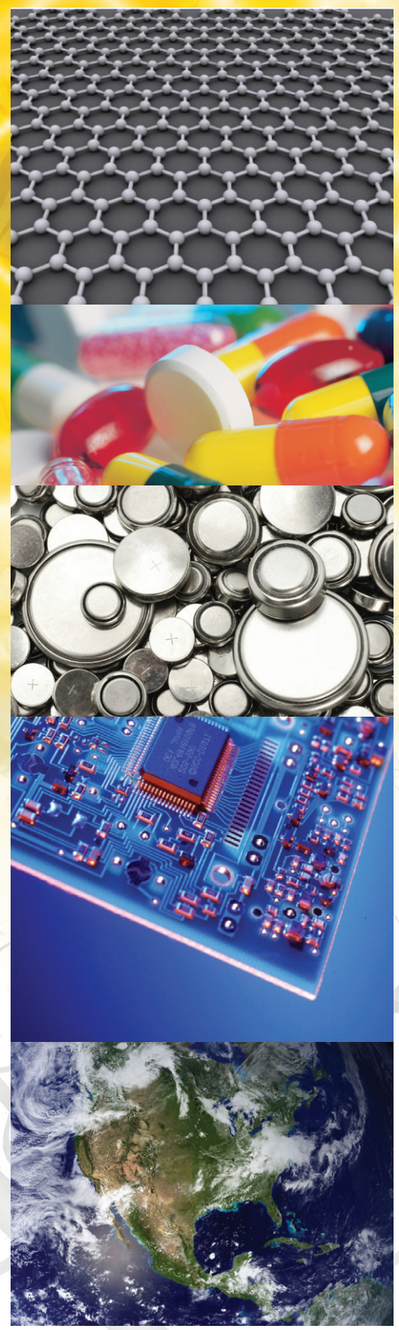
PDF methods are the most sophisticated tool available for characterising local structure.
Because the pair distribution function (PDF) is quantitative, it is unique among experimental local structure probes in its ability to drive the refinement of structural models. Moreover the models obtained are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

XPDF complements the existing portfolio of instruments at Diamond.
XPDF will be the first dedicated X-ray PDF instrument of its kind in Europe. It will interface directly with the current Extended X-Ray Absorption Fine Structure (EXAFS) and diffraction capabilities on offer at Diamond, and will collaborate with the scientific programmes of the Extreme Conditions (I15) and Engineering (I12) beamlines. There is a strong and rapidly growing UK community looking to use X-ray PDF measurements in their research and XPDF aims to serve this vibrant community.

Science Areas

The PDF method is applicable to both non-crystalline and crystalline materials alike. A Fourier transform of the entire spectrum of scattered intensity provides a histogram of all inter-atomic distances: the PDF. This quantitative information can then be used for local structure refinement in much the same way as Bragg diffraction patterns are used for average structure refinement. PDF 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, the X-ray PDF in conjunction with traditional crystallographic approaches can give entirely new insights crucial for the understanding of the physical and chemical properties of these materials. Moreover, the method can be used to produce realistic atomic-scale models of the local structure in a wide range of materials — crystalline, nanocrystalline, amorphous or fluid.



Chemistry and 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.
- Phenomenology of structural phase transitions.

Pharmaceutics & Biomaterials for Healthcare
- Characterisation of local packing in amorphous and nano-crystalline drugs to control, monitor and eventually design new non-crystalline molecular materials.
- Structural finger-printing of amorphous active pharmaceutical ingredients.
- Studies of biomaterials and bio-mineralisation.

Materials for Energy Applications
- Assisting in the development of new battery technologies.
- Characterisation at the local scale of ion transport though disordered materials as a function of time.
- Mapping of structural variations during solvation and flow for ionic liquids.
- Measurements of structural degradation through radioactive decay for damage prediction modelling of nuclear waste storage materials.
- Atomic scale models for fuel cells processes.

Materials for the Digital Economy
- 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.

Physics of Condensed Phases
- Studies of multiferroics, magneto-resistant manganites and high-T_c superconductors.
- *In-situ* PDF may allow the first direct observation of variation in polar nano-regions under changes in applied field.
- Studies of phenomena like liquid-liquid phase transitions and amorphisation processes.

Earth & Environmental Sciences
- Study of cage occupancies and decomposition pathways in methane hydrate clathrates located in the shallow marine geosphere and deep Antarctic ice cores.
- Interlayer water and host-guest interactions in clay minerals.
- Structure-property relationship of solid and fluid silicates.
- Characterisation of nano-materials in fine dust such as volcanic ash.

For more details, to express an interest or to follow the progress of the XPDF project, please visit **http://www.diamond.ac.uk/Home/Beamlines/I15/xpdf.html** or email **xpdf@diamond.ac.uk.**

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