Diffraction

X-ray Powder Diffraction

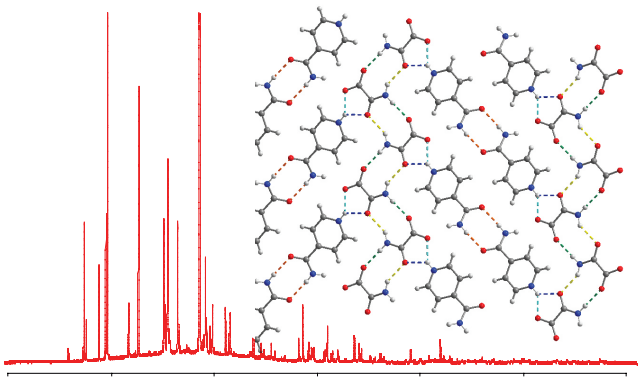
I11 Technical Information

I11 - X-Ray Powder Diffraction

Powder diffraction is the principal technique for determining the structure of materials that do not necessarily form large ordered crystals. It is therefore the technique of choice for the analysis of many naturally occurring materials such as minerals and artefacts as well as novel man-made materials. The technique has the advantage of a relatively simple scattering geometry but has been much enhanced by the development of intense synchrotron sources as well as advances in data analysis, using modelling, direct methods and global optimisation methods.

In recent years powder diffraction has provided crucial structural information for many strategically important materials including high temperature semiconductors, pharmaceuticals, mesoporous materials/catalysts, fullerenes and self-assembled nanoscale arrays. The combination of very high angular resolution, high count rates and controlled environmental conditions on I11 make it possible to carry out detailed structural analyses of such complex materials.

This versatile beamline has the resolving power to probe deep into sample structures, to detect rapid changes under non-ambient conditions as they occur and to perform resonant diffraction in order to solve complex structures containing low electron contrasts.



Beamline Specification

Energy range [keV] / Wavelength Range [Å]	5-30 / 0.4-2.5 (standard setting of 15 keV)
Temperature range	4 - 1000 K
Detectors	Multi-analyser crystal (MAC) detectors (45 channels) Position sensitive detector (PSD): 90° aperture
Beam size at sample [mm]	5 (H) x 0.5 (V)
Angular Range	MAC: 3-150° (2q) PSD: 3-90° (2q)
Geometry	Capillary

For further information please contact the Diamond Industrial Liaison Office on

+44 (0)1235 778797

industry@diamond.ac.uk

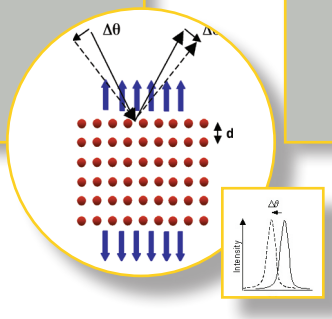
www.diamond.ac.uk/industry

@DiamondILO

I11 Applications

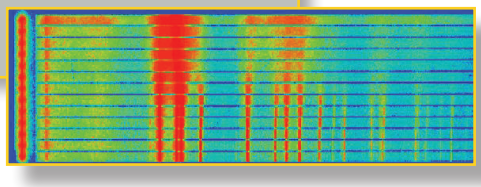
Materials Characterisation

- Measurement of line broadening can give an insight into particle sizes;
- Stress/strain measurements using the $\sin^2\Psi$ method allows post-mortem investigation of fatigued samples.



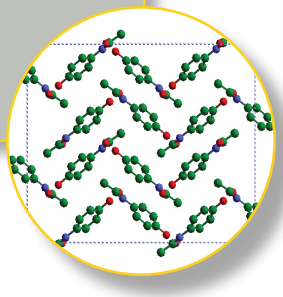
In Situ Measurements

- Data can be collected with millisecond time resolution using the PSD;
- Experiments can be performed at variable temperatures and humidities;
- In combination, these allow the determination of the kinetics of reaction.



Structure Determination

- The high resolution of I11 allows for accurate determination of peak positions for indexing;
- Full structures can be obtained either by Rietveld refinement or by *ab initio* structure determination.



Systems Exploration

- The robot on the beamline can hold up to 200 samples allowing for high throughput experiments;
- High resolution data aids with the identification of phases;
- Combinations of temperature, speed and resolution leads to generation of phase diagrams.

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