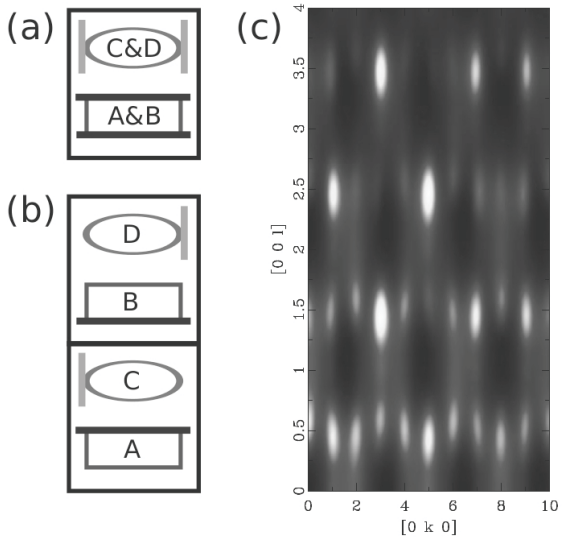
Figure 1:

(a) Refined average unit cell with overlayed components A and B on site 1 and 2.

(b) Possible configuration of disordered unit cells.

(c) Diffuse scattering of 9-Bromo-10-Methylanthracene in the 0kl-layer.



References:

[1] Schmidt, E., & Neder, R. B. (2017). Acta Cryst. A73, 231.
[2] Warren, B. E. (1969). X-ray Diffraction. Courier Corporation.
[3] Welberry, T.R., Jones, R.D. & Epstein, J. (1982). Actra Cryst. B38, 1518–1525.

Keywords: diffuse scattering, disorder, single crystal

MS24-P03

NanoMAX Beamline, a nanoprobe beamline for scattering and imaging at MAX IV

Angel Rodriguez Fernandez[1], Ulf Johansson[1], Gerardina Carbone[1], Alexander Björling[1], Sebastian Kalbfleisch[1], Tomas Stankevic[1], Björn Bring[1], Anders Mikkelsen[2], Ulrich Vogt[3]

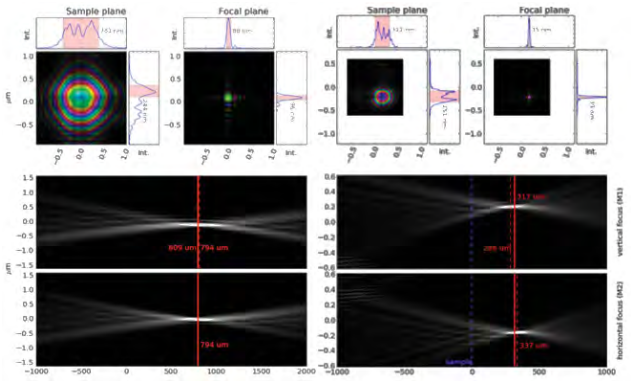
1. MAX IV LABORATORY, Lund University, Lund, Sweden
2. Synchrotron Radiation Research, Department of Physics, Lund University, Lund, Sweden
3. Biomedical & X-Ray Physics, Dept. of Appl. Physics, KTH Royal Inst. of Tech, Stockholm, Sweden

email: angel.rodriguez_fernandez@maxiv.lu.se

NanoMAX is a hard X-ray nanoprobe beamline at the 3 GeV multi-bend achromat storage ring MAX IV, Lund, Sweden [1]. The beamline is designed to utilize the uniquely high brilliance of the facility to achieve nanometer-sized coherent foci with high photon intensity. The small focus is used for scanning imaging with the main methods nano-diffraction, phase and absorption contrast, coherent diffractive imaging and ptychography - in forward and Bragg condition. The beamline optics has been briefly presented earlier [2].

The beamline will have two experimental stations when the buildup phase ends 2019/2020. One experimental station using Kirkpatrick-Baez mirror optics (KB) for focusing. The KB system gives a diffraction limited probe of 40 nm (24 keV) - 200 nm (5 keV) with 100 mm working distance from optics to sample position. The generous space will allow for versatile sample environments. Three main detectors are planned for or installed at the station; a megapixel photon counting area detector in forward direction, a compact photon counting area detector in off-axis position on a commercial industry robot and a 3-element Germanium X-ray fluorescence detector. A compact two axis high precision goniometer will allow advanced studies of ordered samples with diffractive methods. Continuous sample scanning is implemented in a basic version and will be further developed for efficient data acquisition. The design of the second experimental station is ongoing and first tests are anticipated early 2019.

We have provided beamtime to a handful user experiments during the first year of operation. Experiments in X-ray fluorescence, wide-angle scattering, nano-diffraction and ptychography have been executed. To achieve optimal performance from the super-polished KB-mirrors we have developed a simple procedure to measure focus astigmatism by scanning a Siemens star like test structure in ptychographic mode. The test sample image and the probe are reconstructed at the sample position using diffraction data from an inline pixel detector [3]. The probe is then propagated along the beam direction to show the beam profile, in vertical and horizontal plane, as seen in figure 1 bottom parts.



References:

[1] P F Tavares et al, (2014), J. Synchrotron Rad., 21, p. 862.
[2] U Johansson, U Vogt and A Mikkelsen, (2013),Proc. SPIE 8851, 88510L.
[3] B. Enders P. Thibault, (2017), Proc. R. Soc A 472 20160640

Keywords: Nanofocus, Hard X-ray, diffraction

MS24-P04

Correlated disorder in a metal-organic framework

Emily Reynolds[1], Mia Baise[2], Alistair Overy[1], Arkadiy Simonov[3], Jamie Gould[4], Ben Slater[2], Andrew Goodwin[1]

1. University of Oxford, Oxford, United Kingdom
2. University College London, London, United Kingdom
3. University of Freiburg, Freiburg, Germany
4. University of Leeds, Leeds, United Kingdom

email: emily.reynolds@chem.ox.ac.uk

At the heart of creating and developing functional materials is understanding structure - a task often complicated by disorder, be it compositional or orientational, static or dynamic. Whilst diffraction techniques have become adept at describing periodicity and understanding atomic structure, deviation from perfect order occurs in most real materials. Traditional crystallographic techniques fail to describe such deviations from periodicity, and while we understand the importance of disorder we are yet to understand how to describe, characterize and control disordered states.

A very specific disordered state is correlated disorder. This state arises when dominant interactions - i.e. chemical bonding - dictate fixed local atomic arrangements that need not result in long-range 3D order but may result in aspects of the structure being correlated. These correlations can produce signature patterns in the measured diffraction pattern in the form of diffuse scattering. In a class of materials known as metal-organic frameworks (MOFs), the local interactions driving formation usually result in long-range periodic arrangements. However, we can introduce disorder in MOFs through asymmetry in the linker, which acts in an analogous way to cyanide in transition-metal cyanides,[1] second-order Jahn-Teller displacements in $BaTiO_3$ [2] and hydrogen bonding in square ice.[3]

We substitute terephthalate linkers with asymmetric pyrazole-carboxylate and show that while powder and single crystal diffraction data suggest the linkers are disordered, the highly structured diffuse scattering visible in single-crystal X-ray patterns indicates correlated disorder along the linker rows. By comparing experiment with models calculated using simple local rules, we are able to understand the specific type of correlations giving rise to the diffuse, and prove the presence of correlated disorder in a MOF-5 analogue. The fixed local arrangements in the structure results in specific pore chemistry and binding sites important for adsorption and catalytic applications. More generally, these results contribute to the ability to identify specific types of correlated disorder within analogous systems, and therefore a greater understanding of structure on the nanoscale.

References:

[1] Karyakin, A. (2001). Electroanalysis, 13, 813-819.
[2] Senn, M., Keen, D., Lucas, D., Hriljac, J. & Goodwin, A. L. (2016). Physical Review Letters, 116, 207602.
[3] Pauling, L. (1935). Journal of the American Chemical Society, 57, 2680–2684.

Keywords: Disorder, framework, diffraction