ESRF	**Experiment title:** Simulation of SwissFEL broad bandpass beam on SNBL to develop a suitable methodology for single-shot diffraction on small unit cell materials	**Experiment number**: 01-02 1026
Beamline: BM01A	**Date of experiment**: from: 21/05/14 to: 22/05/14	**Date of report**:
Shifts: 6	**Local contact(s)**: Phil Pattison	*Received at ESRF:*

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Report:

New opportunities for studying (sub)microcrystalline materials with small unit cells, both organic and inorganic, will open up when the X-ray free electron laser (XFEL) presently being constructed in Switzerland (SwissFEL) comes online in 2017. The SwissFEL facility [1] will have a unique feature: the bandpass of the X-ray beam will be adjustable to give as much as a 4% energy spread. To evaluate the possibility of exploiting this option for microcrystal diffraction of crystals with relatively small unit cells (≤ 25000 Å^3), we simulated data for typical inorganic structures and found that with the 4%- energy-bandpass mode, not only can more reflections be recorded per shot, but the intensities can also be measured more reliably [2].

To test the viability of these simulations experimentally, we took advantage of the flexibility of the single-crystal diffractometer on SNBL (ESRF-BM01A) to mimic the SwissFEL setup. The broad bandpass mode was simulated by collecting a diffraction pattern while the monochromator was scanned over a 4% energy range. Three relatively large test crystals with unit cells typical of small-molecule and inorganic structures were measured: the zeolite ZSM-5, a hydrated cesium cyanoplatinate, and the mineral sanidine. Patterns with several crystals diffracting simultaneously were also collected (Fig. 1).

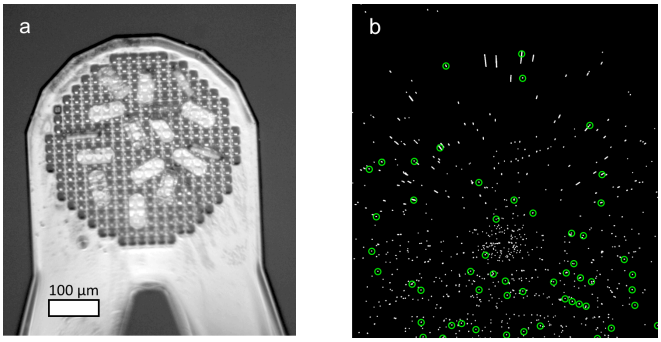

Figure 1. (a) 15 crystals of ZSM-5 dispersed on an MiTeGen grid. (b) Typical frame showing data collected on 15 crystals of ZSM-5. There are a total of 664 observed reflections, and 58 that originate from one of the crystals, are indicated with green circles.

In order to index the resulting, relatively sparse, single-shot patterns of randomly oriented crystals, we developed two indexing algorithms, one using Laue diffraction concepts and the other starting with a monochromatic approximation. Both algorithms were optimized to deal with multicrystal patterns. We could show that the individual patterns of up to 10 crystals measured simultaneously can be indexed. The partially measured reflections near the two boundaries of the energy range and close to the origin of the reciprocal lattice were identified and eliminated (Fig.2). The intensities could be extracted reliably for structure analysis (Fig. 3). This means that even with a single shot (a single pulse at SwissFEL), at least a partial analysis of the crystal structure will be possible, and this offers tantalizing possibilities for time-resolved studies.

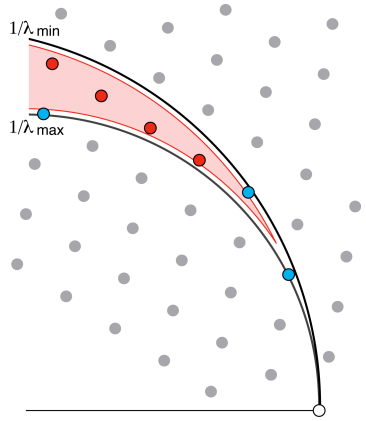

Figure 2. Ewald construction showing the 4%-energy-bandpass experiment (proportions exaggerated to show more detail). The reciprocal lattice points are shown as large dots to indicate that the intensities associated with them have a finite width. For simplicity, the reflections here are assumed to be isotropic and the widths identical for all reflections. The white borders between the Ewald spheres delimited by 1/λmin and 1/λmax and the shaded area correspond to half the reflection width. Here, four reflections are fully measured (red) and three partially (blue).

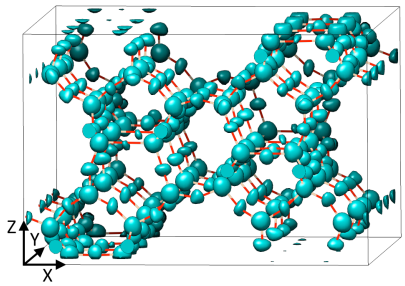

Figure 3. Electron density map generated by the charge-flipping algorithm in Superflip using 4%-energy-bandpass data (full dataset) collected on the zeolite ZSM-5. The refined structure has been overlaid for comparison.

While our algorithms were developed with SwissFEL in mind, they can be applied to any diffraction data collected in single snapshot mode with a broad bandpass beam.

More details can be found in: C. Dejoie, et al., *IUCrJ*, 2015, **2,** 361-370.

[1] B. D. Patterson, *et al.*, *Chimia*, 2014, **68,** 73-78.

[2] C. Dejoie, *et al.*, *J. Appl. Cryst.,* 2013, **46**, 791-794.