Oral Contributions

[MS1-03] Using a non-monochromatic microbeam for serial snapshot crystallography.

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New X-ray free-electron laser (XFEL) sources that create X-ray pulses of unprecedented brilliance open up new possibilities for the structural characterization of crystalline materials. By exposing a small crystallite (from nano- to a few micrometers in size) to a single ultrafast pulse, a diffraction pattern can be obtained before the crystal is damaged. If such single-pulse diffraction patterns, collected sequentially on many randomly oriented crystallites, are combined, it is possible to determine the structure of the material accurately [1]. One of the drawbacks of this approach is that only a single position of the Ewald sphere is accessed in each pattern, so, because reflections have a finite width, the diffraction condition is not satisfied completely for any of the reflections recorded. The new X-ray free-electron laser source (SwissFEL), which is currently being developed at PSI (Switzerland), will provide a broad-bandpass mode with an energy bandwidth of about 4% [2]. By using the full energy range of the SwissFEL beam, a new option for structural studies of crystalline materials may become possible.The use of such an 'extra pink' beam in a diffraction experiment with stationary crystallites should not only increase the number of reflection intensities that can be collected in a single shot, but also overcome the problem of 'partial reflection' measurement that is inherent to the monochromatic experiment. In order to take advantage of the full SwissFEL beam for crystallographic studies, we propose a new approach, inspired by the Laue single crystal (micro)diffraction technique and the experimental setup on BL12.3.2 at the Advanced Light Source in Berkeley [3]. Diffraction patterns for 100 randomly oriented stationary crystallites of the MFI-type zeolite ZSM-5 were simulated assuming several energy bandwidth values and 2 detector positions. These necessarily sparse diffraction patterns could be indexed using a pattern recognition algorithm. The number of accessible reflections that are not affected by the partial reflection intensity problem increases significantly with bandwidth. On average with a 4% (0.5%) bandwidth, there are 140 (17) reflections per pattern with a 2D 1M Pilatus detector positioned at 90° (2θ) relative to the incident beam and 46 (6) reflections with the detector at 45° (2θ). Combining the simulated reflections from the 100 patterns and the 2 detector positions, a completeness value of 73% is obtained for a 0.65-8.02 Å resolution range. Structure solution using the reflections from these patterns was performed using both direct methods and a dual-space method [4]. Our prime interest is in the area of inorganic and small molecule structures, where the diffraction patterns are sparse, but this new approach could also be of benefit to the protein community. We believe that the 'extra pink' beam mode option offers a clear opportunity to ease the data acquisition and subsequent evaluation in femtosecond time-resolved experiments at an XFEL facility.

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