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Advanced diffraction techniques for operando and ex-situ studies of real systems

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The well-established diffraction techniques of classical single crystal and powder diffraction have been hugely influential in the study of materials structure and of functional relationships to that structure. However, the characterization challenge for materials scientists is always to bring the conditions of our experiments as close as possible to the real conditions under which the systems we study operate. To that end, it is necessary to study samples of physical and chemical interest in the state in which they function. To do so, we must probe the time and length scales characteristic of the properties of interest, on non-optimized samples in terms of crystallinity and morphology, and to do so in an environment as close as possible to that under which the process under study takes place in a real setting.
We will describe the range of techniques which have been recently developed to characterise the atomic-level structure of far-from ideal samples such as amorphous, poorly crystalline or micron scale samples. We will also describe the use of tomographic approaches to crystallographically study the components of working systems.
This technique, X-Ray Diffraction Computed Tomography (XRD-CT) offers much richer information on the chemical and microstructural characteristics of the sample than absorption or phase-contrast tomography, as each reconstructed voxel contains not a scalar quantity but an entire diffraction pattern. Recent technical advancements in X-ray optics and high-speed/high-efficiency photon counting detectors have greatly reduced data collection times, allowing the study of real working devices under operando conditions with three-dimensional resolution of several micrometres. Furthermore, implementation of pair distribution function methods allow even amorphous samples to be characterized in this way.
We will present the principles of the methods used, drawing from recent examples of samples measured within operating catalytic reactors, batteries, and other devices.

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