Drinking from the firehose of synchrotron powder diffraction experiments

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The ability of modern powder diffraction beamlines with area detectors to rapidly (0.1 - 10 s) acquire high quality data can be transformative for many in situ and operando experiments aimed at understanding the synthesis and performance of functional materials. This is especially true when the goal is to simultaneously follow the time-evolution of a reaction across multiple positions on a sample or across multiple samples. However, much of the current hardware and software infrastructure for the collection and analysis of powder diffraction was born in the dark ages when the time for a pattern acquisition was orders of magnitudes longer. Over the past five years, we have been developing methods for the rapid acquisition and analysis of powder diffraction data. This has enabled us to collect about 100,000 patterns in the course of a 3-day beamtime experiment as well as to rapidly fit the data - in some cases with the ability to follow physical parameters extracted from the data (for example, reaction rate constants or local temperature in a heterogeneous sample) essentially in real time. Some examples will be given with respect to our ongoing research on synthesis science and/or batteries.

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