Image Segmentation and Advanced Processing of 2D Diffraction Data

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Area detectors are widely used for in situ and operando powder diffraction and PDF experiments, as their fast data collection rate can keep up with the kinetics of most transformations that we study in chemistry and materials science. The reduced 1D data usually have very good signal-to-noise ratio as the detectors capture as many diffracted photons as possible in the space, as compared to 1D or 0D detectors. However, when it comes to data analysis, people often overlook the original 2D data but only focus on the 1D data, especially when live integration of 2D data has become a routine at synchrotron powder beamlines. In the meanwhile, as a result of brighter X-ray source, more advanced detectors, and easier access to vast capacity of data storage, the data volume per experiment becomes larger and larger. It is becoming very difficult to comprehend the massive amount of 2D data, though there can be important information very visible in a 2D image not passed down to the reduced 1D pattern, such as the sample graininess and texture. It is therefore very helpful to have an output file flagging appearance and disappearance of unusual diffraction features, record their concentrations as they evolve, and to generate multiple integrated profiles per image based on the features, which can help with phase identification later on. We have developed programs to identify and segregate different features in 2D data with machine learning methods, and expect to deploy them at the Structural Science Group beamlines after the APS upgrade.