Sample absorption and background: optimizing signal/noise ratio for synchrotron and neutron diffraction

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In situ and *in operando* synchrotron and neutron diffraction experiments are typically carried out using a transmission geometry in which the beam passes through the entire thickness of a cylindrical sample on the way to the detector. Suboptimal intensities will occur when samples are either too thick (excessive attenuation) or too thin (small volume in beam). For this reason, a quantitative understanding of absorption effects is necessary to design optimal experiments. We have recently revisited the classic problem of the calculation of absorption correction factors for cylindrical sample geometries in a novel manner that takes full advantage of the radial symmetry of the problem. Using this approach, we have calculated not just absorption correction factors but also the relative diffraction intensities for different potential sample configurations. Our predictions for optimizing relative intensities have been validated using experimental data collected on synchrotron beamlines. Additionally, our methods have been extended beyond classic results in two ways. First, code has been developed for annular sample geometries (nested cylinders) to calculate both absorption correction factors and relative intensities. Second, our code has been adapted to enable the calculation of absorption correction factors when scattering occurs outside the conventional plane of diffraction. These calculations are critical for all diffraction experiments carried out using 2D area detectors – the configuration most commonly used for *in situ* and *in operando* studies – as the majority of the measured scattering occurs outside of the diffraction plane. In this talk, we will discuss calculation methods, practical methods for optimally preparing samples for experiments, and some successes in the collection of *in situ* and *in operando* studies for the study of energy materials.