A survey of applied corrections to measured Bragg and diffuse diffraction intensities for meaningful structure factor amplitudes

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Powder and single crystal diffraction are analytical methods that have developed into widely used tools for material analysis on molecular and atomic level. Dependent on the sample symmetry, the material to be investigated and the question to answer, X-ray diffraction and increasingly also neutron diffraction are the investigative tools of choice due to their complementary sensitivity to heavy and light elements. Data collection with area detectors is more and more automated. Bragg diffraction intensities are collected highly efficiently and data reduction is streamlined. For single crystal structure analysis, raw diffraction intensities are reduced to an extracted structure factor amplitude for each measured Bragg reflection, and the reduced data set represents the composition and symmetry arrangement of the sample. The measured Bragg intensities are raw intensities and need to be corrected for sample absorption due to chemical composition and size, the experimental setup that might add extra scattering, for example glue used to secure the sample, or the detectors that might have variations in detection sensitivity and electronic noise. Those are just a few examples for sample and instrument specific corrections. Other corrections that are dependent on the radiation (X-rays or neutrons) and on monochromatic or polychromatic incident beams are Lorentz and polarization corrections, scaling and normalization. Being aware of the various corrections and when they are applied in the data reduction workflow can help to solve issues that surface during data analysis. Understanding the effects of various corrections are even more important, when relatively weak superlattice intensities or diffuse scattering are studied.

This contribution aims to shed light on which corrections are applied to diffraction data, at which step of data reduction they are applied and they might impact the structure factor amplitudes and data analysis.