Approaches towards Phase Quantification with Full Profile Matching and SQUALL

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A number of methods exist for quantifying relative phase amounts via powder X-ray diffraction (PXRD) – these include the use of reference intensity ratios (RIR) using database calibration values and quantitative Rietveld refinement from known crystal structures. Here, we highlight the use of SQUALL, a new quantification method utilizing a user-defined database of full powder diffraction patterns as references. This provides a rapid, simple approach for cases where (1) users do not want to evaluate large numbers of diffraction data in detail or (2) peak shapes cannot be easily described due to complex behavior like stacking faults. Relevant case studies will be provided along with a discussion of typically achievable accuracies.