

High-throughput PXRD data analysis

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Traditionally X-ray powder diffraction patterns are analyzed one by one to extract the useful information like cell parameters, phase composition, structure details or sample related properties like stress, strain or texture.

With the advent of fast 1D/2D detection systems this analysis scheme is no longer feasible, because hundreds or even thousands of scans can be collected in a very short time. This fast data collection can be useful in application areas like polymorph screening, salt screening, non-ambient experiments and many others. However, the very large amount of data requires a different analysis approach than before. Multivariate statistics methods like agglomerative hierarchical cluster analysis, principle component analysis or fuzzy clustering are used first to sort the data into classes of similar scans and to visualize their relationships. Later on only representative scans of cluster and/or outliers are analyzed in detail.

In this presentation the high-throughput data analysis workflow using multivariate statistics methods is explained and examples that prove the usefulness also for protein X-ray powder diffraction patterns are shown.