

XRPD PATTERN MATCHING: PROBABILITY BASED VERSUS IMAGE COMPARISON

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Cluster analysis is an indispensable tool for high throughput data analysis. Almost all cluster analysis methods (agglomerative, divisive, k-means, fuzzy...) require a correlation matrix that has to be calculated by comparing all involved objects. In addition, techniques like MMS (**M**etric **M**ulti-dimensional **S**caling) or PCA (**P**roincipal **C**omponent **A**nalysis) calculations can be carried out on such a correlation matrix to extract and visualize the systematic variation in the data.

The basic question is, however, how to properly calculate the similarity of two X-ray powder diffraction patterns?

We will compare a probability-based approach, where the probability curves are constructed on a point-by-point basis from the signal-to-noise ratio of the supplied profile data, against a so called image comparison approach that does not take into account the counting statistics of the XRPD raw data.