Phase Mixture Detection by Fuzzy Clustering of X-ray Powder Diffraction Data

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For application areas ranging from pharmaceutical research (polymorph screening, high-throughput screening) through classical non-ambient experiments to zeolithe research it is necessary to measure a large number of X-ray powder diffraction patterns. The goal is to create a dense grid of measurements that not only offer a reliable overview, but also ensure that information that may be important is not missed

Nowadays this is easy to achieve using modern, fast X-ray diffraction equipment. However before analysis, the massive amount of datasets needs to be reduced. Here full pattern cluster analysis is nowadays seen as a very valuable approach.

However, cluster analysis is not only a data reduction tool, it can also be used to discover hidden patterns in data as well as exposing phase relationships in series of scans of complex mixtures.

In order to be able to deal with phase mixtures without prior knowledge of the possible constituents we have added fuzzy clustering to our other clustering methods in our latest software package [1].

We will use the data from a high temperature phase decomposition experiment on $CuSO_4$ ·5H₂O to show how fuzzy clustering in conjunction with hierarchical agglomerative cluster analysis and principal components analysis can help to reveal the phase relationships and detect phase mixtures in a complex multiphase system.

[1] PANalytical X'Pert HighScore Plus V2.x

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