ADVANCED DATA ANALYSIS ON HIGH-THROUGHPUT, HIGH-RESOLUTION XRPD DATA

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XRPD scans from high-throughput experiments are usually only analysed by multivariate statistics methods like clustering and/or Principal Component Analysis (PCA). The reasons for this somewhat limited approach are the bad counting statistics and the poor angular resolution of such data, which prevents the further crystallographic analysis like Indexing or Rietveld refinements.

Since the introduction of PANalytical's new high-throughput solution based on a standard X'Pert PRO MPD, equipped with a programmable XYZ stage, the X'Celerator detector and the focusing elliptical mirror, this situation has changed. Data from high-throughput measurements with short data collection times, now shows resolutions down to 0.045 degree 2Theta (depending on the type of sample), together with reasonable counting statistics. This allows for a completely new/refurbished approach to analysis.

In this contribution we will show how our advanced software package X'Pert HighScore Plus can help to take advantage of a large number of high-resolution XRPD patterns, by combining multivariate statistics methods and crystallographic analysis methods to obtain a much more complete view of the properties of the measured samples.