Poster Presentation

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Analysis of hidden information - PLSR on XRD raw data

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Usually in XRPD we are paying lots of attention to accurately describe profile shapes. We do that to eventually extract/predict information from the full pattern using physical models and fitting techniques. Sometimes this approach is stretched to its limits. That usually happens, when no realistic physical model is available, or when the model is either too complex or doesn't fit to reality. In such cases there is one very elegant way out: multivariate statistics and Partial Least-Squares Regression. This technique is rather popular in spectroscopy as well as in a number of science fields like biosciences, proteomics and social sciences. PLSR as developed by Herman Wold [1] in 1960 is able to predict any defined property Y directly from the variability in a data matrix X. In the XRPD the rows of the data matrix used for calibration are formed by the individual scans and the columns are formed by all measured data points. PLSR is particularly well-suited when the matrix of predictors has more variables than observations, and when there exists multi-collinearity among X values. In fact with PLSR we have a full pattern approach that totally dismisses profile shapes but still uses the complete information present in our XRPD data sets. We will show a number of cases where PLSR was used to easily and precisely predict properties like crystallinity and more from XRPD data.

[1] *Wold, H. (1966). Estimation of principal components and related models by iterative least squares. In P.R. Krishnaiaah (Ed.). Multivariate Analysis.(pp.391-420) New York: Academic Press.*

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