More features, improved integration, HighScore(Plus) V4.6 and beyond

Thomas Degen, Mustapha Sadki, Egbert Bron, PANalytical B.V. Lelyweg 1, 7603EA Almelo, The Netherlands

HighScore(Plus)[1] is an extremely versatile software package for the treatment and analysis of X-ray and now also Neutron powder diffraction data. HighScore(Plus) tightly integrates phase identification, quantitative phase analysis, crystallography and multivariate statistics features, like cluster analysis and PLSR into one consistent User Interface. In the latest versions we improved the Rietveld kernel for diffractometers with smaller radii, like the Aeris benchtop, by adding a model for specimen transparency. Specimen transparency effects get more pronounced with smaller goniometer radii and low Z samples. Other additions are the option to create isotropic starting coefficients for the Stephens Model[2], Support of the CSD database[3] (Search/Match and retrieval of starting models for Rietveld refinements) with more than 850.000 organic patterns, support for Neutron TOF data and strongly enhanced support for the automated handling and analysis of many similar scans. In this presentation we will shed some light on these and some other new features.

1) *T. Degen, M. Sadki, E. Bron, U. König, G. Nénert*, The HighScore suite, Powder Diffraction (2014), **29**, 13-18.
2) *P.W. Stephens*, Phenomenological model of anisotropic peak broadening in powder diffraction, J. Appl. Cryst., 1999, **32**, 281 – 289.
3) *C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward*, The Cambridge Structural Database, Acta Cryst. (2016). **B72**, 171-179