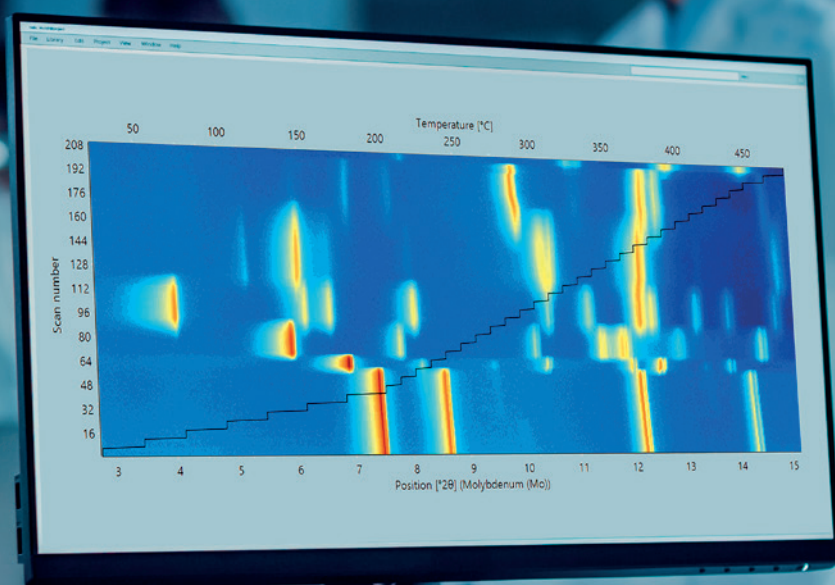




**Malvern  
Panalytical**  
a spectris company

## The HighScore suite

From phase identification to Rietveld analysis,  
from single scans to parametric refinements



# The HighScore suite

## Designed with flexibility in mind

Whether you are interested in improved process control, or doing research and development, understanding your materials very often starts with understanding the XRD powder diffraction pattern. Whether you are pushing techniques to their limits or establishing a regular and routine assessment, the HighScore suite will always suit your requirements.

The HighScore suite contains three modules: HighScore, the Plus option and RoboRiet.

While HighScore is a comprehensive phase identification program with profile-fitting capabilities, the Plus option has the additional functionalities of Rietveld fits, crystallographic and extended cluster analysis. RoboRiet performs automatic analysis in an automated environment.

Thanks to the combined efforts of powder diffraction communities worldwide, databases of powder patterns are growing rapidly, extending the scope of powder pattern search-match analyses.

In addition, new statistical methods such as partial least squares regression (PLSR) are emerging, providing a rapid and targeted analysis for the reproducibility and quality control of materials.

HighScore comes with a comprehensive help file, support material and access to education and training.

With local applications specialists at hand to answer your questions you are never far from help.

## The most comprehensive powder diffraction software

We continuously innovate and update the HighScore suite to offer you the most comprehensive and user-friendly toolbox for XRD.

Users will benefit from:

- Complete integration of all tasks within one user interface
- Powerful search-match algorithm
- Simultaneous use of reference databases
- Document-based structure with history and multiple datasets
- Automated analyses
- Automatic reporting
- State-of-the-art profile fit with 3 model functions and options
- Extensive help system and tutorials for self-study
- Data exchange by XRDML, text and binary scan file formats from all major suppliers

# HighScore

## Full-pattern approach for phase identification and much more

Determination of the crystalline components in your material:

### Phase identification

#### Search-match

Powerful search-match algorithm that combines peak and profile data and instantly re-scores an existing candidate list.

#### Automatic identification

Best matches for candidates can be automatically accepted using a sophisticated filter.

#### Chemistry calculator

The chemistry calculator breaks down phase chemistry into simple elements, oxides, sulfides or other compounds. It can be used for single phases or for phase mixtures with known phase concentrations.

#### Reference databases

All reference databases are supported, including those created by the user.

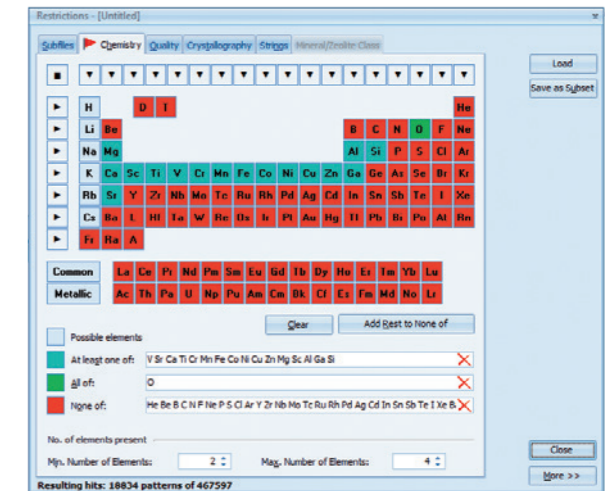


Figure 1. Selection example of chemical elements from the periodic table.

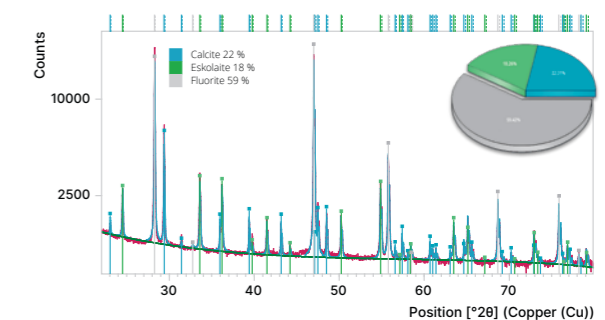
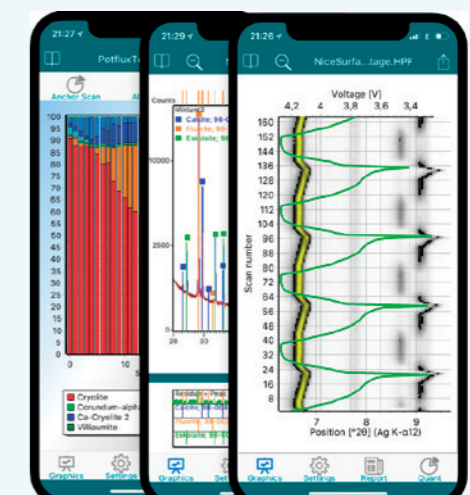


Figure 2. Phase identification of a minerals mixture. All phases are color-coded and their peaks are displayed with their corresponding markers for improved readability. The semi-quantification is done with reference intensity ratios.



### HSvu: the world's first X-ray powder diffraction app

- Display all kinds of X-ray diffraction scans in various formats
- Show and reports all details from an X-ray diffraction analysis, performed by the HighScore software from Malvern Panalytical
- Open a scan or a diffraction analysis from your email account
- Share powder diffraction data with friends by Dropbox, Facebook and email
- Report details from a HighScore analysis document



**Discovering hidden information or correlations:**

**Partial least squares regression method**

The partial least squares regression (PLSR) method in HighScore:

- User-friendly
- Truly statistical approach that compares data to real-life calibrations and does not require the lengthy simulation and fitting of a sample model
- Rapid and direct correlation of measured data to the sample of interest

As illustrated in Figure 3, the PLSR method offers considerable time-savings over wet chemistry and is just as reliable.

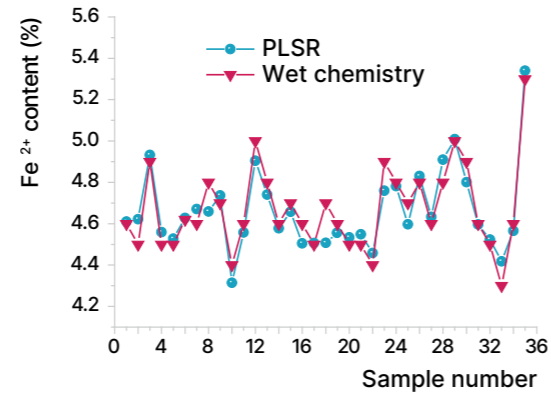


Figure 3. Comparison between wet chemistry and the PLSR method for the determination of the Fe<sup>2+</sup> content in a series of mineral samples [1].

**Investigating the microstructure:**

**Strain & size analysis**

Information on the microstructure of crystalline materials is obtained from the width and shape of X-ray single peak profiles. Before analysis, HighScore can correct for the instrumental contribution of line broadening.

The results are microstrain and/or crystallite size information for each peak. For multiple peaks, a Williamson-Hall plot can be shown with the average values [2].

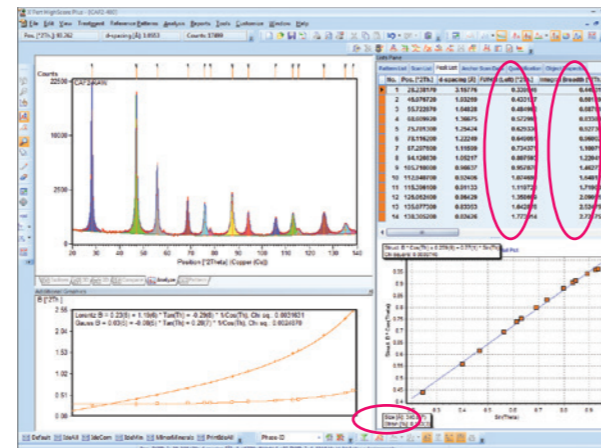


Figure 4. Fitted profile and peak list with full width at half maximum (FWHM) and integral breadth (top part) and Gaussian and Lorentzian broadening contributions with Williamson-Hall plot (bottom part).

**Accessing insights into disorder and local structure:**

**Pair distribution function**

The derivation of the reduced structure function and the corresponding atomic pair distribution is integrated and made easy.

With a few clicks, you can correct for:

- Absorption
- Bremsstrahlung
- Compton and multiple scattering
- Lorentz polarization

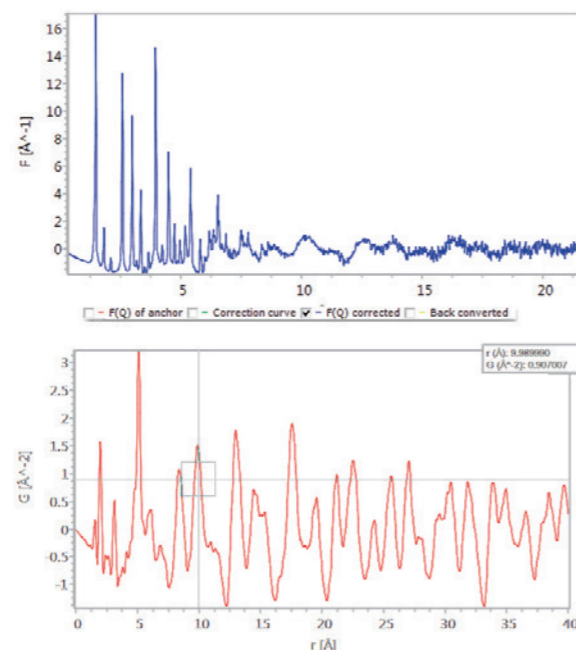


Figure 5. a) Reduced structure-function of Zn(CN)<sub>2</sub> measured at room temperature and b) its corresponding atomic pair distribution function calculated within HighScore.

[1] U. König, T. Degen, N. Norberg, Powder Diffraction 29 (S1), pp 578-583 (2014)  
 [2] G.K. Williamson, W.H. Hall, Acta Metall. 1, 1953, pp 22-31

**Handling big data:**

**Cluster analysis**

Modern X-ray diffraction equipment allows rapid measurements resulting in large amounts of data to be analyzed. The best way to tackle data evaluation relies on identifying and grouping similar data sets, and selecting most representative data sets while pointing out outliers.

The cluster analysis tool implemented in HighScore makes this analysis smooth and easy.

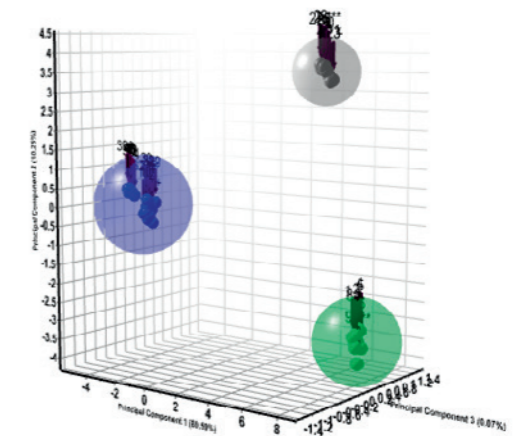


Figure 6. Cluster analysis of fly ash raw materials coming from different sources.

**Deconvoluting overlapping reflections:**

**Profile fitting**

For improved determination of the peak parameters, profile fitting allows the deconvolution of severely overlapping reflections.

Improved extractable parameters:

- Position
- Intensity
- Width
- Shape

Useful information for:

- Crystallite size
- Microstrain

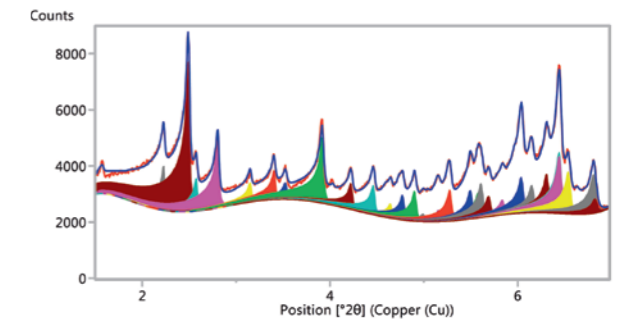


Figure 7. Profile fitting of a microcrystalline lysozyme sample.

**Digitalizing powder diffraction patterns:**

**Bitmap-to-scan converter**

A tool to quickly and easily convert pictures of scans into raw data.

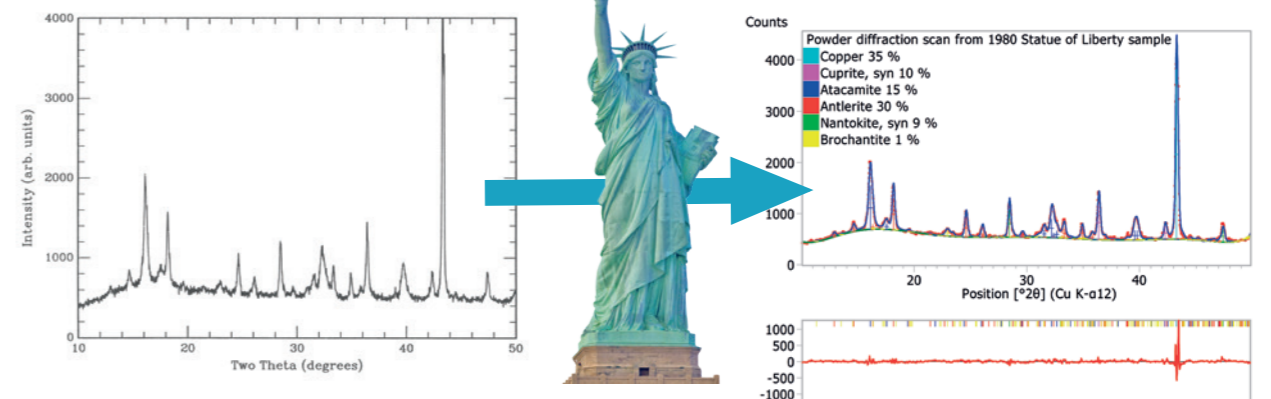


Figure 8. Original graphic of the X-ray diffraction pattern of a rust sample of the Statue of Liberty published in Powder Diffraction 1, 299 (1986) [3].

Figure 9. Rietveld refinement on the converted scan.

# HighScore and the Plus option

## The ideal tool for crystallographic analysis and more

By adding the Plus option to HighScore, you will have a true all-in-one package including unit cell refinements, PLSR, crystal- and microstructure analysis, DDM and PONKCS phase quantifications, next to profile fitting and phase identification, and many other tools integrated in a user-friendly package.

### For structural analysis and quantification:

#### Rietveld and Pawley, DDM and PONKCS

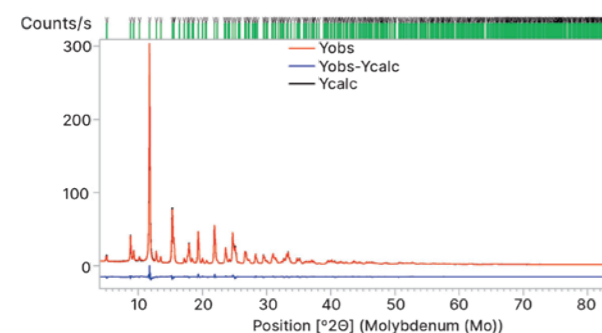


Figure 10. Rietveld refinement of  $\text{Fe}(\text{IO}_3)_3$  measured with Mo K $\alpha$  radiation, using HighScore Plus.

Data fitting using the Rietveld kernel has been significantly improved by employing:

- Layer displacement and layer thickness models
- Description of the full emission spectrum including K-edges and white radiation
- 64-bit technology and parallel fitting mode for fitting one model to many similar scans

As illustrated in Figure 3, the PLSR method offers considerable time savings over wet chemistry and is just as reliable.

For the quantification of a phase with an unknown crystal structure, the direct derivative method (DDM) or the PONKCS methods are alternatives [3,4], that can be as efficient as the Rietveld method.

The minimization routine permits the combination of different models (structure-based, DDM, PONKCS, Pawley, individual peak fits) in one run to quantify any phase, as illustrated in Figure 11 with a slag cement sample.

The Rietveld method compares a measured diffraction profile and a calculated profile and, by varying a range of parameters, the difference between the two profiles is minimized (see Figure 10). A standard Rietveld refinement requires atomic positions, space group and cell parameters for each phase.

Malvern Analytical's Rietveld algorithm is an advanced implementation of widely accepted and proven technology, continuously developed over the past decades.

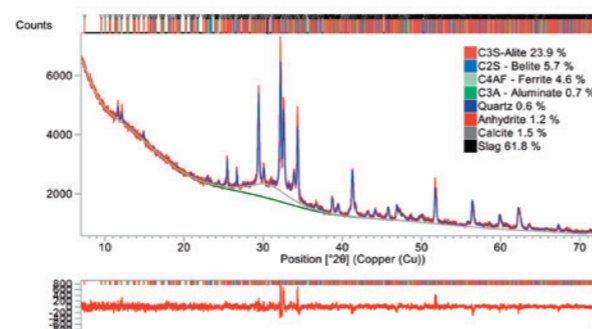


Figure 11. Quantification of a slag cement sample using multi-phase model fitting.

### New crystalline phases:

#### Indexation and space group determination

The most popular and powerful indexing programs are incorporated in HighScore and the Plus option:

- Dicvol
- Treor
- ITO
- McMaille

Extinction Symbol	Log Probability Score	Long Herman Ma...	Space grou...	Frequency Inorg...
P n - -	74.4084			6895
P 4/n	74.4084		85	481
P 4/n m m	74.4084		129	6414

Figure 12. After performing a Le Bail or Pawley fit, in just a few clicks, the possible space groups can be determined using the most advanced algorithm ExtSym [5].

### Speeding up your data processing:

#### Automatic data treatment

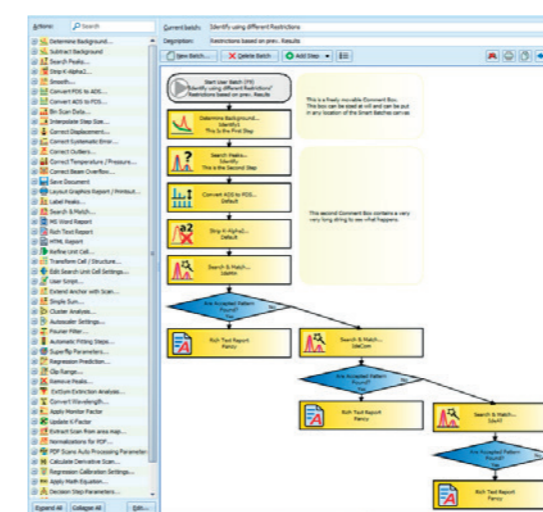
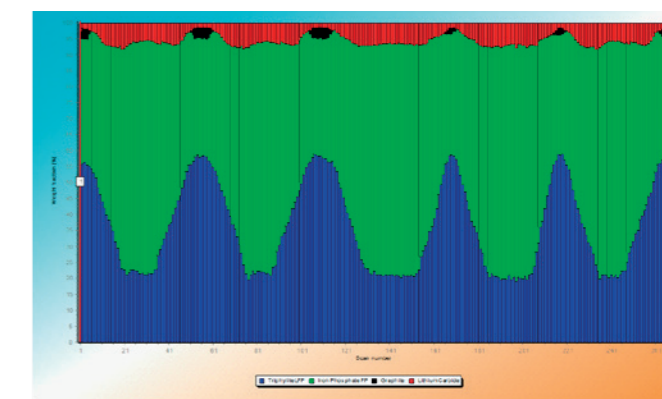


Figure 13. To quickly assemble an automation, actions with either pre-defined or custom parameters can simply be dragged from the left-hand side action list and added or inserted into the flowchart.

Any type of data analysis can be automated in a user batch and is executed on any number of scans. Editing batches is done in a flowchart with easy drag and drop of predefined and custom processing steps. This can include decisions (conditional branching). An example of a batch is shown in Figure 13. The bargraph picture shows the condensed output of an automatic analysis of a battery charge-discharge experiment with the quantification of four phases.



## For process control and more: Industrial applications

All HighScore (Plus) functions can be automated and run unattended. Batch programs can contain any sequence of data treatments and analytical functions. Scripting is available to provide dedicated output for any Laboratory Information Management System (LIMS).

Another version of the software – RoboRiet – executes pre-programmed Rietveld analyses in a production environment. It automatically detects new measurements and communicates the results to a printer, a disk drive, Excel lists or directly to a LIMS system.

### Ensuring regulatory compliance

HighScore can now be used in combination with OmniTrust, our complete solution for the regulated environment. OmniTrust ensures record accuracy and data integrity by ensuring users can only perform the auditable actions that the workflow requires.

System controls help users avoid errors and prevent the falsification of data, ensuring compliance with all current regulatory guidance, including the USFDA's 21 CFR Part 11.



[3] N. V. Y. Scarlett, I. C. Madsen, Powder Diffraction, 21(4), 278-284 (2006)  
[4] A. J. Markvardsen et al.; J. Appl. Cryst. (2008). 41, 1177-1181



## Why choose us?

**When you make the invisible visible, the impossible is possible.**

Our analytical systems and services help our customers to create a better world. Through chemical, physical and structural analysis of materials, they improve everything from the energies that power us and the materials we build with, to the medicines that cure us and the foods we enjoy.

We partner with many of the world's biggest companies, universities and research organizations. They value us not only for the power of our solutions, but also for the depth of our expertise, collaboration and integrity.

With over 2200 employees, we serve the world, and we are part of Spectris plc, the world-leading precision measurements group.

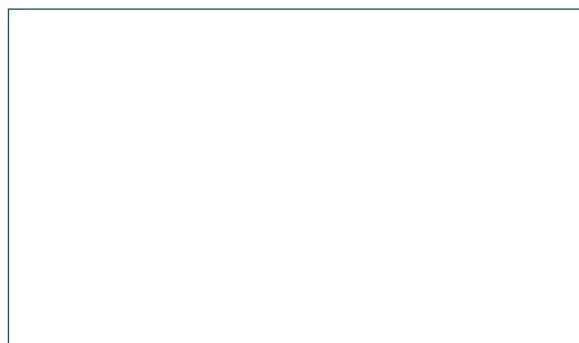
**Malvern Analytical. We're BIG on small™**

## Service & Support

Malvern Analytical provides the global training, service and support you need to continuously drive your analytical processes at the highest level. We help you increase the return on your investment with us, and ensure that as your laboratory and analytical needs grow, we are there to support you.

Our worldwide team of specialists adds value to your business processes by ensuring applications expertise, rapid response and maximum instrument uptime.

- Local and remote support
- Full and flexible range of support agreements
- Compliance and validation support
- Onsite or classroom-based training courses
- e-Learning training courses and web seminars
- Sample and application consultancy



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