

BIOVIA MATERIALS STUDIO REFLEX QPA DATASHEET

BIOVIA Materials Studio Reflex QPA allows you to determine the relative proportion of different phases, including both inorganic as well as organic systems, in a mixture based on powder diffraction data. It is a widely used analytical method for phase characterization in various industries.

Quantitative phase analysis (QPA)¹ refers to the determination of relative amounts of different phases in multi-phase samples. X-ray powder diffraction is perhaps the most powerful method of obtaining quantitative phase information from multi-component mixtures in the fields of science and engineering for materials research. It is also an important tool for quality and process control in the industry. The power of the method lies in its simplicity and speed. Its applications include the characterization of pharmaceuticals, corrosion products, intermetallics, and contaminants, as well as forensic analysis, mineral assays, and fiber analysis.

WHAT DOES BIOVIA MATERIALS STUDIO REFLEX QPA DO?

BIOVIA Materials Studio Reflex QPA has been developed to determine the relative amounts of different phases in a mixture by means of a powder diffraction pattern of the mixture.

In BIOVIA Materials Studio Reflex QPA, the pure component phases that comprise the mixture may be represented by:

1. Crystal structures (The Rietveld method^{2,3,4}) The experimental diffraction pattern is characterized as the superposition of powder diffraction patterns simulated from the crystal structures of the component phases. Pattern, sample, lattice, and structural parameters for each phase are refinable during a calculation.

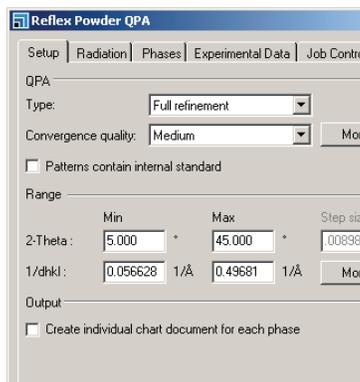


Figure 1: The BIOVIA Materials Studio user interface displaying the BIOVIA Materials Studio Reflex QPA control panel.

2. Experimental powder diffraction patterns BIOVIA Materials Studio Reflex QPA supports the use of the standardless method and the internal standard method. For each phase, parameters associated with line shift corrections may be refined. The standardless method^{5,6} assumes that all the patterns are recorded under an identical experimental setup. For the internal standard method^{7,8}, a fixed weight fraction of a standard material is added to all pure component phases as well as the mixture phase before their powder diffraction patterns are recorded.

3. A combination of scenarios of 1 and 2 This approach combines the standardless QPA method using crystal structures as input (the Rietveld method) with the standardless QPA method using experimental powder patterns as input.

THE BIOVIA MATERIALS STUDIO ADVANTAGE

BIOVIA Materials Studio Reflex QPA is part of BIOVIA Materials Studio Reflex product, providing a seamless integration with other modules in BIOVIA Materials Studio Reflex (Powder Diffraction, Powder Indexing, and Powder Refinement) and BIOVIA Materials Studio Reflex Plus for a full crystal structure determination. Experimental powder diffraction patterns are readily visualized using the BIOVIA Materials Studio Visualizer. BIOVIA Materials Studio's integrated model building and editing tools enable you to construct, visualize, and manipulate molecular fragments in the asymmetric unit of a crystal structure representing for systems such as drugs, pigments, metal oxides, and zeolites.

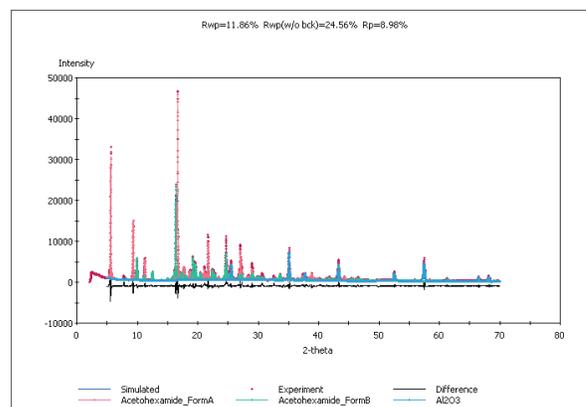


Figure 2: A decomposition of input experimental powder diffraction pattern of the phase mixture in terms of the patterns of all the individual component phases.

Results generated by BIOVIA Materials Studio Reflex QPA can be analyzed using BIOVIA Materials Studio's spreadsheet-like study table environment. The study table provides an easy association of the crystal structure or experimental powder diffraction pattern for each pure component phase with its estimated contribution in the mixture phase (e.g. integrated intensity, intensity fraction, weight fraction). It also offers powerful sorting and plotting functionality. Chart documents containing the decomposition of the input easy incorporation into documents created by standard word processor, spreadsheet, and presentation packages. In addition, high quality images can be easily produced.

Structural information, diffraction data, and chart documents can be readily exported to and imported from other PC applications allowing easy sharing of the results with colleagues and an easy incorporation into documents created by standard word processor, spreadsheet, and presentation packages. In addition, high quality images can be easily produced.

FEATURES

Setup

- The initial crystal structures can easily be imported from other sources or created using the Crystal Builder within the BIOVIA Materials Studio Visualizer.
- Read in a variety of diffractometer file formats, including 3CAM, Bruker, Galactic SPC, GSAS raw, ICDD PD3, ILL, JCAMP, PAnalytical XRDML, Philips, Scintag, and Stoe.
- Allows for different radiation sources with multiple wavelengths and user-defined polarization.
- Ability to pre-process experimental data, for example via background subtractions, data smoothing, scaling, and Ka2 stripping.
- No limit on the number of pure component phases.
- Crystal structures or experimental powder diffraction patterns for the pure component phases are stored in a spreadsheet-like study table.
- Multiple default settings allow for simple operations, or advanced users can adjust individual simulation parameters as necessary.
- For pure component phases represented by crystal structures, pattern, lattice, sample, and structural parameters are refinable.
- For the pattern parameters, a versatile range of peak profiles is provided, including Gaussian, Lorentz, Mod. Lorentz#1, Mod. Lorentz#2, Pseudo-Voigt, Person VII, Thompson-Cox-Hasting, David-Voigt and Tomandl pseudo-Voigt. Choice of asymmetry correction consists of Rietveld, Howard, Berar-Baldinozzi, and Finger-Cox-Jephcoat. For the sample parameters, sample and instrument broadening effects are simulated. Isotropic and anisotropic temperature factors can be accounted for, as well as the effects of preferred orientation. The structural parameters include rotational, translational, and torsional degrees of freedom for any molecular fragment in the unit cell.
- For pure component phases represented by experimental powder diffraction patterns, parameters associated with line shift corrections may be refined.
- Ability to propagate the refinement settings from one pure phase component document to any or all of the others in the input study table.
- The background contribution of the mixture experimental powder diffraction pattern can be fitted as part of a QPA calculation.

CALCULATION FEATURES

- Ability to treat both organic and inorganic systems.
- Pure component phases can be represented by (1) crystal structures, (2) experimental powder diffraction patterns, or (3) the mixture of (1) and (2).
- Ability to determine the scaling factor required for normalizing the powder diffraction patterns with respect to the internal standard.
- Full refinement calculates the relative contents of a number of specified pure phases in a given mixture from the powder diffraction pattern of the mixture, performing a Rietveld refinement of the input parameters through a specified number of iterations and obtaining the weight fraction for each component phase.
- Refine weights calculates the relative contents of a number of specified pure phases in a given mixture from the powder diffraction pattern of the mixture, but does not refine any of the input parameters. The effect is the same as performing a full refinement calculation with all the refinement options turned off.
- Calculate integrated intensity, intensity fraction, and weight fraction for each component phase.

Running Jobs

- All BIOVIA Materials Studio Reflex QPA jobs are run in the background freeing up the BIOVIA Materials Studio client for other research.
- All BIOVIA Materials Studio Reflex QPA jobs can be submitted to local or remote compute servers.

Results

- Calculated integrated intensity, intensity fraction, and weight fraction for each component phase as well as a chart document containing the calculated powder diffraction patterns for the pure phases and its estimated contributions to the mixture pattern are stored in a study table.
- Parameter settings are automatically saved for each simulation.

Analysis

- Analysis is carried out with the help of spreadsheet-like study tables.
- Each atomic structures or experimental powder diffraction patterns for any given pure component phase is embedded in the study table, allowing for independent viewing using the 3D Viewer tools in the BIOVIA Materials Studio Visualizer.
- Chart documents showing the contribution of each potential phase to the experimental mixture pattern can be analyzed with the Chart Viewer tools in the BIOVIA Materials Studio Visualizer.
- A user specified subset can be filtered out from a study table into a new table.
- Flexible graph plotting enables plotting properties against each other, and plotting to a selected subset.
- All or part of a study table can be copied and pasted into Microsoft Excel® and Microsoft Word®.
- Structures and chart documents can be exported to bitmap files, and also be printed on grayscale or color PostScript printers.

SYSTEM DETAILS

Operated through the BIOVIA Materials Studio Visualizer on Windows® 2000 and XP, BIOVIA Materials Studio Reflex QPA calculations can be executed on Windows® 2000, Windows 2003 Server, Windows XP, SGI IRIX, Red Hat Linux (Intel IA32, EM64T, and compatibles), and SuSe Linux (Intel IA32, EM64T, and compatibles) operating systems.

To learn more about BIOVIA Materials Studio, go to accelrys.com/materials-studio

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