

DIFFRAC.EVA

The next era in phase analysis

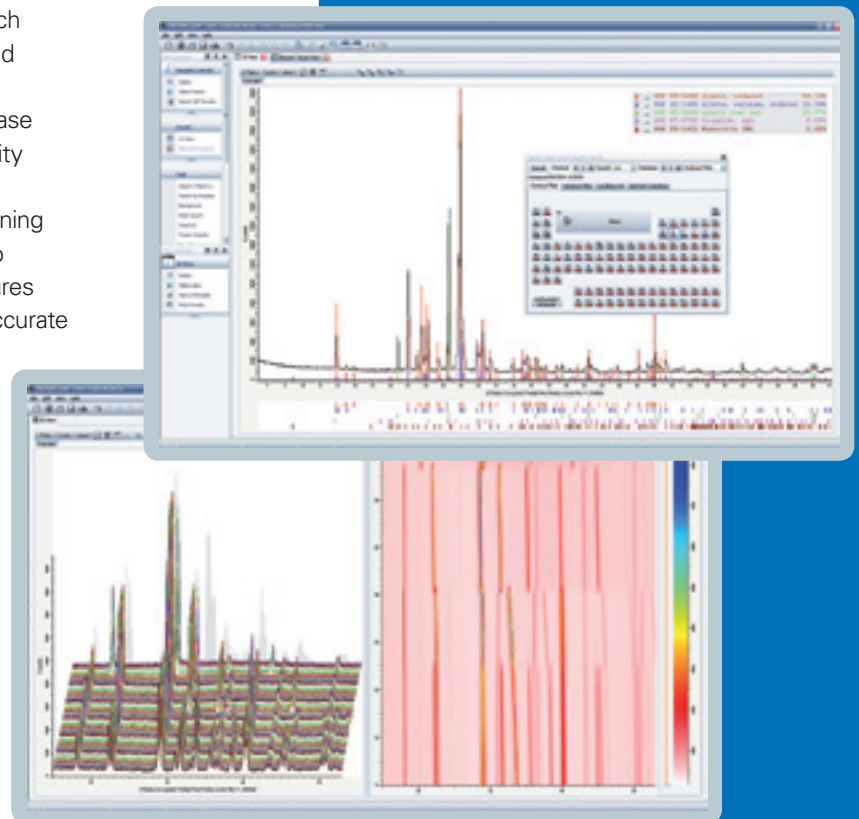
DIFFRAC.EVA defines a new benchmark for phase analysis by making interpretation of XRD data easier, faster, and more accurate than ever. Most remarkable is EVA's complete collection of the best algorithms for data evaluation, blended with an new and innovative design and operation concept for maximum simplicity and flexibility.

The real beauty of EVA is in its full-pattern-approach to phase identification using the most powerful and successful search/match module on the market, seamlessly integrated with unique quantitative phase analysis capabilities. Of significance is the possibility to optionally include element information, e.g. obtained via XRF. Simultaneous analysis by combining complementary XRD and elemental data allows to successfully handle even the most complex mixtures and trace phases with ease, providing the most accurate results possible.

EVA also delivers features for user-interface, graphics and analysis report customisation never seen before. Furthermore, EVA represents a professional graphing and reporting systems for creation of cutting edge, publication-ready graphics and analysis reports.

An extensive step-by-step tutorial makes EVA easy to use from the very beginning. The tutorial also serves as an excellent teaching tool to introduce newcomers to XRD analysis, getting them started with ease in the shortest time possible.

- Simultaneous phase identification and quantification for automated phase analysis
- Combined XRD-XRF analysis for unambiguous phase identification and accurate quantification
- Fully customizable GUI for easy and intuitive data evaluation and presentation



Evaluation methods for all applications

EVA provides a complete collection of the best algorithms for XRD data analysis with full access to all function parameters. Seeing is believing - thanks to a unique real-time-preview of all evaluations for visual validation, thus guaranteeing most reliable and accurate results. Reversing an action? No problem! EVA allows to undo and redo all operations.

Reliable and accurate phase analysis

Since its first release, EVA's search/match module is generally appreciated as the most reliable and most accurate tool for phase identification. Correspondingly, EVA performed best in an international Search-Match Round Robin (Le Meins et al., 2002, <http://www.cristal.org/smrr>). Since then numerous improvements have further differentiated EVA from conventional software for phase analysis:

- Phase identification and accurate quantitative phase analysis based on RIR (reference intensity ratio) values can be performed in one go. Additionally the spiking method is supported, allowing to put all quantitative results on an absolute scale.
- Highly sophisticated residual search with respect to already identified phases, thus greatly improving analysis of minor phases
- Support of Variable Counting Time (VCT) data for highly accurate trace phase analysis thanks to significantly decreased Lower Limits of Detection (LLoD)
- Simultaneous search in multiple reference databases, such as the ICDD PDF2/PDF4+/PDF4 Minerals/PDF4 Organics databases
- Grouping of candidate phases to handle the ever-increasing number of similar or nearly identical reference database entries

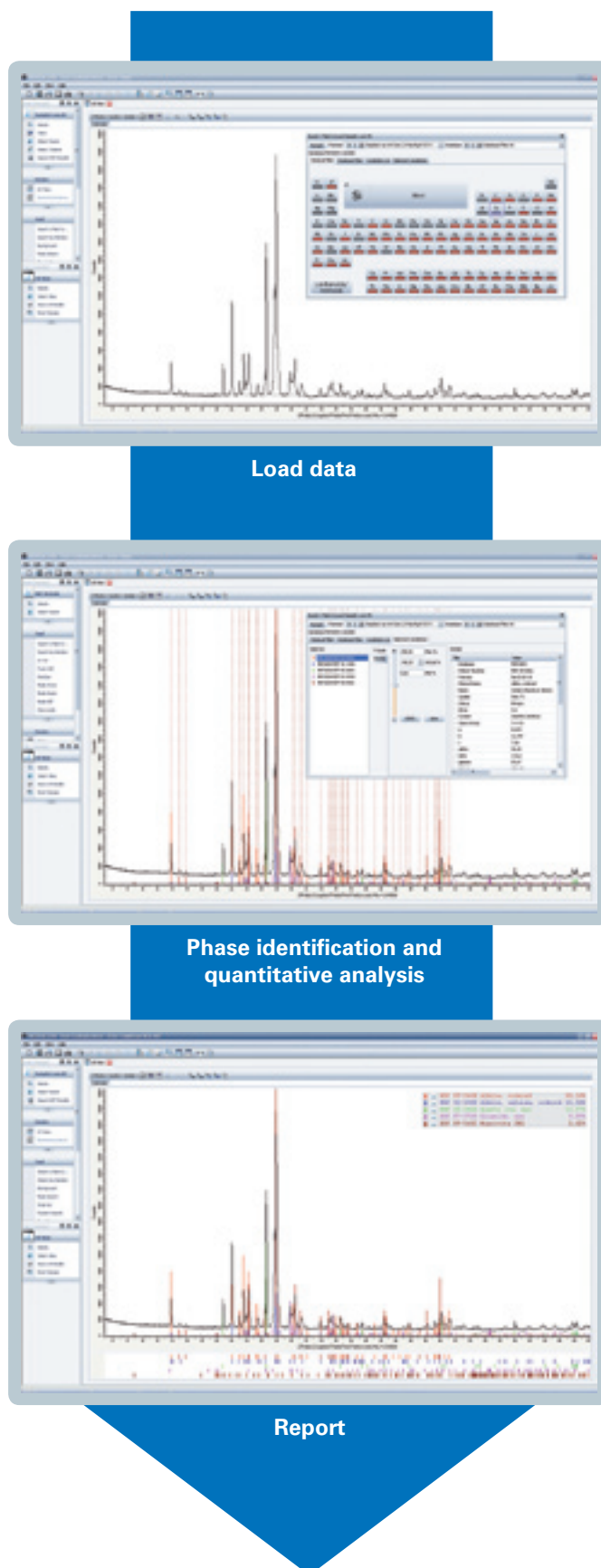
User friendly, convenient and versatile

EVA comes with a new and innovative user-interface providing for maximum simplicity and flexibility enabling cutting-edge data evaluation and presentation.

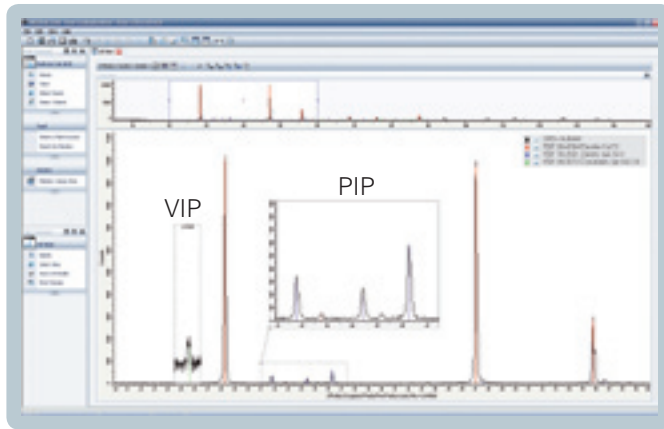
Each individual user can completely customize the user-interface to perfectly fit to his application needs, available screen size, or simply personal taste. Windows can be visible or hidden, changed in size, combined with other windows to form a tabbed window, docked or displayed as floating views.

EVA also offers powerful graphing tools to create customized, publication ready figures and analysis reports. Advanced Vertical-In-Place (VIP) and Picture-In-Picture (PIP) zoom options allow highlighting of important data regions. The contents of any VIP / PIP zoom windows and the main window are synchronized in real-time. Similar to professional graphing software, EVA provides access to graphics properties and text attributes (font formats, colors, and much more).

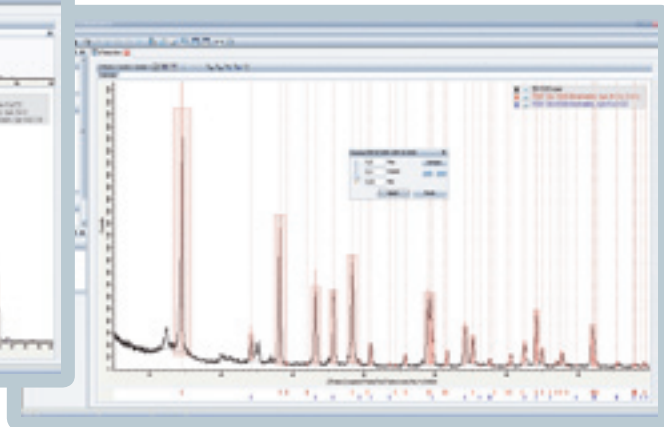
Phase analysis workflow



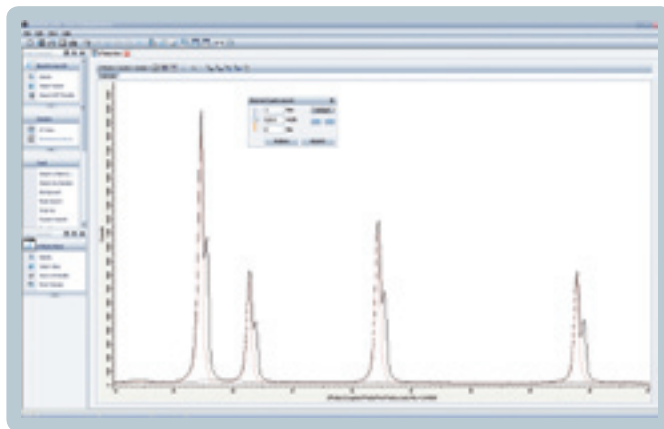
Powerful data evaluation and visualization options



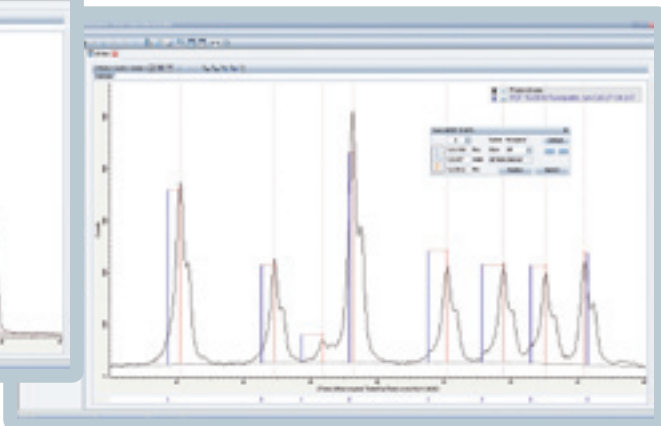
Extended zoom options: Vertical-In-Place (VIP) and Picture-In-Picture (PIP) zooms to highlight regions of interest



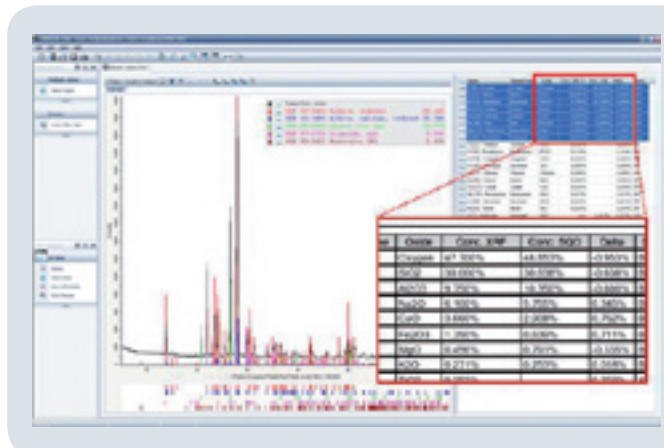
Residual search: Automatic exclusion of identified peak regions (red scan areas) for powerful trace phase analysis on the remaining sections of the scan



Real-time preview: $K\alpha_2$ - stripping (red curve)



Real-Time preview: Graphical adjustment of lattice parameters obtained from a reference data base (blue pattern) to match those of the sample (red pattern)



Combined XRD-XRF analysis

A particular highlight is EVA's ability to simultaneously analyse XRD and elemental data (e.g. obtained via XRF). Automatically restricting search/match to phases consisting of only actually present chemical elements dramatically improves phase identification success rates, specifically for samples with completely unknown composition and origin. For quantitative phase analysis, EVA calculates both phase and element concentrations, and compares the latter with the actually measured element concentrations. Combined XRD and elemental analysis thus serves as an extremely powerful tool to confirm phase identification and to improve the accuracy of quantitative phase analysis results.

General data evaluation options:

- Peak search and creation of peak data, e.g. for phase identification
- Manual and fully automatic background subtraction
- Data smoothing (Savitzky-Golay method or Fourier filtering)
- $K\alpha_2$ -stripping (enhanced Rachinger method)
- 2θ -offset and sample displacement corrections
- Calculation of profile parameters such as line position, center of gravity, integrated area, half width and more
- Crystallite size determination (Scherrer method)
- Addition, subtraction, scaling, normalisation and merging of scans
- Simultaneous evaluation of multiple scans
- Undo / redo of all operations

Data display options:

- Self explaining user interface, fully customizable by each individual user
- Advanced Vertical-In-Place (VIP) and Picture-In-Picture (PIP) zoom options
- Customizable 2D and 3D data representations (iso-intensity plots, waterfall plots)
- Free customization of graphics and text properties for creation of publication-ready figures

Data exchange and reporting options:

- Creation of customizable, high quality analysis reports
- Data exchange options to and from any other Windows application: copy and paste, Windows bitmaps and metafiles
- Display and printout of all reference database patterns

Phase identification and quantitative phase analysis options:

- Supports ICDD PDF2 and PDF4 reference databases
- Simultaneous search in multiple reference databases
- Search working on full-pattern and peak data
- Search for solid solutions and isostructural phases
- Highly sophisticated residual search
- Consideration of 2θ -offset and sample displacement errors
- Search by various selection criteria such as chemical composition, card quality marks, subfiles, and more
- Graphical adjustment of peak positions via tuning of lattice parameters e.g. to describe solid solutions
- Interactive overlay of the search results with the measurement data for easy evaluation
- Display of stick patterns as well as „Rietveld-type“ tick marks with hkl-indices
- Quantitative analysis based on RIR (reference intensity ratio) and spiking methods
- Degree of crystallinity determination
- „Combined XRD-XRF analysis“: Validation and improvement of search as well as quantitative phase analyses results using elemental analysis results; direct access to SPECTRA^{plus} XRF databases, formatted ASCII-files, and more.
- Support of Variable Counting Time (VCT) data for accurate trace phase analysis