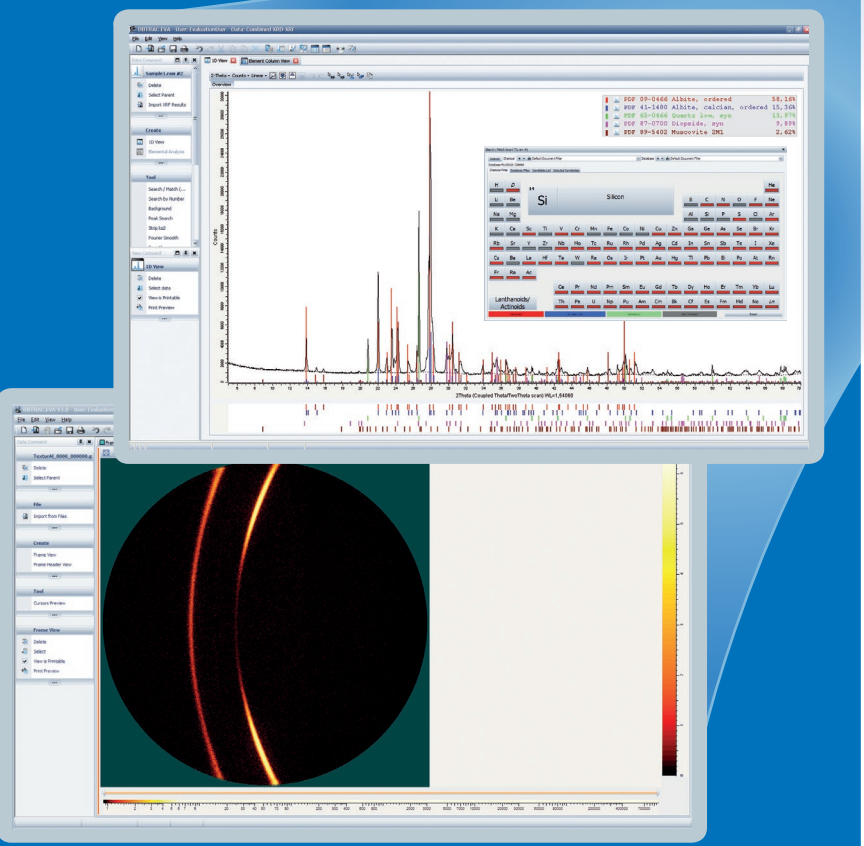
DIFFRAC.EVA

The next era in phase analysis



- Seamlessly integrated interpretation of 1-D and 2-D data sets
- Simultaneous phase identification and quantification for automated phase analysis
- Combined XRD-XRF analysis for unambiguous phase identification and accurate quantification

DIFFRAC.EVA defines a new benchmark for phase analysis by making interpretation of one- and two-dimensional XRD data easier, faster, and more accurate than ever. Most remarkable is EVA's complete collection of the best algorithms for data integration and evaluation, blended with a 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.

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.

Seamless integration of 1-D and 2-D data interpretation

Unique to EVA is its ability to fully exploit the advanced capabilities of XRD² for phase analysis. Preferred orientation and spotiness effects can be seen at a glance and dealt with by appropriate integration. A multitude of integration tools are available for single and multiple frames at the touch of a button to obtain the best data quality XRD can deliver.

Reliable and accurate phase analysis

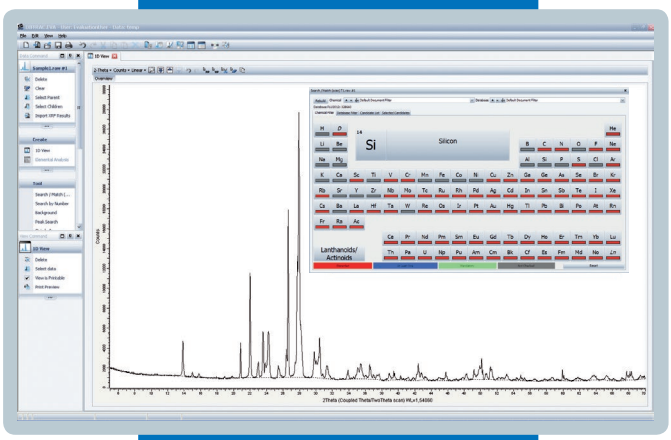
Since its first release, EVA's search/match module is generally appreciated as the most reliable and most accurate tool for phase identification. Correspondingly, EVA performed best in an international Search-Match Round Robin (Le Meins et al., 2002, http://www.cristal.org/smrr). Since then numerous 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. Additionally, the spiking method is supported, allowing absolute scaling of quantitative results.
- Highly sophisticated residual search with respect to 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

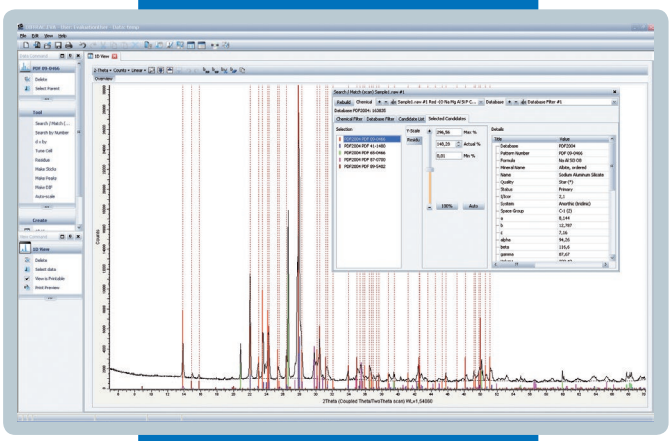
Powerful graphing tools

EVA offers powerful graphing tools to create customized, publication ready figures and analysis reports from 1-D and 2-D data. Advanced picture-in-picture (PIP) and vertical-in-place (VIP) zoom options allow highlighting of important data regions. The contents of any PIP / VIP 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).

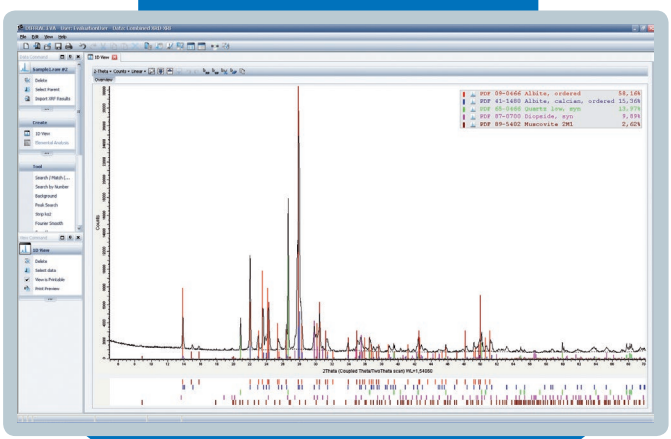
Phase analysis workflow



Phase identification

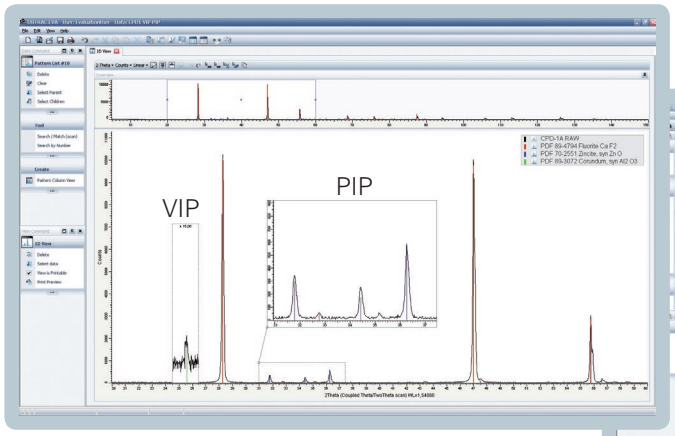


Quantitative analysis

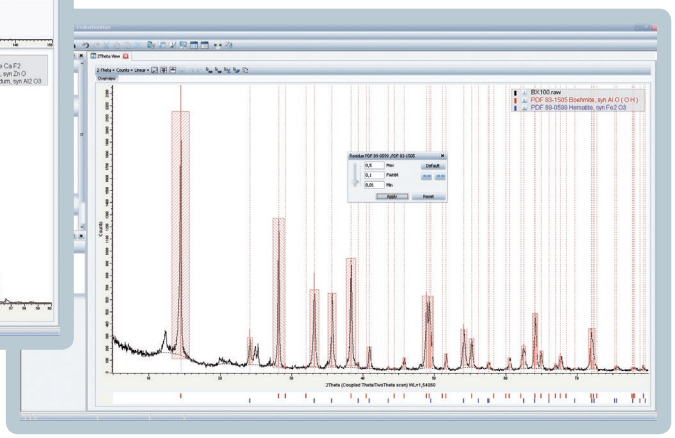


Report

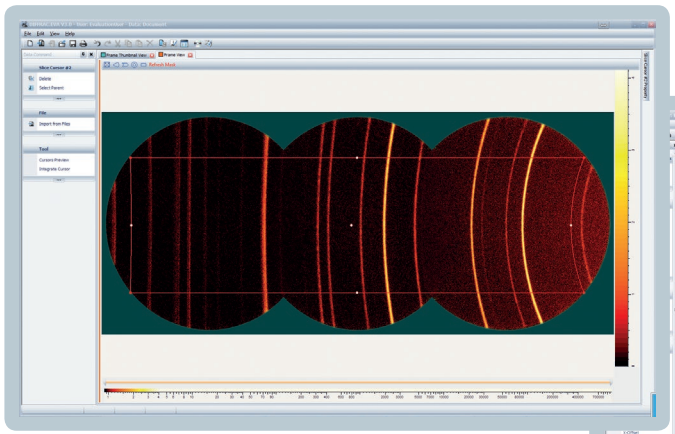
Powerful data evaluation and visualization options



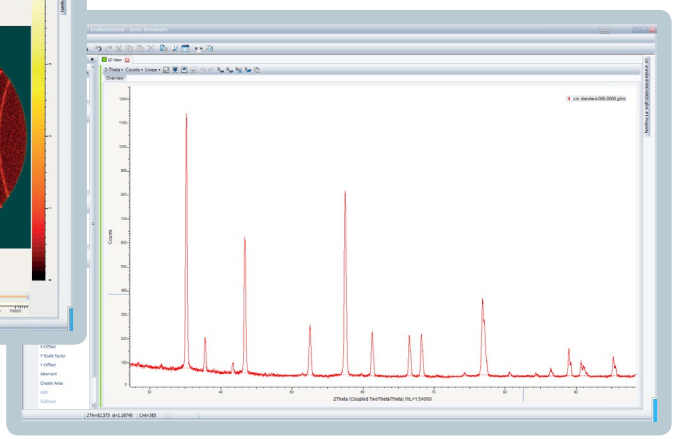
Extended zoom options: Vertical-in-place (VIP) and picture-in-picture (PIP) zooming to highlight regions of interest



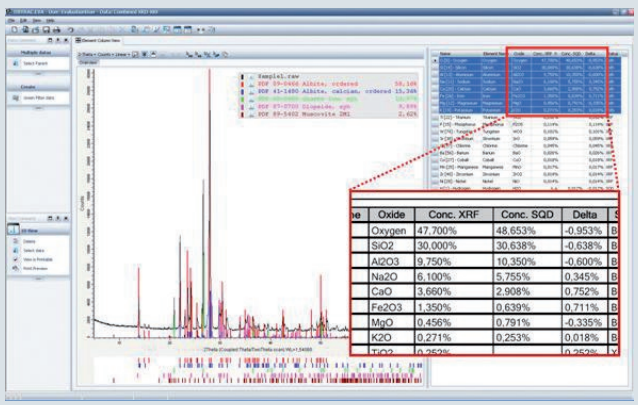
Residual search: Automatic exclusion of identified peak regions for powerful trace phase analysis



2-D frame view with three merged frames



Resulting 1-D scan after data integration



Combined XRD-XRF analysis

A particular highlight is EVA's ability to simultaneously analyze 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 phases 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 mass absorption coefficients and corresponding X-ray penetration depth into the specimen
- 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 picture-in-picture (PIP) and vertical-in-place (VIP) zoom options
- Customizable 2-D and 3-D 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
- Data can be exported as Bruker's .raw file format, an ASCII 2 column XY file or a 3 column XYE file

Advanced XRD² data evaluation and display options

- Single 2-D frame integration over gamma and 2Theta with full frame, wedge, ring and line cursor
- Integration on merged 2-D frames with slice, wedge und ring cursor
- Multiple integrations on stackable 2-D frames with one click
- User configurable masks with angular or pixel coordinates
- "Rocking curve analysis" on stackable 2-D frames with various frame properties
- Frames are automatically grouped into mergeable or stackable lists
- For large zoom factors the 2-D view displays the number of counts inside the pixel areas

Phase identification and quantitative phase analysis options:

- Supports ICDD PDF2, ICDD PDF4 and the COD reference databases
- Simultaneous search in multiple reference databases
- Search 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
- Hkl-generator for calculating peak positions based on lattice parameters and space group to aid identification of missing or redundant specimen peaks
- 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, if available
- 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 SPECTRAplus XRF databases, formatted ASCII-files, and more
- Support of variable counting time data

Multilanguage support

- Chinese, English, French, German, Japanese

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