



X-RAY DIFFRACTION

DIFFRAC.EVA V8

Software Feature Overview

DIFFRAC.EVA provides tools for the analysis of one and two-dimensional diffraction data. It supports all types of Bruker detectors and scan types. The EVA functionality covers a broad analytical spectrum from data reduction, basic scan evaluation and presentation, detailed peak analysis, phase identification and quantification, to crystallinity and crystallite size determination. EVA interfaces with all relevant databases for phase ID but can also use crystal structures and complementary information from e.g. XRF based chemical analysis for its award-winning species identification.

In addition, DIFFRAC.EVA supports the evaluation of large amounts of data generated by today's state-of-the-art fast detectors, the use of in-situ environments, or high-throughput screening studies. The software provides specific plots as well as advanced chemometrics tools for cluster analysis and pattern-matching based species identification and phase quantification.

It fully supports traditional file-based tasks, but also integrates the DIFFRAC.SUITE database infrastructure for day-to-day work, even in controlled environments as required by the 21 CFR Part 11 regulations for the pharmaceutical industry. Finally, DIFFRAC.EVA is used to produce publication-ready graphs and custom reports, either directly in EVA or using the DIFFRAC.SUITE RESULTS-MANAGER and the instrument database.

Typical EVA analysis include:

- Peak and phase monitoring
- Crystallinity determination
- Crystallite size
- Phase identification
- Quantitative phase analysis
- Crystallographic lattice determination
- Cluster analysis
- Reference scan matching
- Rocking curve evaluation

General data evaluation options

- Scan arithmetics (add, subtract, combine, normalize, merge, re-bin)
- Peak search and creation of peak lists, e.g. for phase identification
- Manual and fully automatic background determination
- Data smoothing (Savitzky-Golay method or Fourier filtering)
- $K\alpha_2$ -stripping (enhanced Rachinger method)
- 2theta-offset and sample displacement corrections
- Peak/Background and Signal/Noise calculation
- 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 (area tool)
- Analytical profile analysis for single peaks and patterns (fit tool)
- Automatic 2theta-offset detection
- Crystallite size determination (Scherrer method)
- Simultaneous evaluation of multiple scans
- Undo / redo of view operations

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 and 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

Pattern matching

- Combine up to four datasets: XRD, XRF, IR, Raman, TGA/DSC, numeric data
- Automatic Weighting Scheme
- Five clustering methods
- Cluster Validation Tools
- Customizable Analysis Methods
- Re-run selected analysis
- Interactive Dendrograms
- Cell view
- 3-D MMDS and PCA plots
- 6-D plots of sample prep info
- Numerical Results
- Amorphous Phases Identification
- Reference patterns for mixtures
- Quality Control mode
- Report Writer
- Online documentation, Program Tutorial
- SQUALL: semi-quantitative analysis based on reference scans
- PMI: Positive Materials Identification

Species identification and quantitative phase analysis options

- Supports ICDD PDF2, PDF5, Web PDF and PDF4 AXIOM, user databases and the COD reference database
- User update of COD search and structure database
- Search by various selection criteria such as chemical composition, card quality marks, subfiles, and more
- Simultaneous search in multiple reference databases
- Search on full-scan or individual peak data
- Search for solid solutions and isostructural phases
- Highly sophisticated residual search with Match peaks supporting the identification of minor phases or alternatively Profile Fit Residual Search (PFRS) after automated pattern fit
- Wavelength cursor for interactive identification of spectral aberrations (tungsten, $K\beta$ lines)
- Consideration of 2theta-offset and sample displacement errors
- 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 or "Rietveld-type" tick marks with hkl-indices, if available
- Display of calculated profiles of the individual species in a mixture
- Quantitative analysis based on RIR (reference intensity ratio) and spiking methods
- Matching lines view for individual peak analysis
- 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 Bruker XRF databases, formatted ASCII- files, and more
- Support of variable counting time data
- Use of crystal structures (cif- and DIFFRAC. TOPAS str-format) for pattern generation
- Pattern fit with intensity, lattice parameter fit, preferred orientation correction and amorphous determination, size/strain calculation. Sequential fit of scan lists.
- TOPAS connectivity (STR export of the selected candidates)
- Create and/or execute TOPAS PRO file
- STR information added to COD und User DB
- Auto phase ID

Data display options

- Self-explaining user interface, fully customizable by each individual user (dockable panels, configurable tool-bars; save/load general settings, tool-bar layouts and application specific screen layouts)
- Advanced picture-in-picture (PIP) and vertical-in-place (VIP) zoom options
- Customizable 2-D and 3-D multi-scan representations (iso-intensity plots, waterfall plots, 3D surface plot)
- Free customization of graphics and text properties for creation of publication-ready figures
- Side view to for charting additional information (non-ambient properties, time, crystallinity) to combine with multi-scan presentations
- Bragg 2D: Two-dimensional visualization of sample inhomogeneities (large crystallites, preferred orientation), measured with a 1-dimensional detector

Data exchange and reporting options

- Creation of customizable, high quality analysis reports including charts, tables, and complimentary information
- 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 conversion from/to Bruker's proprietary file format to ASCII single Y, 2 column XY file or a 3 column XYE file
- Comprehensive measurement parameters reporting
- Predefined and customizable table layouts
- Connection to DIFFRAC.SUITE instrument database for multi-sample reporting of scan, peak and pattern properties via RESULTS-MANAGER
- LabNotes
- User defined pattern color schemes to match with complimentary techniques (SEM, microXRF)

Workflow automation

- Workflow live recording
- Workflow runner for editing or step-by-step execution of pre-recorded actions in EVA
- Workflow selection in toolbar for immediate execution
- Workflow execution from Measurement Software START JOBS and RESULTS-MANAGER

Pair Distribution Function

- Generation of experimental Pair Distribution Functions
- Automatic corrections for Compton scatter, fluorescence, background, absorption, polarization
- Interpretation of PDF by matching individual interatomic distances cursor
- Distances Histogram View overlaying distances distributions calculated from crystal structures in search databases, selected via chemical filter
- Export PDF to TOPAS for quantitative analysis

Compliance

- DIFFRAC.EVA is part of the DIFFRAC.SUITE Part 11 package. The software fully complies with the cGxP/21 CFR Part 11 requirements of the pharmaceutical industry

Multilanguage support

- English
- French
- German
- Japanese

Supported computer operation systems

- Windows 10 and 11 (64 bit)
- Supporting multi-core CPUs

Update and upgrade policy

- Free maintenance updates (without access to new features) are available from brukersupport.com
- Bug fixes are cumulative and can be applied via maintenance update to any previous version
- Upgrades are paid versions with a higher license level that provide new functionality

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