

Display and Capabilities

▶ Search Results

*PDF-4 only

*PDF-4/Sieve+ only

- User-selectable display fields
 - Color coded quality marks
 - Formula and nomenclature fields
 - Strongest and longest lines
 - Unit cell data
 - Atomic coordinates flag*
 - And many more...
- All fields can be sorted
- Calculations for all numeric fields (mean, median, and ESD)
- User-defined graphing of most fields (x-y graphs, histograms, and category graphs)

▶ PDF Card

- d-spacing table and graph for fixed slit intensity, variable slit intensity, and integrated* intensity
- Simulated diffraction pattern*
- Formula and nomenclature fields
- Temperature of data collection
- Unit cell data
- Cross referenced atomic coordinates*
- Crystal (Symmetry Allowed) data field
- References table with DOI's (Digital Object Identifiers)
- XML export

▶ Simulated Diffraction Patterns*

- X-ray diffraction, neutron diffraction, and electron diffraction
- Bragg-Brentano or Debye-Scherrer geometry
- Particle size profile function
- 2θ zero correction
- 2θ , Q, d, and $1/d$ options for x-axis
- Linear, logarithmic, and square root intensity options for y-axis
- JPEG, PNG, and TIF exports

▶ Raw diffraction (PD3) patterns*

▶ Temperature series *

▶ 2D structure diagrams

▶ 3D molecular structures*

▶ Bond lengths/angles display*

▶ Selected Area Electron Diffraction (SAED) patterns*

- Overlay image for visual comparison and spot indexing

▶ Electron Backscatter Diffraction (EBSD) patterns*

▶ Ring patterns*

- Overlay image for visual comparison
- Option to simulate uniaxial preferred orientation

▶ Total pattern analysis*: Similarity index compares imported experimental data to simulated diffraction patterns

▶ Sieve/Sieve+

- Phase identification plugin
- Automatically import experimental data for all major XRD file types
- Support for importing 2D diffraction (ring) patterns from image files*
- Custom data processing sets for background removal, smoothing, $K\alpha_2$ stripping, and peak finding
- Semi-quantitative analysis using RIR method*
- "Smart I/Ic Substitution" uses dynamically cross referenced I/Ic values*