

# 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
- $2\theta$  zero correction
- $2\theta$ , 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\*