Advantages of Using PDF-4+ Q&A

Q: Can we simulate diffractograms with more than one phase?

A: You can display multiple simulated patterns and change crystallite size and/or orientation on one or all displayed simulated patterns. Also Answered Live at 57:25 in recorded video – available here.

Q: What is the difference between crystallite size which obtained by XRD phase quantification and crystallite size which obtained by scanning electron microscopy (SEM). For example - C3S clinker crystallite size is: 140 nm and C3 clinker crystallite size is 60 micron.

A: SEM analysis will reveal the particle or grain size. XRD will reveal the crystallite size. A grain can be comprised of one crystallite (single crystal) or several crystallites. The crystallites would be separated by grain boundaries, defects etc. within a grain. XRD crystallite size will always be equal to or less than grain size. As a guide, XRD is good to measure crystallite size up to 1000-1500 angstroms. Larger than that, the peak broadening due to crystallite size gets lost in the inherent instrument broadening.

Q: What are the main differences between PDF-4/Axiom and PDF-4+? Can you upgrade before the 3-year license of PDF-4/Axiom has expired?

A: PDF-4/Axiom features 70,318 entries with I/I_c values for quantitative phase analysis by Reference Intensity Ratio. PDF-4/Axiom is useful for routine phase identification and quantitation, but focuses on ambient phases and has a selected group of entries versus PDF-4+. You can pre-purchase 6 or 9 year packages, but I would strongly suggest you contact our sales team in order to obtain customized quote for your organization (sales@icdd.com).

Q: Can we perform the Rietveld quantification with this software? If so, how?

A: This software does not do full Rietveld quantification. You are able to do semi-quantification using I/I_c values (which is done in SIeve). You can utilize the PDF entries to identify phases, and extract atomic coordinate & crystal structure info to use during a Rietveld analysis. You may purchase a very powerful software tool called JADE that can do Rietveld Refinement and Whole Pattern Fitting as well as many other things. JADE was originally created by Materials Data, and is used in labs all over the world on data collected on every type of diffractometer. ICDD and Materials Data are now one organization working together for the benefit of our scientific community. Next month's InSession will highlight our JADE XRD software. Learn about JADE here.

Q: Is it possible to view past InSession webinars? It is very useful for me as a PDF-4+ user.

A: Yes, all past InSession webinars about the PDF are viewable on the ICDD website - https://www.icdd.com/in-session/.

Q: Is the Similarity Index the same as the Figure of Merit?

A: Answered Live at 1:01:20 in recorded video – available here.

Q: What if the pattern matching with raw pattern requires kα2 strip?

A: For the similarity index, it will depend on what processing was performed on the reference raw data pattern. As a first step, for polymer, nano, clay disordered phase type try without α2 stripping first since you would likely be comparing to raw data.

Q: How do you get the CIF files in PDF-4+?

A: When looking at a PDF entry (card) with atomic coordinates, in the upper left corner is an icon to EXPORT. Click on the dropdown arrow and there is an option to save as a CIF, TOPAS STR or XML file. For entries with no atomic coordinates you can create a simulated pattern CIF (no atomic coordinates) by opening a simulated pattern, in the upper left corner of the pattern click on FILE, click on SAVE, then you can save the pattern as a CIF pattern.

Q: Is it possible to generate/export a CIF file for a compound for which the 3D structure is available?

A: Answered Live at 1:02:50 in recorded video – available here.

Q: Does microanalysis also work for mixtures/blends? i.e. multiple phases.

A: Generally, the microanalysis option as a complement to phase identification is not designed for blends or mixtures...at this time. Currently the assumption is the microanalysis XRF data is from a single grain or small region of a sample that is single phase. There is a task group of ICDD members that are working on application of XRF data resulting from a multiphase specimen and correlating with phase identification.

Q: Is it possible to import raw neutron diffraction data? If yes, what file type?

A: You can import neutron diffraction data, constant wavelength and time-of flight. For PDF-4 entries with atomic coordinates, one can simulate CW and ToF data to compare to raw data. For ToF, the default instrument parameters are set for POWGEN, and the user has the option to import instrument parameters from another instrument. Though datafile types can vary depending upon the source, several XRD vendor formats are accepted along with CIF, CSV, XY, XYY, XYE, and GSAS GSA, GSAS, raw formats. ASCII files can typically be read and setup for import.

Q: Hi, we're using PDF 4+. Is there a way to access the database from my own program (Could I connect to PDF 4+ and search for patterns from a python program that I write myself)?

A: To protect the database from piracy and to maintain the data integrity per our ISO management system, the database is not set up to be accessed by an individual program. Doing so would be a violation of the software agreement.

Q: In micro-XRF, can we determine weight ratio close to our sample by compare with the database?

A: Possibly, if the user is certain it's a pure phase material. For a multiphase sample, the microanalysis-XRD result currently would not correlate.

Advantages of Using PDF-4+
Q&A

Q: How can you export your quantification as an image?

A: In SIeve+, right-click the graph and select "Copy". This will copy the graph image and legend to the clipboard and you can paste the image into any image editor.

Please Visit ICDD InSession Online for a List of Future Webinars:

https://www.icdd.com/in-session/