Navigating a Powder Diffraction File™ Entry
Q&A

Q: Is it possible to do refinement for quantitative analysis of different phases?

A: The built-in PDF® software can estimate the quantitation of phases using the RIR method, which can be refined using a least squares algorithm. However, in order to do a more accurate phase quantitation using the Rietveld method, you will need to use 3rd party software that is compatible with the PDF database.

Q: How is a PDF card evaluated when it is starred quality? Some starred PDF cards lack atomic sites which makes it hard to perform quantitative analysis?

A: Diffraction patterns are reviewed based on several criteria. One of the criteria for a Star pattern is a known unit cell, all reported peaks can be indexed based on the unit cell, and the observed minus calculated peak positions are less than $0.06°$ 2Θ for diffraction peaks. It is possible that a pattern without atomic coordinates can be a Star quality pattern when all peaks meet this criteria, as well as additional criteria. When atomic coordinates are present an additional (of many) criteria includes a review of atomic coordinate and thermal parameter errors.

Q: What are the differences to PDF-2?

A: The demonstration today is using our premier product (PDF-4+), and several of the simulations that will be demonstrated are unfortunately, not available in PDF-2. Additionally, PDF-2 databases, are primarily used for qualitative analysis (and not quantitative analysis).

Q: Is it possible to have whole pattern fitting use the actual diffraction patterns instead of theoretical? I frequently characterize halloysite and have a hard time fitting it with the theoretical pattern.

A: Yes, if the actual diffraction pattern exists in the PDF database. However, only a small number of PDF entries have the actual diffraction patterns.

Q: The RIR value can be obtained for all the structure. If not how to get that value?

A: RIR values are available for ~77% of all PDF entries, so in most cases you should be covered.

Q: What is the difference between calculated and structural density?

A: Calculated comes from the unit cell and the formula. Structural comes from unit cell and the coordinates.

Q: Resources are free, we are allowed to download?

A: Several free resources are available on our website (www.icdd.com) under the "Resources" menu.

Navigating a Powder Diffraction File™ Entry
Q&A

Q: Is there a way to perform search match from an experimental electron pattern in order to identify an unknown sample?

A: You can using the SIeve+ plugin if you have a list of d-spacings and intensities that were obtained/extracted from an SAED pattern. The search/match works well for a single phase pattern, but not as well for a multi-phase pattern.

Q: Is there any PDF about all preferred orientation for all minerals?

A: There is a minerals subfile within the PDF-4+. You can filter the database to display all entries that are flagged as a mineral. Within each entry you can manipulate the pattern to simulation preferred orientation effects.

Q: Other than RIR, what are the possible quantification methods in the PDF?

A: PDF-4+ allows users to carry out semi-quantification based on the RIR values. If an individual is interested in full quantitative analyses, they can export the structure information for each phase of interest, and use that information to perform full profile analysis in the refinement software of their choice. This panelist recommends utilizing MDI's JADE whole pattern fitting, as this software seamlessly allows the user to carry out a search/match or whole pattern fit once the PDF-4+ product is linked. This will be demonstrated in an upcoming ICDD In Session webinar.

Q: Is it possible to do multiple phase match and search from a raw data using PDF4+?

A: This can be accomplished in PDF-4+ by using the SIeve+ plug-in. In SIeve+ a user can import their raw diffraction pattern, carry out various data processing steps (optional), and then complete a multiphase search/match analysis. For additional details, please review our tutorial about importing data located here: https://www.icdd.com//wp-content/uploads/2018/04/Importing-ASCII-Pattern.pdf. Please note that the tutorial indicates how to import data using ASCII file format; however, PDF-4 does accept various raw data formats.

Q: Can I make diffraction of my monocrystal with powder diffraction without changing the information? What's the difference between monocrystal and powder?

A: When analyzing materials using powder diffraction and identifying the phase(s) present, there is an assumption that the sample is a powder with a randomly oriented distribution of lattice planes resulting in the powder diffraction pattern. One can run a single crystal on a powder diffractometer, however the crystal will have a preferred alignment of lattice planes so that one or very few diffraction peaks are observed in the diffraction pattern, when compared to the powder diffraction pattern. The ability to identify a phase will be hindered when the single crystal is analyzed on a powder diffractometer. If the crystal were to be ground to a powder and then analyzed using the powder diffractometer, there is a better chance to produce a powder pattern and identify the phase. Sample preparation techniques are covered in our XRD1 Clinic, and will prove useful in understanding the effect of sample type on powder diffraction data. (https://www.icdd.com/virtual-x-ray-diffraction-clinic/)

Q: I have problem in renewal and for obtaining in India. It's very difficult of embargo fixed on foreign procurement other than a country make. Do you provide an alternate for procurement?

A: ICDD does provide databases to laboratories in India. ICDD has sometimes seen that delivery to India is delayed due to shipping or tax issues. Unfortunately, these issues are outside of ICDD's control. ICDD has been working on electronic delivery of databases, and currently being tested with faculty at IISC Bangalore. Electronic delivery should help with renewal delivery and should be available in the near future.

Please Visit ICDD In Session Online for a List of Future Webinars:

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