Data Mining in PDF-4+
Q&A

Q: How many of the entries also have the neutron data besides the X-ray data?

A: The database contains entries where the data was extracted from neutron experiments, but there is no actual raw data present. However, there are 290,000 entries where one can simulate neutron constant wavelength and time-of-flight patterns.

Q: What is the "alternate" status checkbox?

A: "Primary" patterns are generally highest quality data collected under standard powder X-ray conditions (i.e. laboratory diffractometers) at room temperature. The "alternate" patterns reflect other data obtained under non-standard conditions.

Q: Some PDF cards list a "phase" field, such as gamma-alumina or chi-alumina. Is it possible to search by phase to locate only the gammas out of all other alumina's?

A: Answered Live at 1:11:20 in recorded video – available here.

Q: Can I create a default search that automatically opens every time I start PDF-4+?

A: Answered Live at 1:12:35 in recorded video – available here.

Q: If there are data missing from a PDF, is it included in the search results?
E.g: no ambient/non-ambient data in the PDF, but you choose ambient patterns in the search.

A: This is true. If the data is not present in the database, then it will not be included in search results. If a user encounters this type of situation, we encourage them to reach out to ICDD headquarters to provide such info, in order to make the entry more comprehensive. (info@icdd.com)

Q: Justin keeps saying "highest quality available" when he selects the star quality mark. Is that what it really does? What if no star for a phase is available? Will it give highest available?

A: If no star quality pattern is currently available then you will only receive the highest quality available (i.e "I" or "O"). If you restrict your search to "star" quality mark, you will not see the lower quality patterns available in the database. Thus, one must be careful to not "over" filter your searches.

Q: Isn't the strongest peak generally also the first listed? What distinguishes a "strong line" and "long line"?

A: The strong line will refer to the three most intense peaks, but searched as the d-spacings for those diffraction peaks. Long line will be based on the largest d-spacings, independent of intensity. In an entry (card) opened in PDF-4+, the d-spacings for the three strongest lines will be bold in the d-space list.

Data Mining in PDF-4+ Q&A

Q: Can you get more sig figs on the regression equation? (the x coefficient had only one sig fig)

A: Answered Live at 1:13:50 in recorded video – available [here](#).

Q: What is the difference between XtlCell vs. RedCell?

A: XtlCell is the original defined cell that typically provides the highest symmetry. The reduced cell is a unique, primitive cell based on the three shortest lattice translations. For example, if the initial cell is defined by centering such as F-centered, it can be converted to a smaller primitive cell.

Q: When you open PDF Card, how to export shown XRD pattern as csv or txt file and plot it into let say Excel or Orgin software.

A: If you are interested in exporting XRD data from the database you will need to open the PDF card of interest, then open the "raw diffraction pattern". Once the window opens you will see "File" in the top toolbar, where you can select to save the pattern. There are various file types available for saving. You can use a similar process if you are saving "simulated powder diffraction pattern".

Q: Does the first couple of digits like 00, 01 or 04 in the entry number, reflect some information like the date of publication?

A: The two numbers that are at the beginning of the PDFID represent the database source for each data set (i.e. 00 = ICDD; 01 = ICSD; 03 = NIST, etc).

Q: In Boolean search, I've never understood the difference between "just" and "only" - they sound synonymous.

A: ONLY will indicate searched phases must have only the elements specified, and has all elements specified. JUST will indicate a search for the elements specified but can have 1, 2, or more of all elements.   As an example, a Mg, Fe, O ONLY search will find phases that have all three elements: Mg, Fe, O, whereas a JUST search will have Mg, or Fe, or Mg and Fe, or Mg, Fe, and O etc.

Q: I notice the subfiles selected were 'AND'ed so search results only included patterns in both subfiles. What if you want to 'OR' the subfiles so matches are in any of the subfiles?

A: There is a drop down by the word "Subfile" where you can change from AND to OR or NOT.

Q: What other physical properties are available for the search options?

A: If you check under the "Physical Properties" tab, you can see all of the available searches.

Data Mining in PDF-4+ Q&A

Q: If sample is amorphous can we identify from XRD spectrum?

A: You can use the whole pattern match option in SIeve+ to carry out similarity searches on amorphous materials that have raw data patterns available in the PDF. PDF-4+ and PDF-4/Organics databases have raw data diffraction patterns for more than 100 polymer materials. Some represent varying levels of crystallinity from amorphous to semicrystalline. Though XRD can be used to identify amorphous phases, it is best accomplished when a reference pattern is available. Additional techniques such as IR and Raman are useful as well when there is an amorphous phase present in a sample.

Q: Was the polymer Raw Diffraction Data PD3 collected in Bragg-Brentano or Debye-Sherrer geometry?

A: Bragg-Brentano, reflection mode geometry.

Q: Does PDF contain only minerals? Does it have synthesize thin films?

A: The PDF does contain more than just minerals. It contains a vast number or inorganic and organic materials, many of which are separated into subfiles and subclasses defined chemistry or by their field of application. You can find out which phases are present in PDF databases by going to the web page https://www.icdd.com/pdfsearch/. You can search for a phase and have information provided to indicate which database(s) the phase is available. Using this search tool is useful when determining which database is best for your XRD phase identification needs.

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