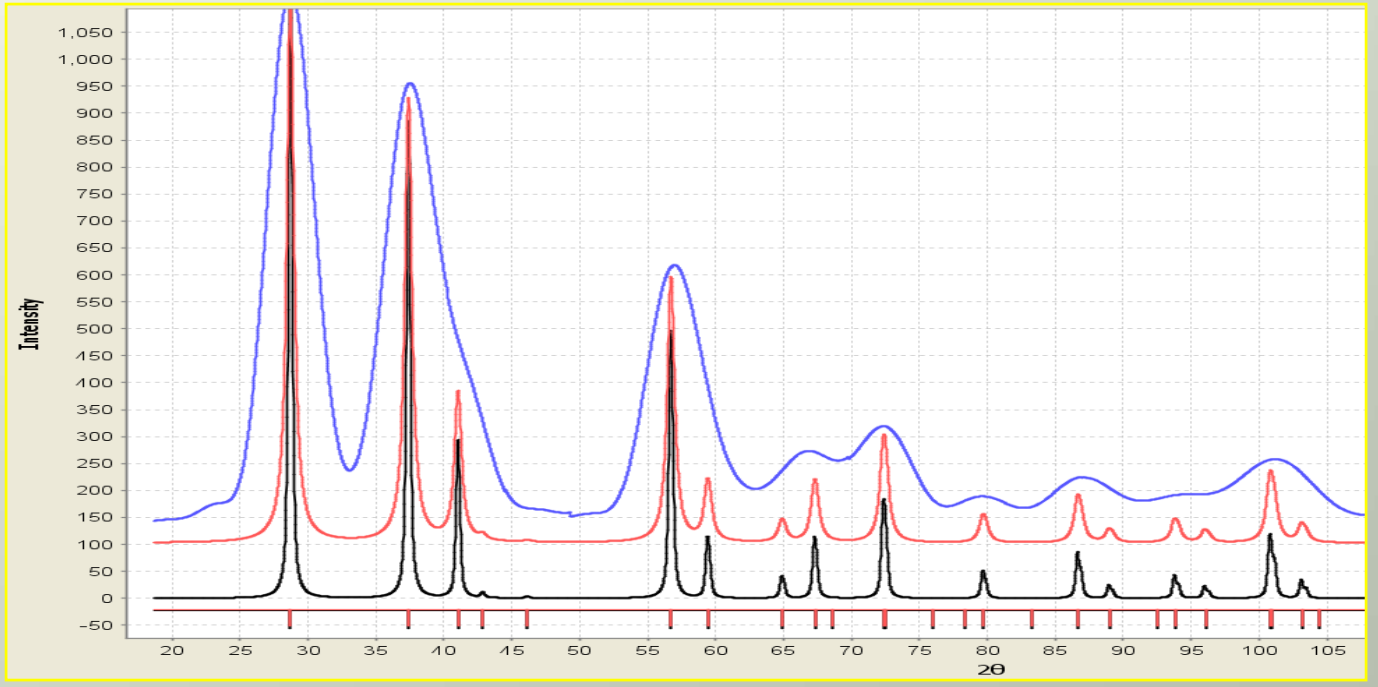
Digital Pattern Simulations

Pattern Simulations



Pattern Simulations

What?

Digital powder patterns can be calculated for all entries in the Powder Diffraction File.

Multiple patterns can be plotted to simulate experimental data.

Pattern Simulations

Why?

Digital pattern calculations can be varied to account for instrumental and experimental conditions normally present in a diffraction experiment.

By using digital patterns, reference data can be adjusted to more closely simulate experimental data for either phase identification or quantitative analysis.

Pattern Simulations

How?

The Powder Diffraction File (PDF) contains 3 basic types of data. Therefore, the simulations use 3 different algorithms to calculate a digital pattern from each type. In the PDF, the software automatically elects the appropriate algorithm based on the information available from the entry data.

Each algorithm can be adjusted for common experimental and instrumental factors.

Pattern Simulations

From Main Menu

Select "Edit" from the Tool Bar.

Use drag down menu to select "Preferences".

Select "Diffraction" from the Preferences drag down menu.

Select either "Experimental" or Calculated".

This changes *all* experimental or calculated patterns in a simulation.

From a PDF Entry

Select either "Experimental Diffraction Pattern or Calculated Diffraction Pattern" from the Tool Bar.

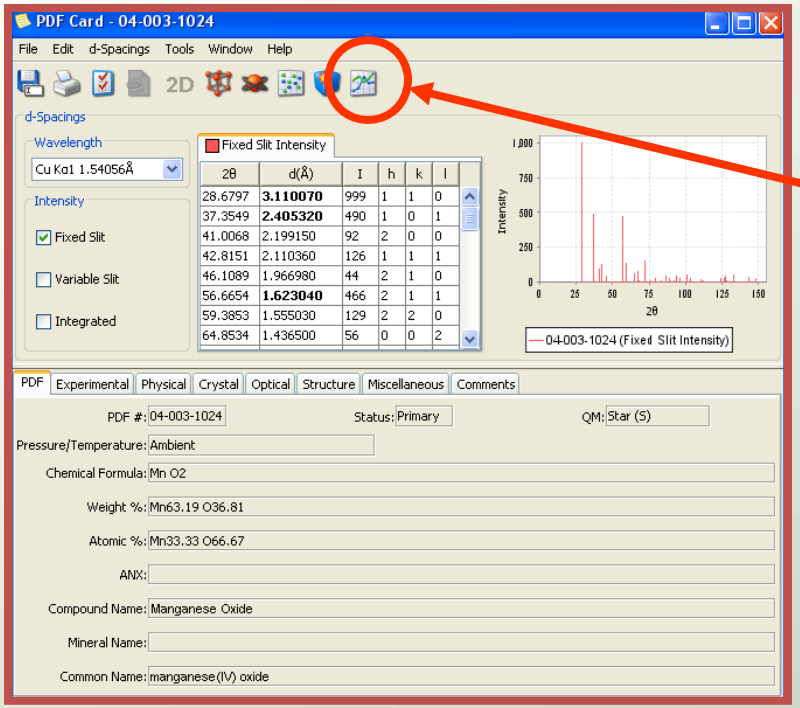
This will produce a digital pattern for the *selected PDF entry*.

Select "Edit" from the Tool Bar of the pattern.

Select "Preferences" from the Edit drag down menu.

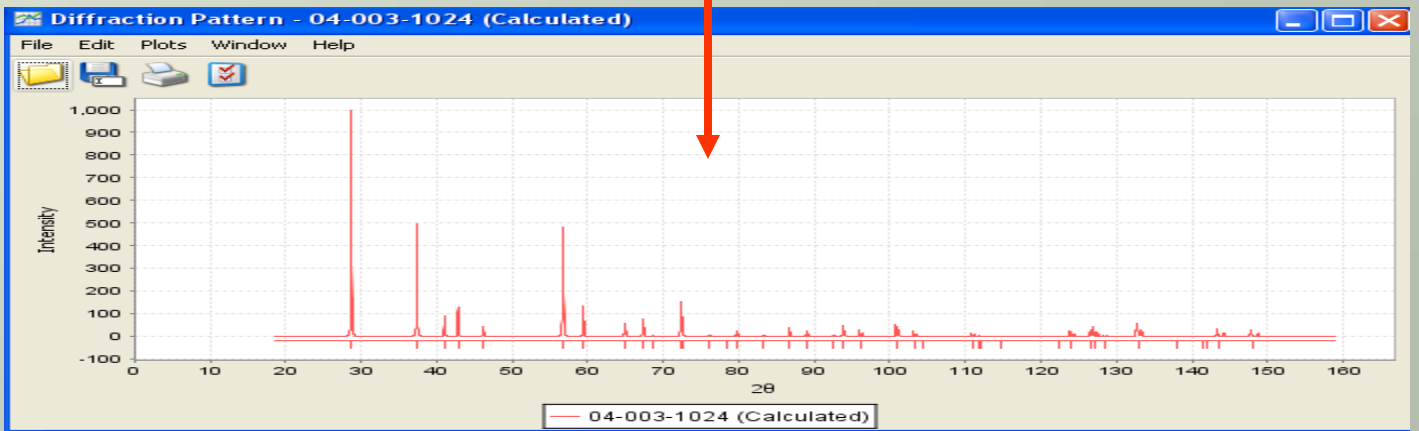
This changes only the selected pattern in the simulation.

From a PDF Entry



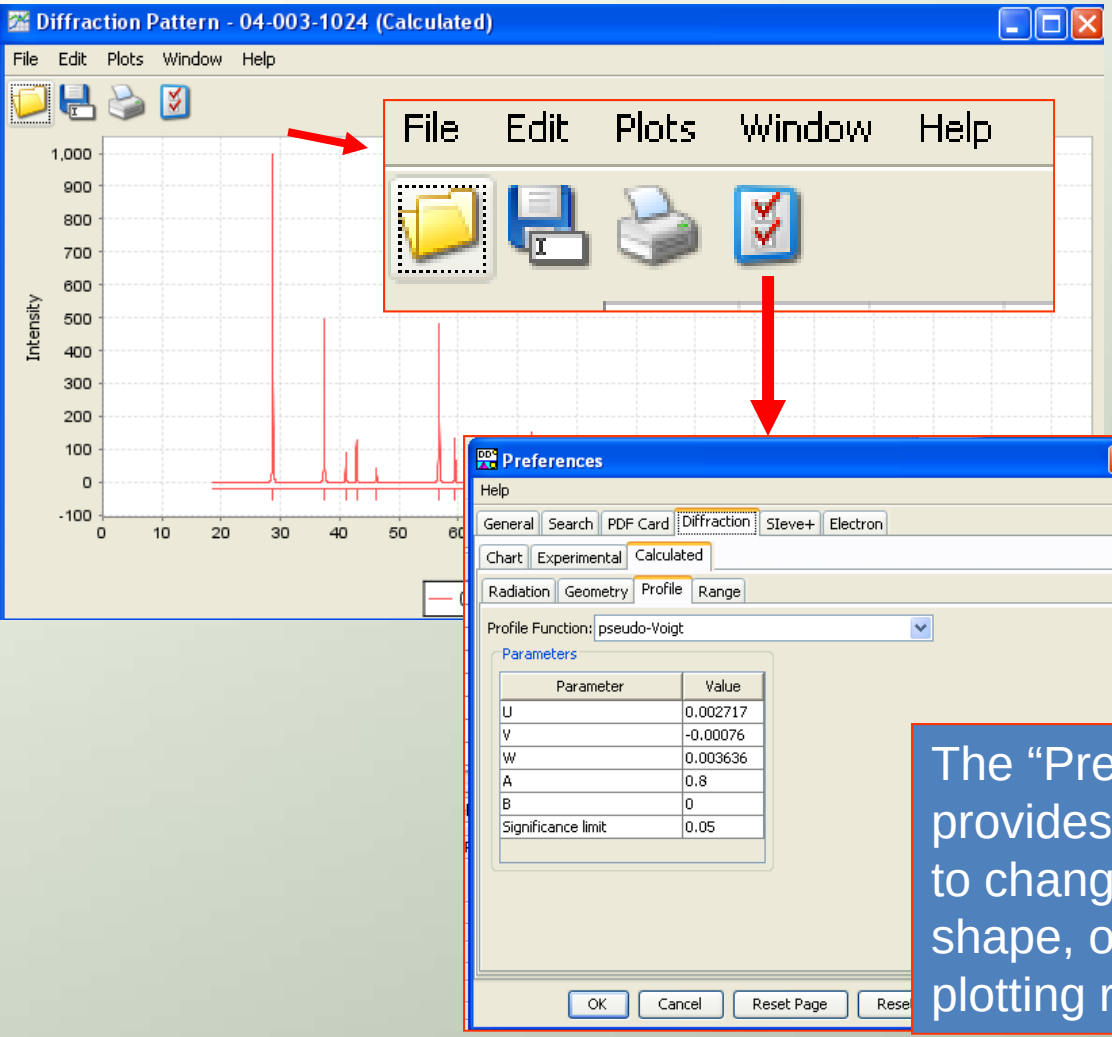
From an entry, select the Graph icon.

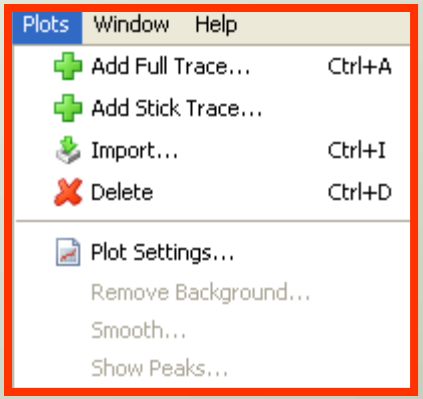
This will produce a digital diffraction pattern using default settings.



Digital Pattern Toolbar

Custom Settings



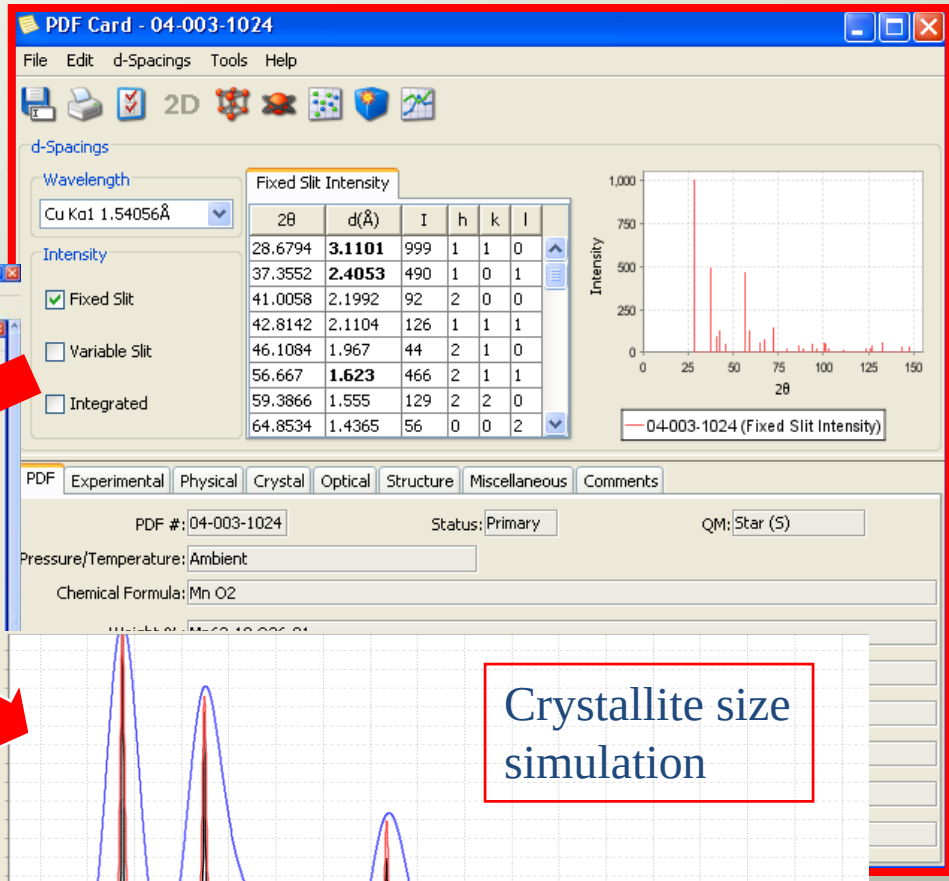


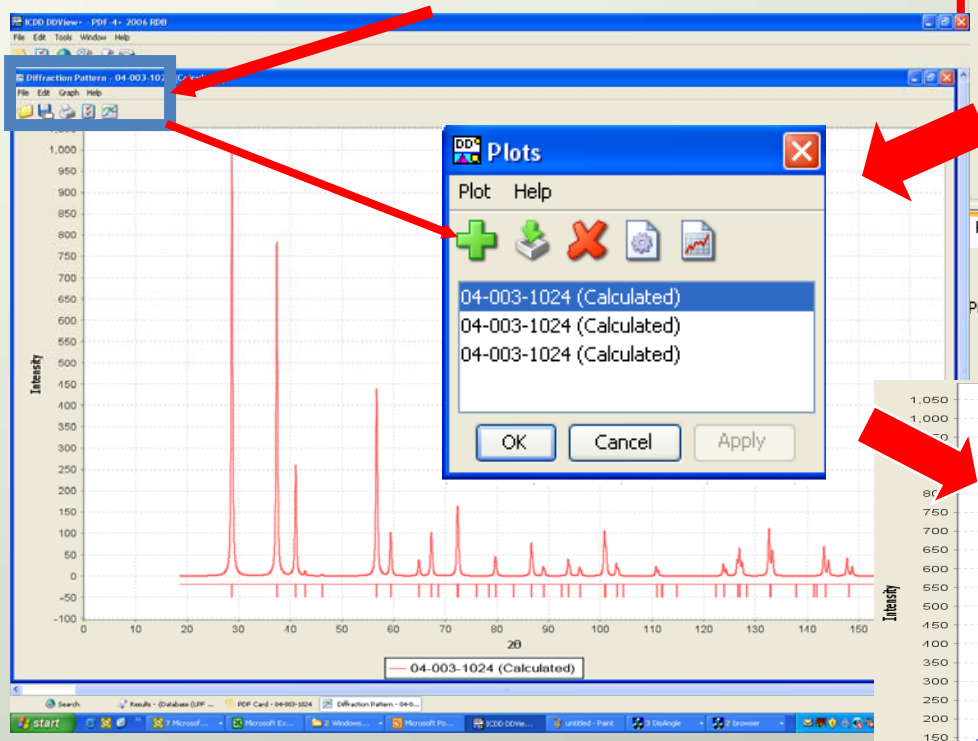
The "Plots" Menu lets you Add or Delete additional patterns and change their settings (color, scale, etc.).

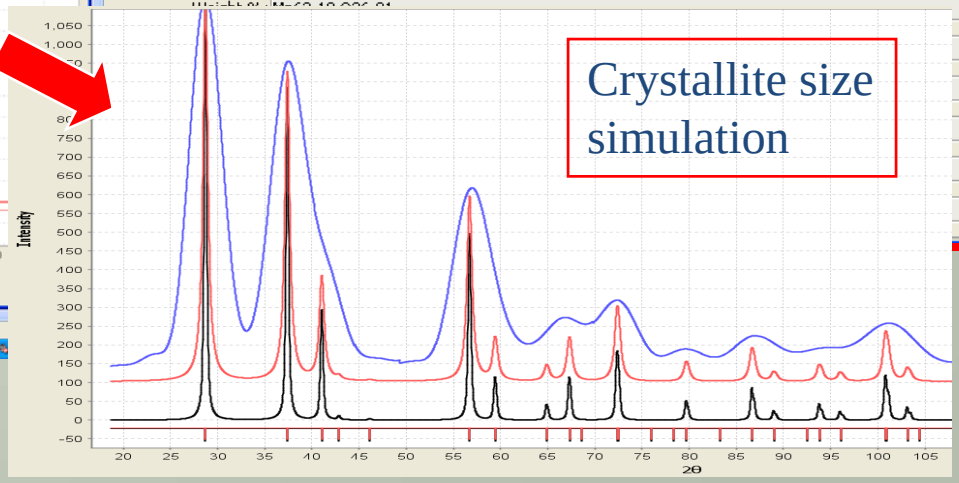
The "Preferences" Menu provides the user with options to change wavelength, peak shape, optical geometry and plotting range.

Pattern Simulations From an Entry

Options for the addition of multiple phases, instrument and specimen factors, wavelengths. Options for import/export and graphic display calculations.

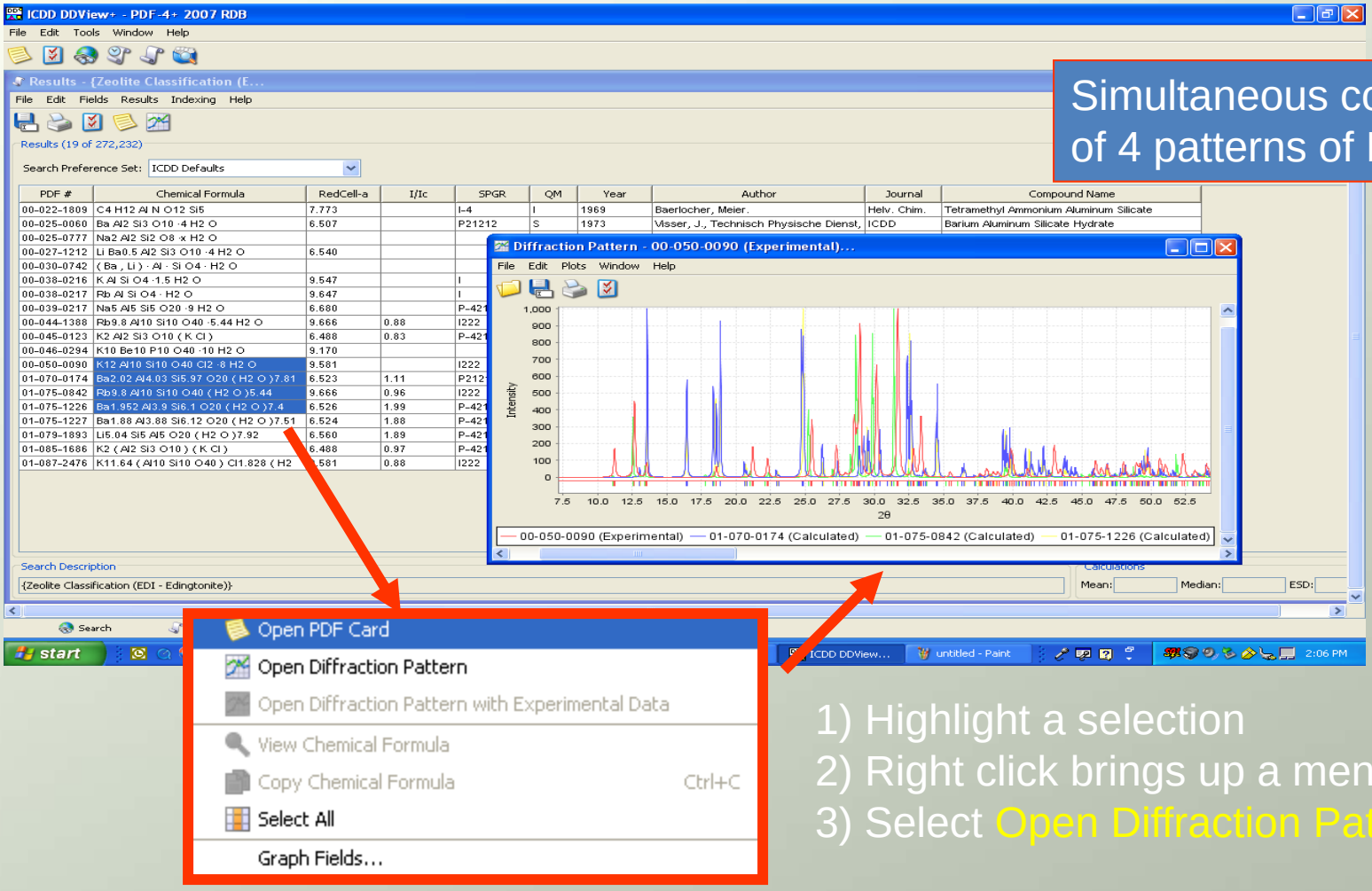






Multi-Pattern Simulations

From the Results Form

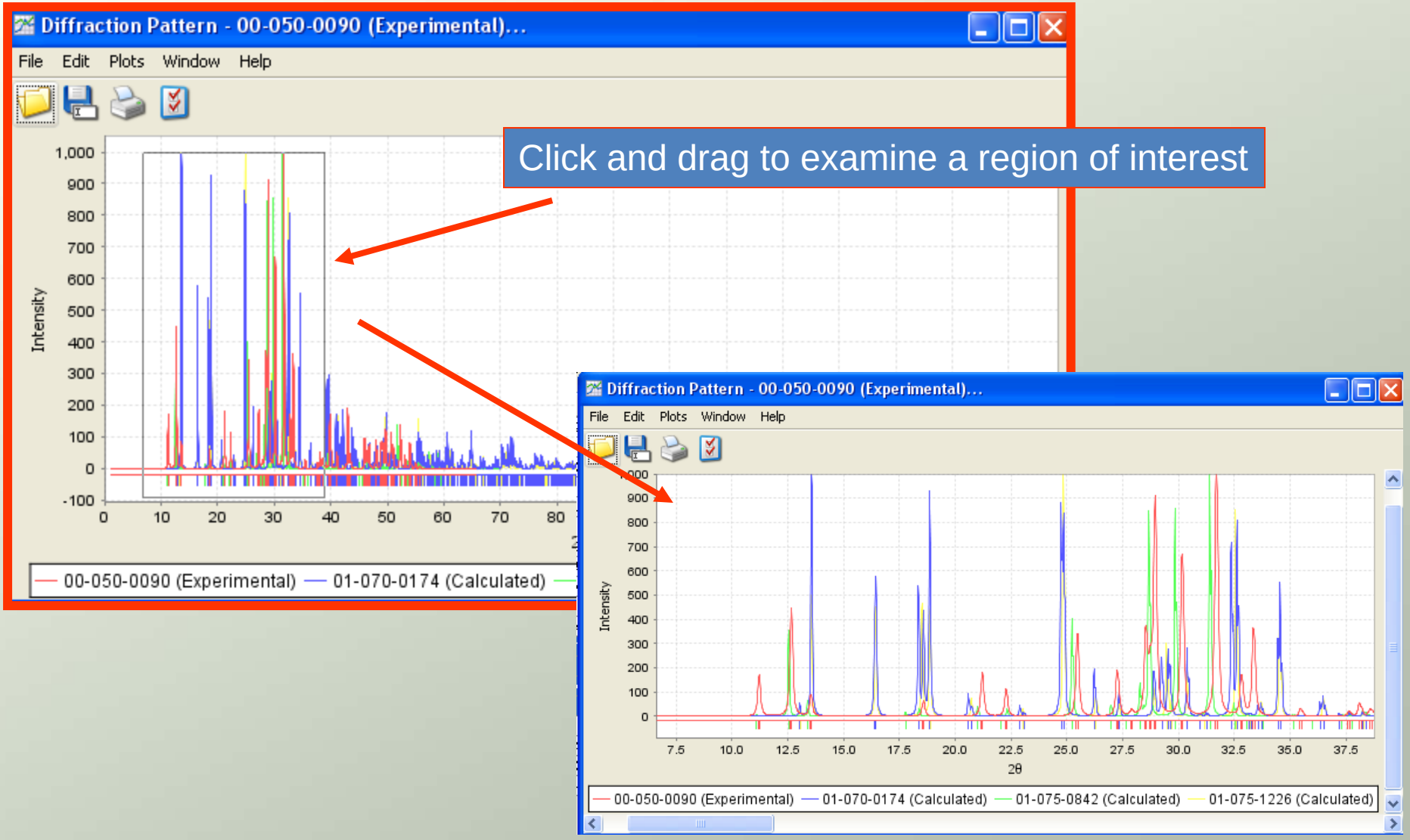


Simultaneous comparison of 4 patterns of Edingtonite

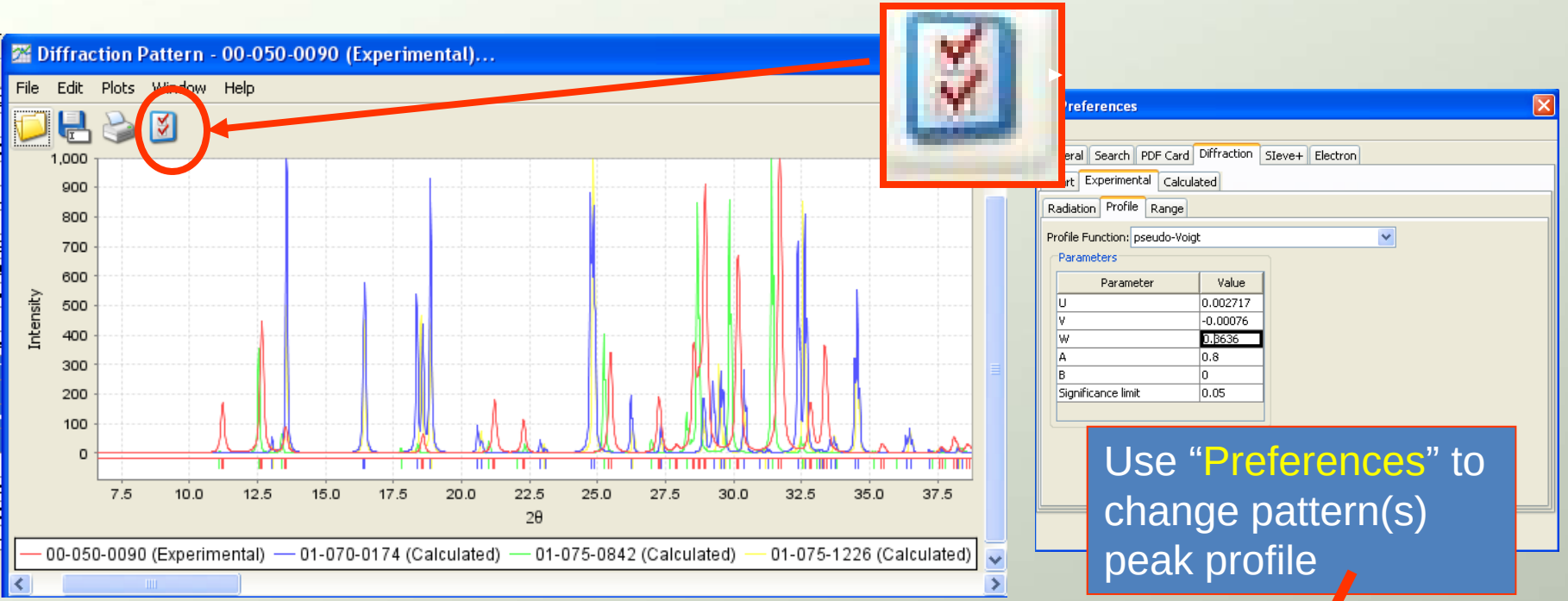
1) Highlight a selection
2) Right click brings up a menu
3) Select Open Diffraction Pattern

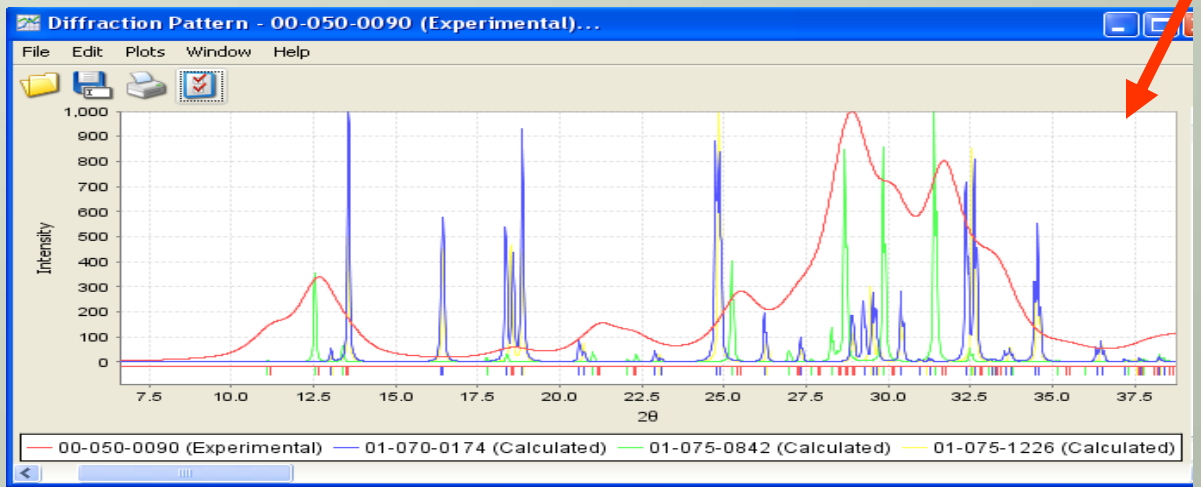
Note: Shift and Ctrl keys highlight selections

Multi-Pattern Simulations



Multi-Pattern Simulations





Simulations with Experimental Data

The digital pattern module can be used interactively with the program SIeve+. (See the Identification – PDF-4 SIeve+ tutorial).

The program SIeve+ will search the database to find matches for experimental data based on Fink, Hanawalt or Long 8 search algorithms.

SIeve+ will examine the peak heights of the reference data and scale them to the experimental data. This scale factor is then input automatically into the digital plotting routines.

Sleve+ and Experimental Data

GOM	PDF #	Compound Name	Chemical Formula	L1	L2	L3	L4	L5	L6	L7	L8	I/Ic	Pat. GOM	Integral In
886	00-002-0571	Magnesium Silicate Hydrate	3 Mg O ·4 Si O2 · H2 O	9.300000	4.600000	3.110000	2.600000	2.480000	2.220000	1.720000	1.520000		212	4.95
886	00-003-0881	Magnesium Silicate Hydroxide	Mg3 Si4 O10 (O H)2	9.300000	4.580000	3.130000	2.620000	2.490000	2.220000	1.720000	1.530000		171	7.03
886	00-009-0474	Calcium Cerium Silicate Hydroxide	Ca2 Ce3 (Si O4) (Si2 O7) (O , O H...	9.300000	5.070000	4.620000	3.500000	3.340000	2.960000	2.830000	2.670000		182	4.47
886	00-013-0118	Calcium Uranyl Silicate Hydrate	Ca3 (U O2)4 Si10 O35 ·24 H2 O	9.300000	5.070000	4.620000	4.470000	3.570000	3.340000	3.210000	3.037000		224	9.17
886	00-014-0155	Potassium Magnesium Vanadium Oxid...	K Mg V5 +5 O14 ·8 H2 O	9.300000	8.200000	7.400000	7.000000	5.000000	4.100000	3.310000	3.130000		212	16.4
886	00-028-2010	Fluorene	C6 H4 C H2 C6 H4	9.300000	5.100000	4.780000	4.590000	4.240000	4.150000	3.350000	2.590000		206	7.18
886	00-029-1659	Diazepam	C16 H13 Cl N2 O	9.300000	6.680000	6.470000	5.130000	5.030000	4.680000	3.893000	3.729000		220	18.18
886	00-031-0273	Calcium Iron Magnesium Aluminum Ph...	Ca Fe Mg2 Al2 (P O4)4 (O H)2 ·8 H...	9.300000	5.590000	4.920000	4.850000	4.660000	3.487000	2.946000	2.789000		228	11.15

Matches Filter

Select...

Filter Description

{Subfile/Subclass (Mineral Or Pharmaceutical)}

Experiment

Search Line(s): 9.29134 Å D1 Range: 9.145 - 9.438 Å Rotation: 1 of 8

Preferences

Search Window: 0.15 ° Match Window: 0.15 °

Search Method: Long8 Lowest Allowable GOM: 500

Wavelength: Cu Ka1 1.54056Å

Phases (6)

#	Accepted	PDF #	Compound Name	Int. Ratio	Int. %	I/Ic	Time
1	☑	04-006-6528	Calcium Carbonate	0.834	34	3.25	127.6s
2	☑	04-002-3211	Potassium Chloride	0.783	31	6.07	21.2s
3	☑	01-070-8072	Zinc Oxide				
4	☑	00-009-0080	Calcium Hydroxide Phosphate				
5	☑	01-086-1155	Titanium Oxide				
6	☐	00-003-0881	Magnesium Silicate Hydroxide				

Open PDF Card

Open Diffraction Pattern

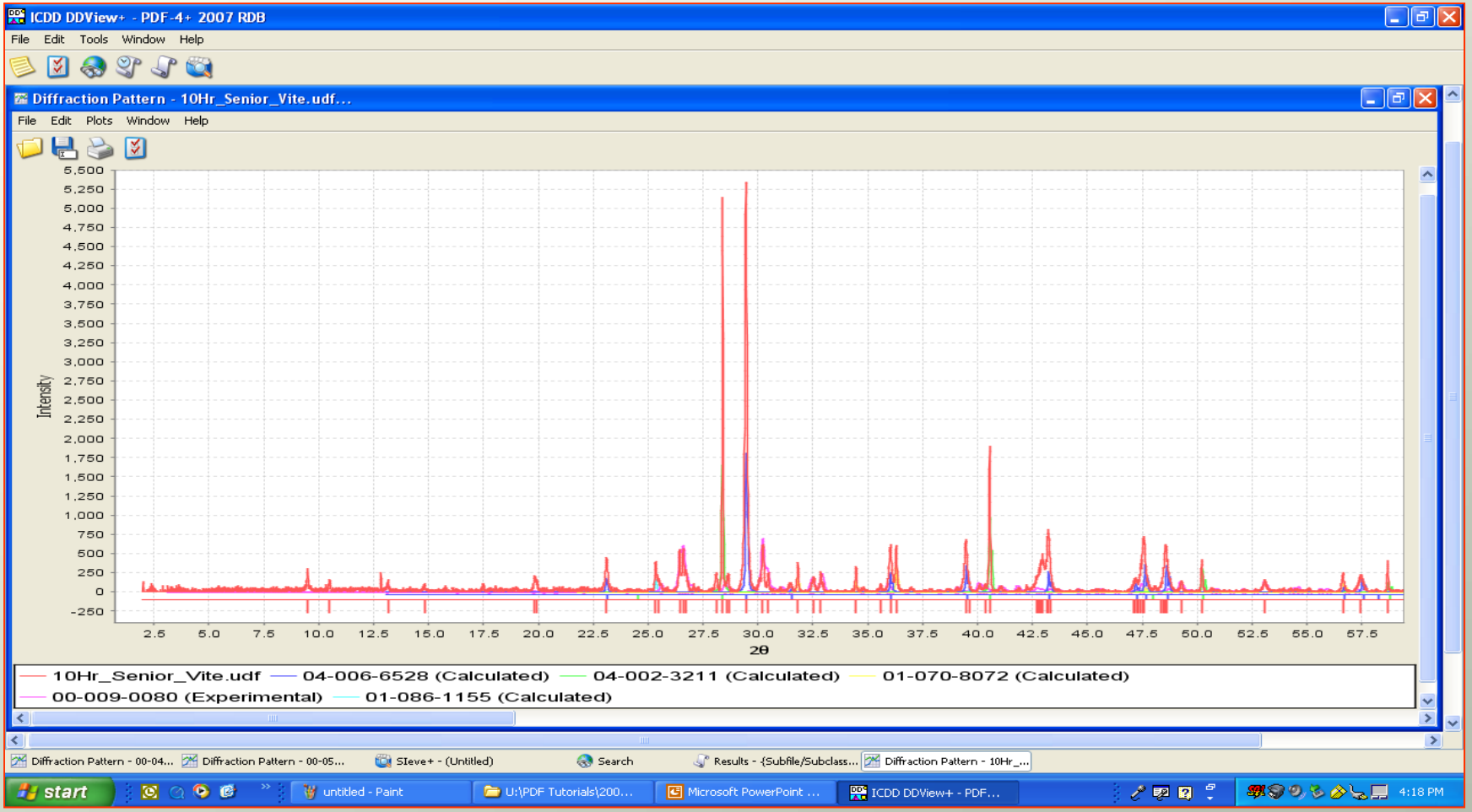
Open Diffraction Pattern with Experimental Data

Lines (40 of 57)

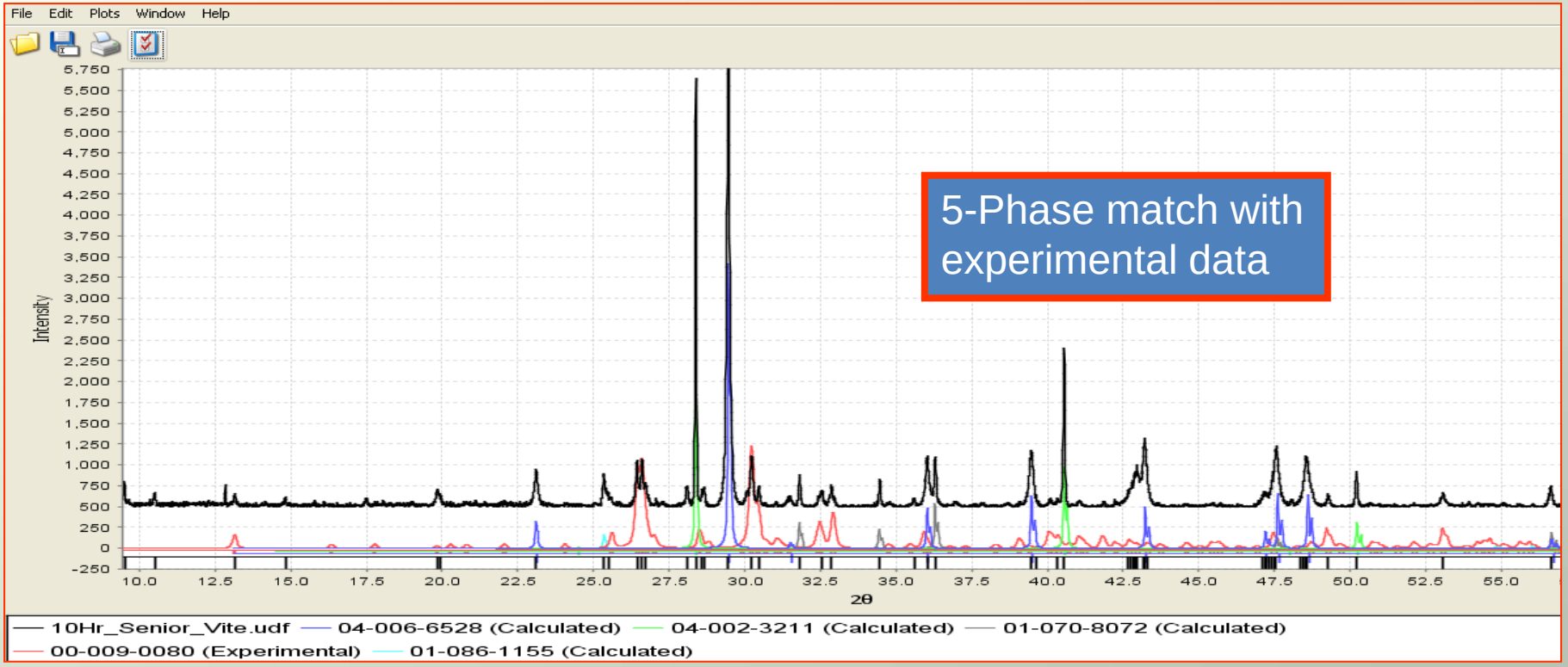
Ex d(Å) ▼	Ex I	P1 d(Å)	P1 I	P2 d(Å)	P2 I	P3 d(Å)	P3 I	P4 d(Å
9.29134	4							
8.41404	3							
6.72086	2							6.74000
5.96723	1							
4.47349	3							4.48000
4.45305	2							
3.84620	8	3.847720	10					
3.51236	6							
3.49085	2							3.48000
3.36829	10							3.37000
3.34751	10							3.35000
3.33210	4							3.33000
3.17173	4							
3.14155	96			3.143300	100			
3.11907	3							3.13000
3.11106	4							3.10000
3.02987	100	3.029430	100					
2.95613	10							2.95800

1) After SIeve search
2) Right click on highlighted results
3) Open with experimental data

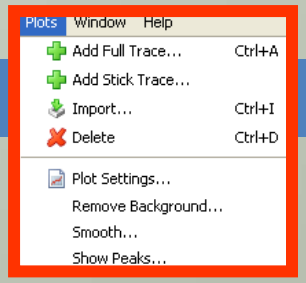
Experimental Data and Digital Pattern Simulations



Adjust Scale, Plot, and Offset Experimental Data



Used Preferences  and Plots



to adjust fit

Digital Patterns

- Can simulate crystallite size and other experimental conditions
- Useful for comparing data mining results
- Can be used to compare multiphase simulations with experimental results

Thank you for viewing our tutorial.

Additional tutorials are available at the ICDD website (www.icdd.com).

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