Electron Diffraction

Applications Using the
PDF-4+ Relational Database

Electron Diffraction in Materials Science

- Electron diffraction is an important technique for crystallographic characterization, a valuable complementary tool to powder and single crystal X-ray diffraction.

- Applications include phase identification and precision determination of subtle structural details for crystals in the micrometer to nanometer size range.

Electron Diffraction with the PDF-4+ Database

- The PDF-4+ database can be used to generate selected area electron diffraction (SAED) and electron backscatter diffraction (EBSD) patterns. This tutorial will deal with SAED patterns.

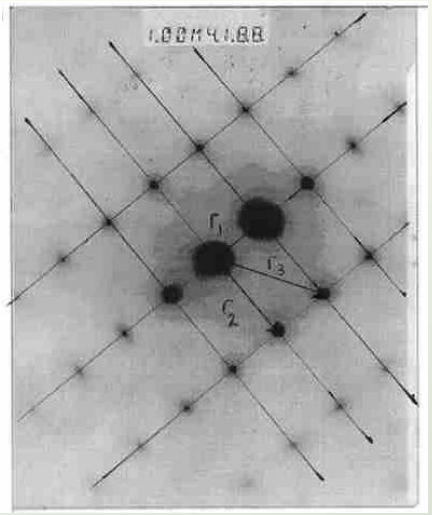
- The SAED patterns simulated by PDF-4+ 2009 use calculated intensities (using atomic scattering factors for electrons) when atomic coordinates are available, and intensities tabulated in the PDF entries when atomic coordinates are unavailable.

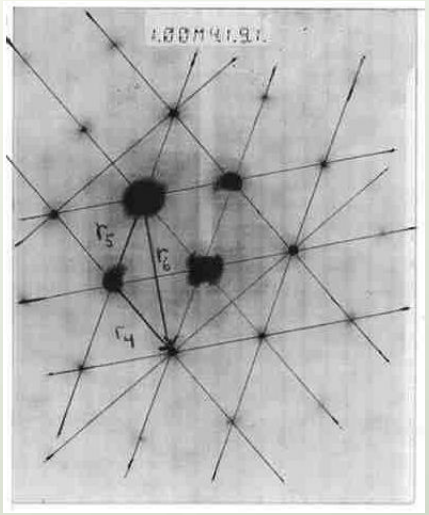
SAED Patterns with the PDF-4+ Database

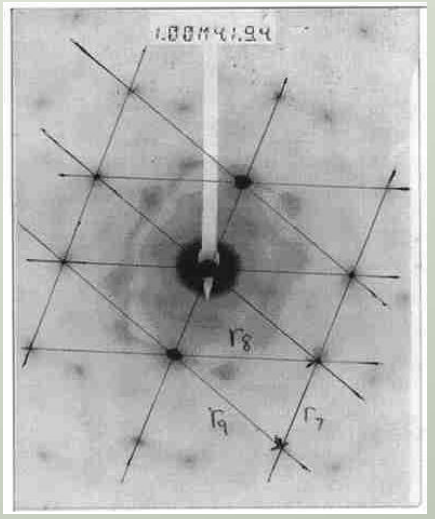
- The PDF-4+ 2009 database does not perform search-match procedures directly on digital SAED patterns. They must first be indexed to obtain a D-spacing-Intensity (D-I) list, then search-match procedures can be performed using Sleve+.

- Obtaining a D-I list and performing search-match using Sleve+ will be illustrated in the following slides.

Prepare a D-I List







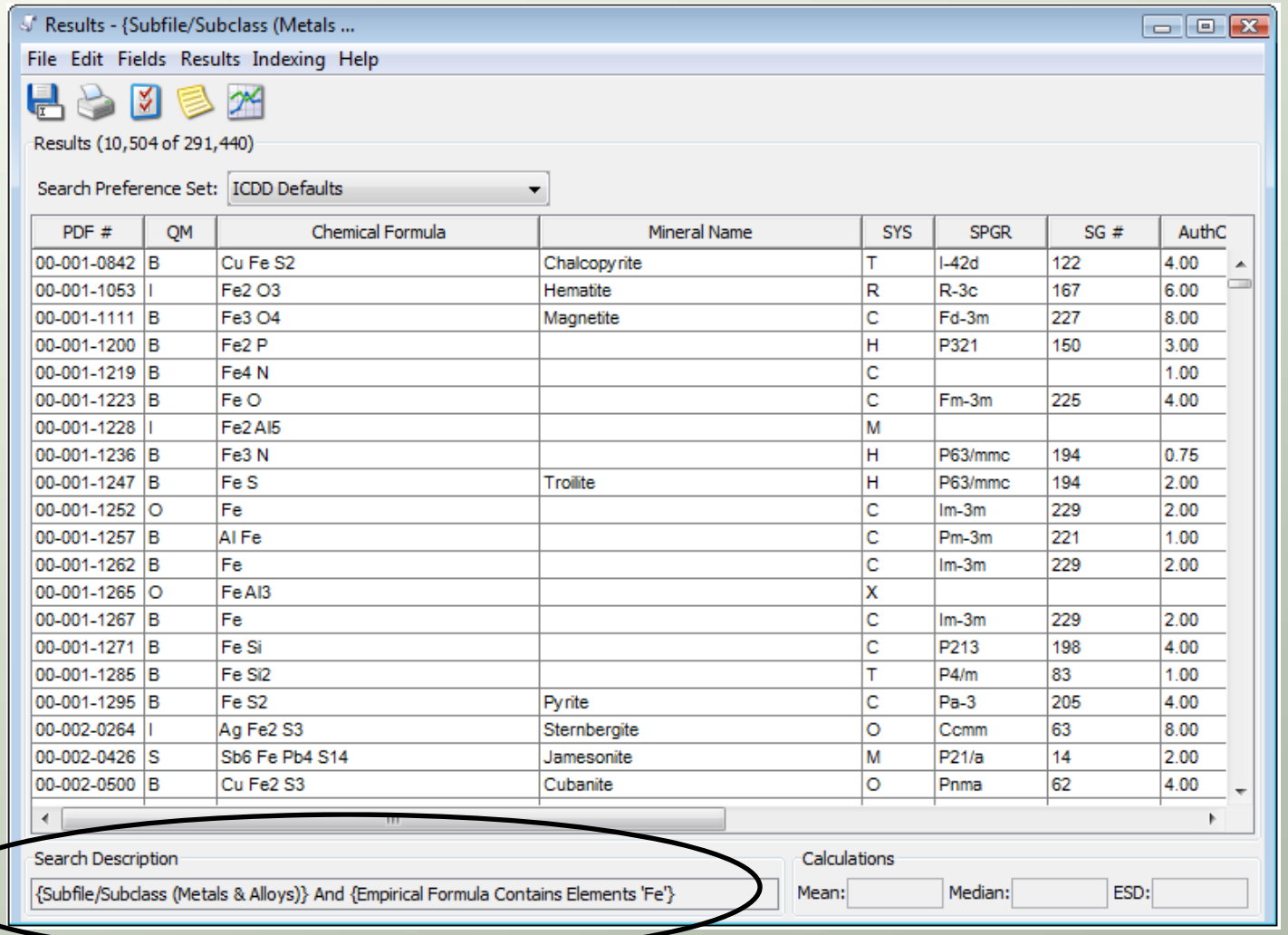
- Use SAED patterns obtained from multiple zone axes with a known camera constant to prepare a D-I list:

d (Å)	I/I_o
2.086	100
1.277	50
1.089	50
0.829	50

Use All Available Information

- The current sample is a metal alloy containing iron (based on EDS analysis).
- Before performing search-match with the D-I list in Sleve+, search the PDF database for compounds meeting the sample criteria:
  - Empirical formula contains ‘Fe’
  - Subfile: Metals and Alloys

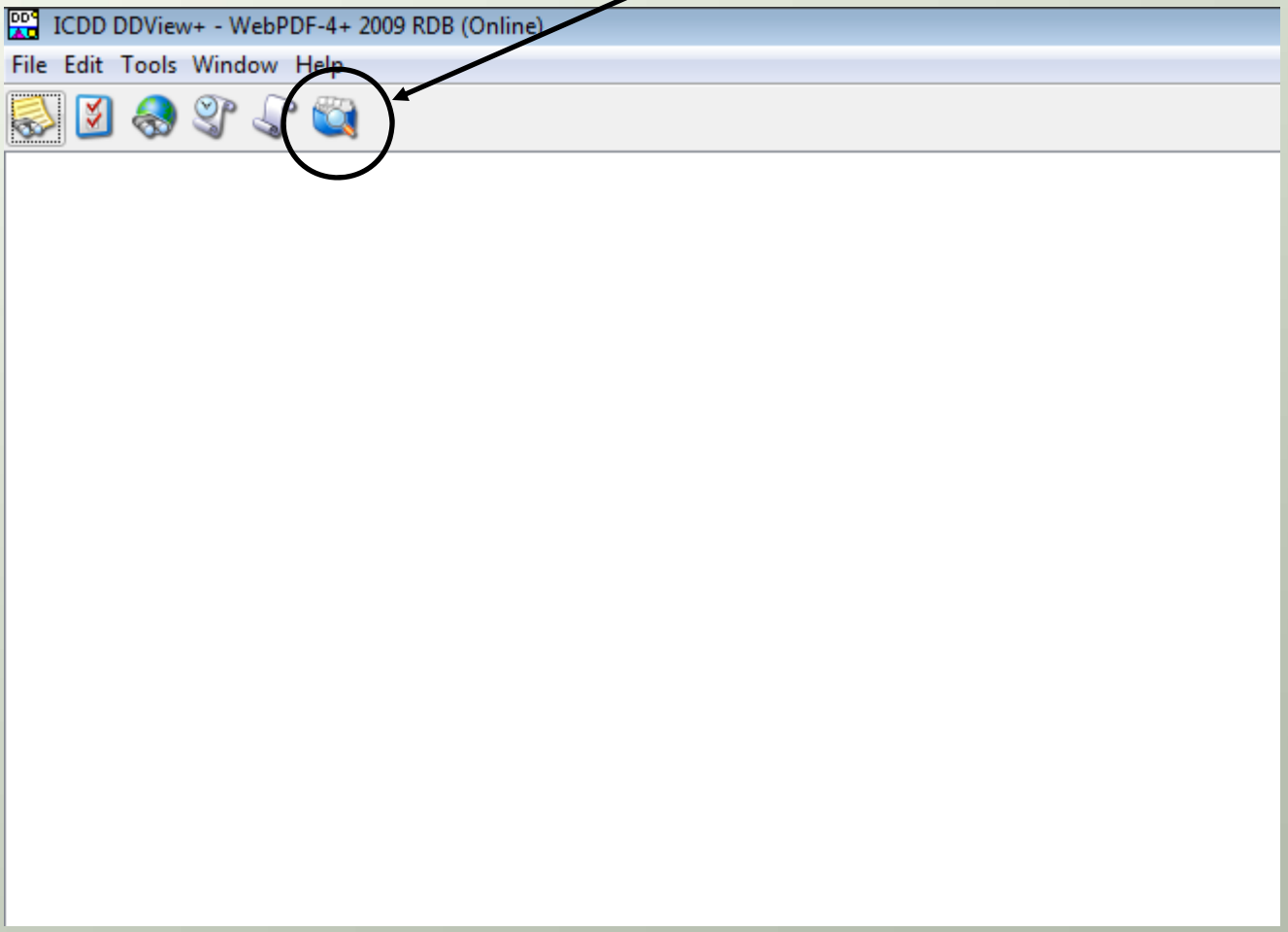
Searching for Iron Alloys



PDF #	QM	Chemical Formula	Mineral Name	SYS	SPGR	SG #	AuthC
00-001-0842	B	Cu Fe S2	Chalcopyrite	T	I-42d	122	4.00
00-001-1053	I	Fe2 O3	Hematite	R	R-3c	167	6.00
00-001-1111	B	Fe3 O4	Magnetite	C	Fd-3m	227	8.00
00-001-1200	B	Fe2 P		H	P321	150	3.00
00-001-1219	B	Fe4 N		C			1.00
00-001-1223	B	Fe O		C	Fm-3m	225	4.00
00-001-1228	I	Fe2 Al5		M			
00-001-1236	B	Fe3 N		H	P63/mmc	194	0.75
00-001-1247	B	Fe S	Troilite	H	P63/mmc	194	2.00
00-001-1252	O	Fe		C	Im-3m	229	2.00
00-001-1257	B	Al Fe		C	Pm-3m	221	1.00
00-001-1262	B	Fe		C	Im-3m	229	2.00
00-001-1265	O	Fe Al3		X			
00-001-1267	B	Fe		C	Im-3m	229	2.00
00-001-1271	B	Fe Si		C	P213	198	4.00
00-001-1285	B	Fe Si2		T	P4/m	83	1.00
00-001-1295	B	Fe S2	Pyrite	C	Pa-3	205	4.00
00-002-0264	I	Ag Fe2 S3	Sternbergite	O	Ccmm	63	8.00
00-002-0426	S	Sb6 Fe Pb4 S14	Jamesonite	M	P21/a	14	2.00
00-002-0500	B	Cu Fe2 S3	Cubanite	O	Pnma	62	4.00

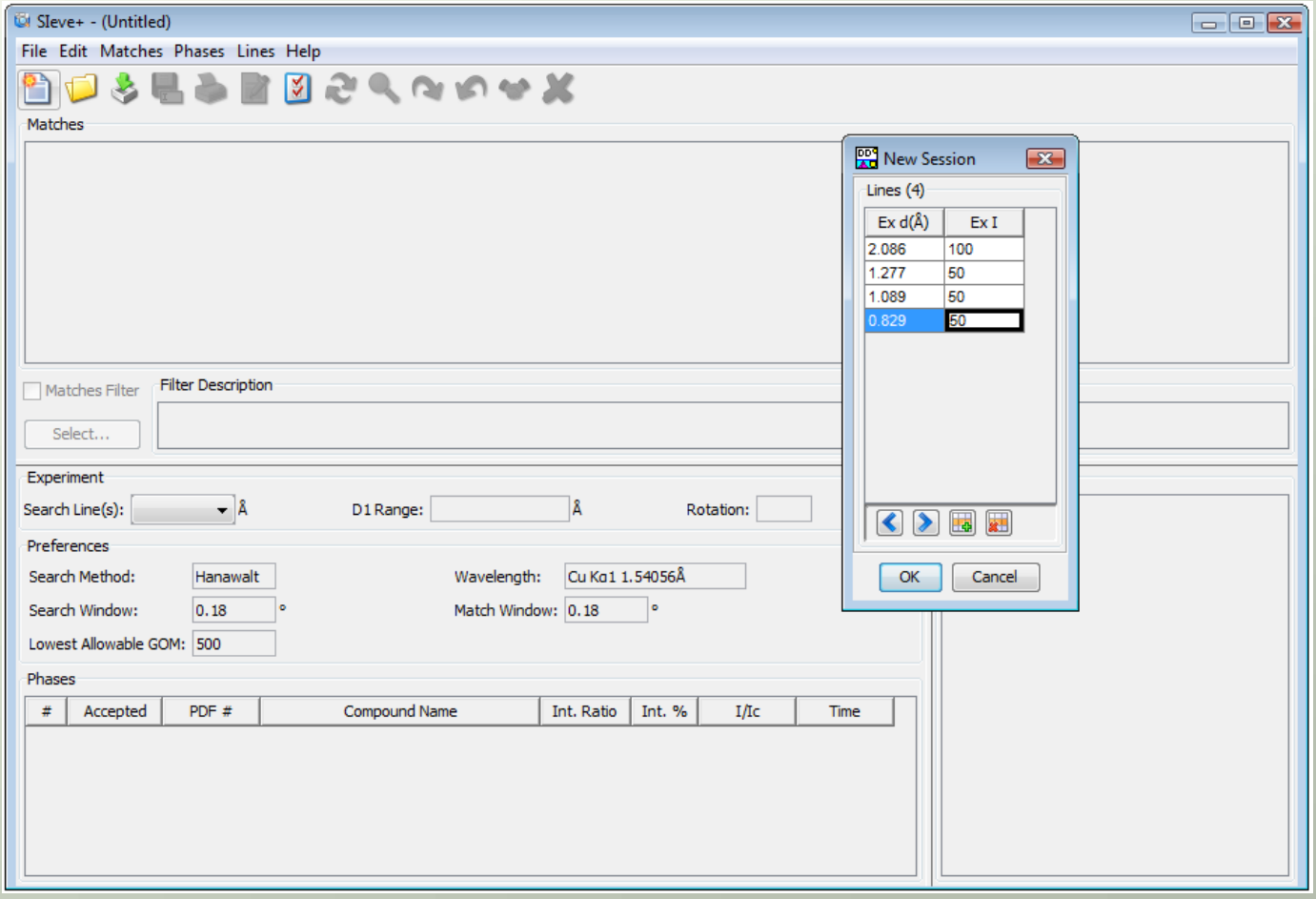
Using SIeve+

Begin a SIeve+ session by pressing the ‘SIeve+’ button…



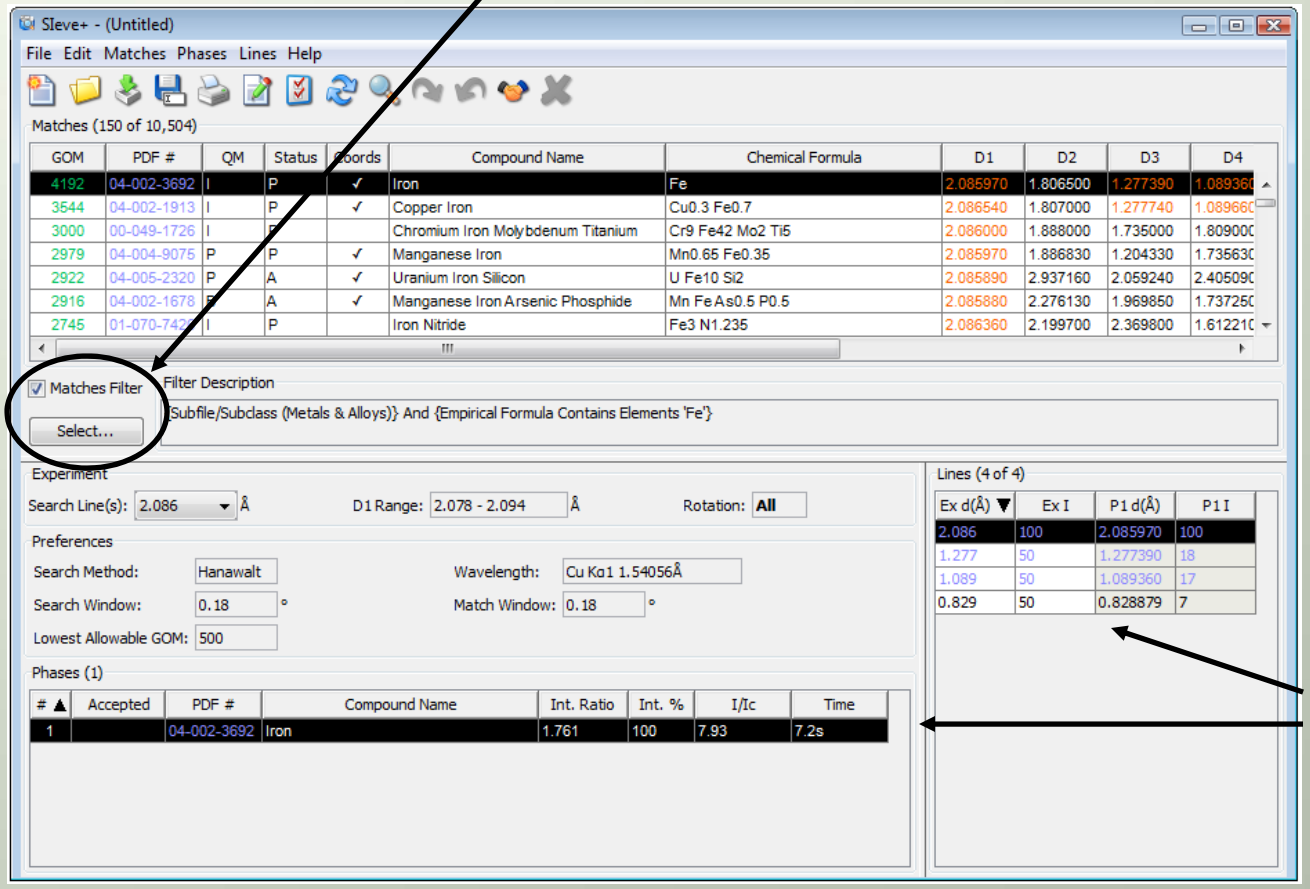
Using Sleve+

…then choose ‘File → New Session’ from the pull down menu, input the D-I list, and press the ‘OK’ button to begin search-match.



Adding the Search Results

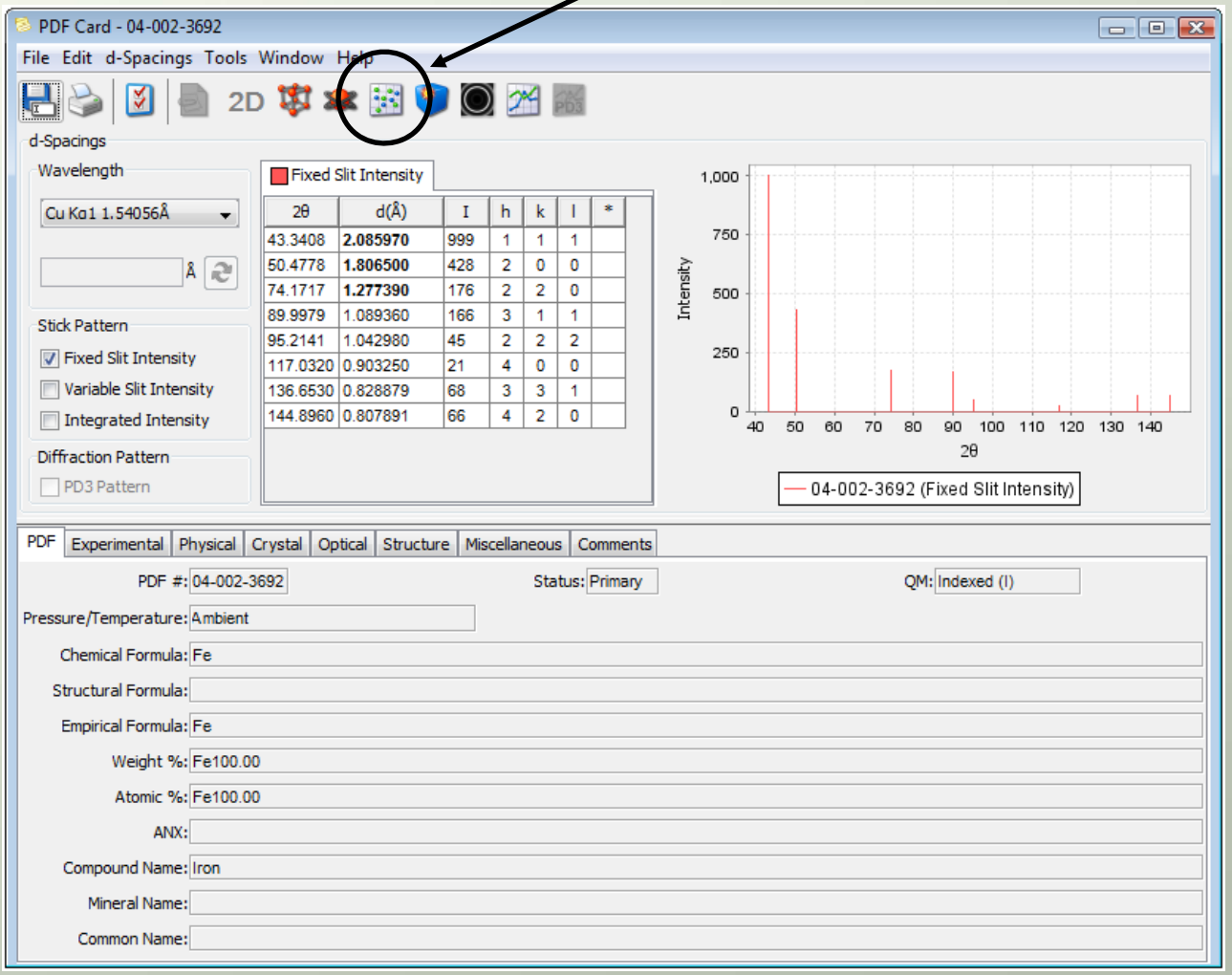
Check the ‘Matches Filters’ box and choose the search for alloys containing Fe to limit the search space.



In this case, we have a very good match for Iron (FCC).

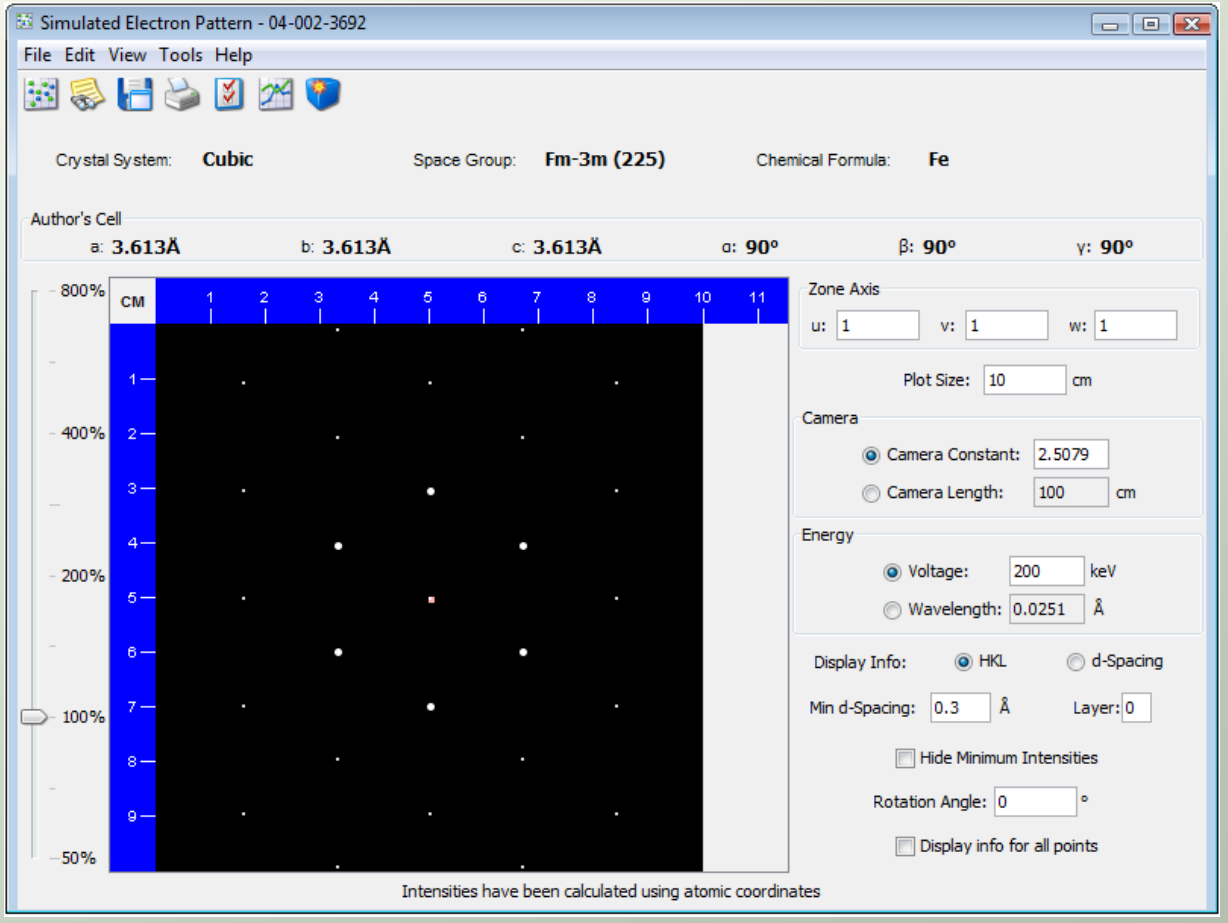
Accessing SAED Patterns

Press the ‘SAED Pattern’ button…



SAED Patterns

…and the Simulated Electron Pattern window will appear.

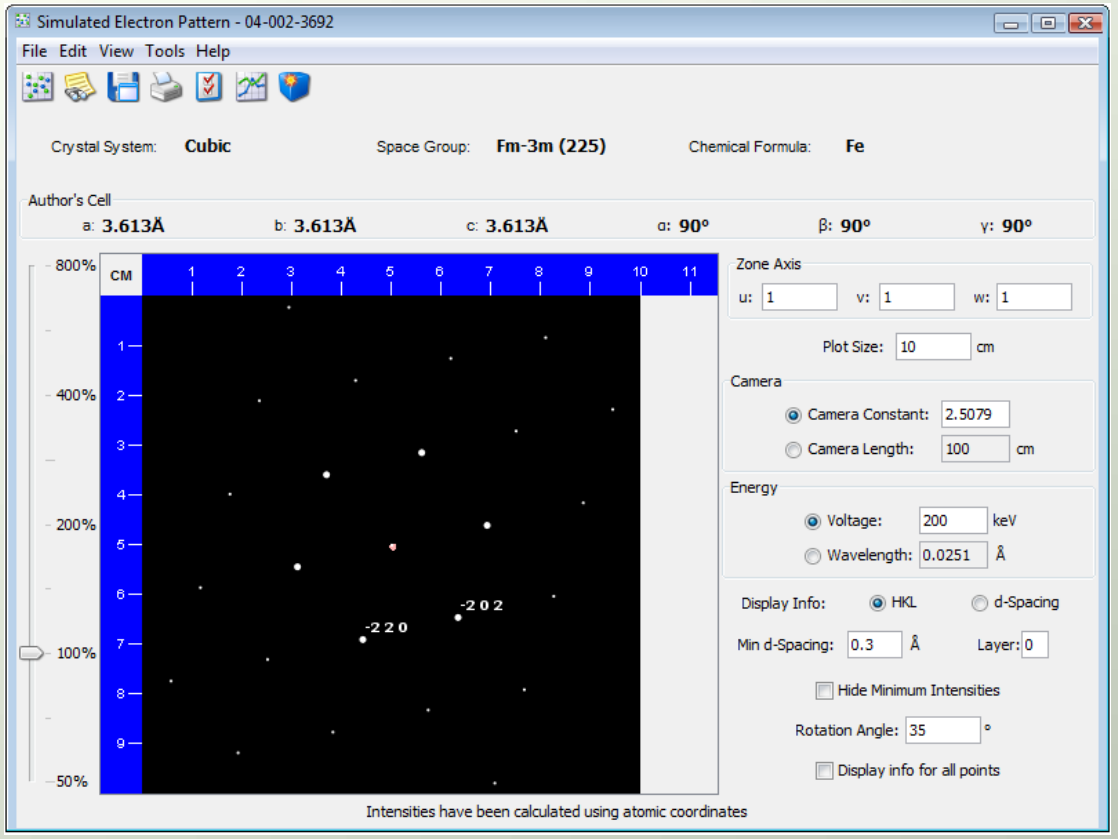


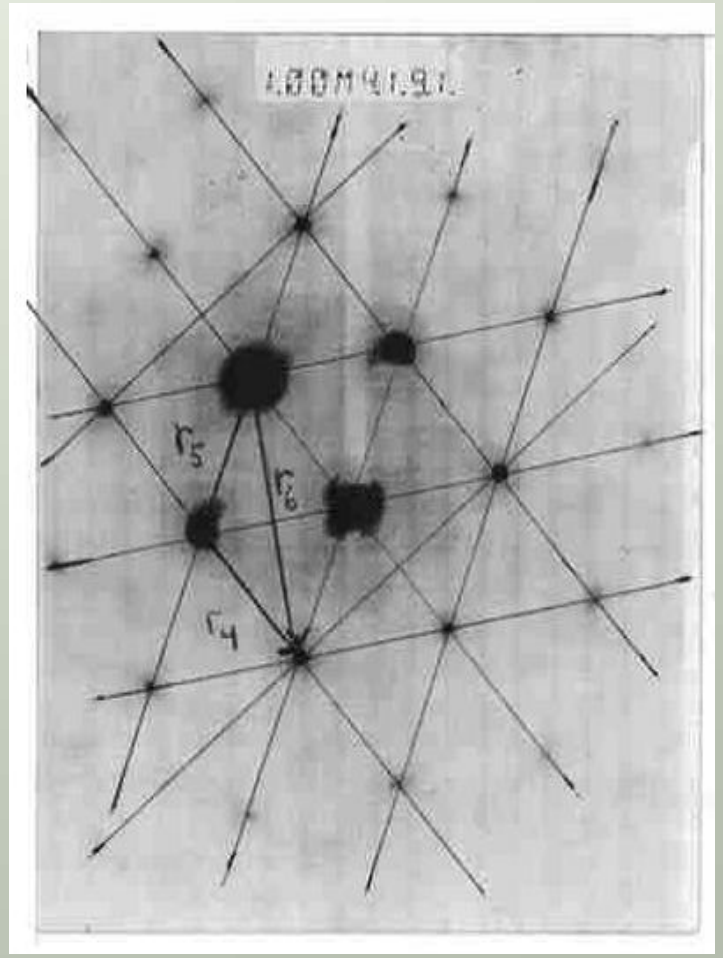
Preferences such as the zone axis, camera constant, and accelerating voltage can be edited with on-the-fly dynamic re-simulation of the pattern.

SAED Patterns for Iron – Simulation & Experiment

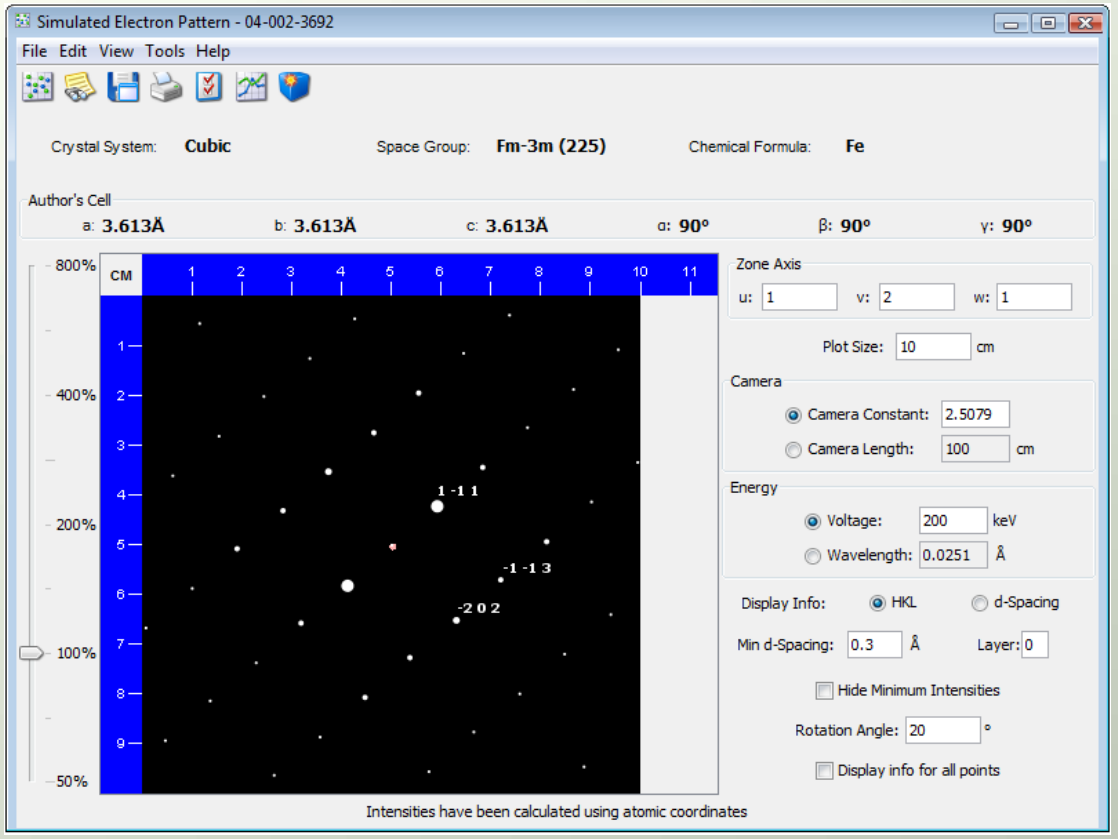
- The following three slides compare simulated and experimental SAED patterns for FCC Iron (Fe, space group Fm-3m) for three zone axes using PDF card 04-002-3692, which was one of the top two matches to the D-I list using search-match with Sleve+.

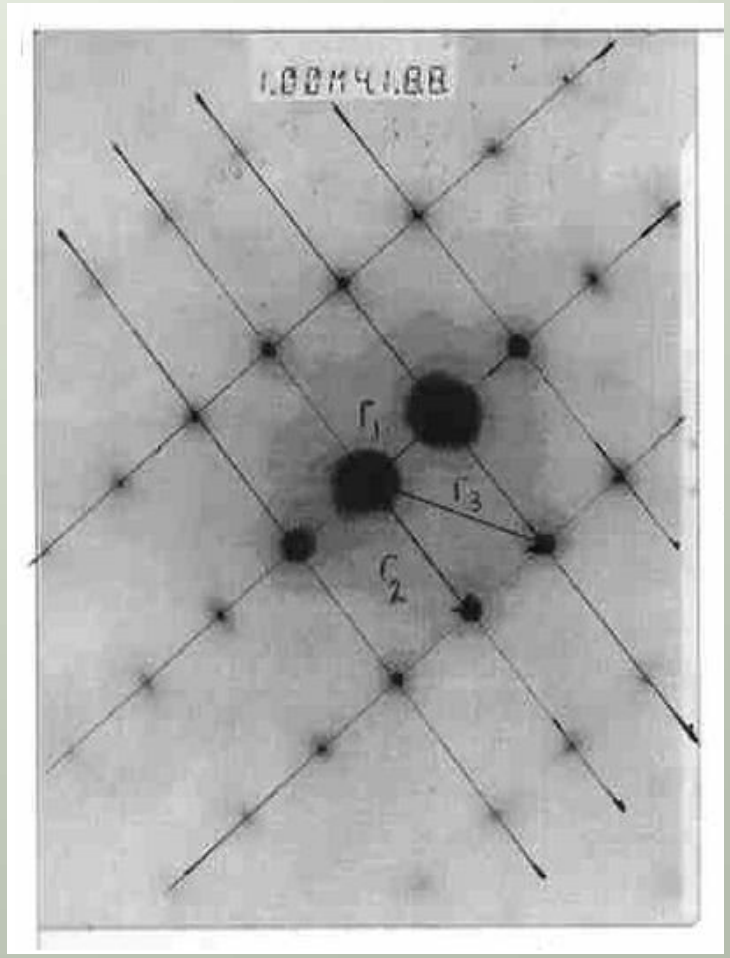
FCC Iron (Fe, Fm-3m)
[111] Zone Axis



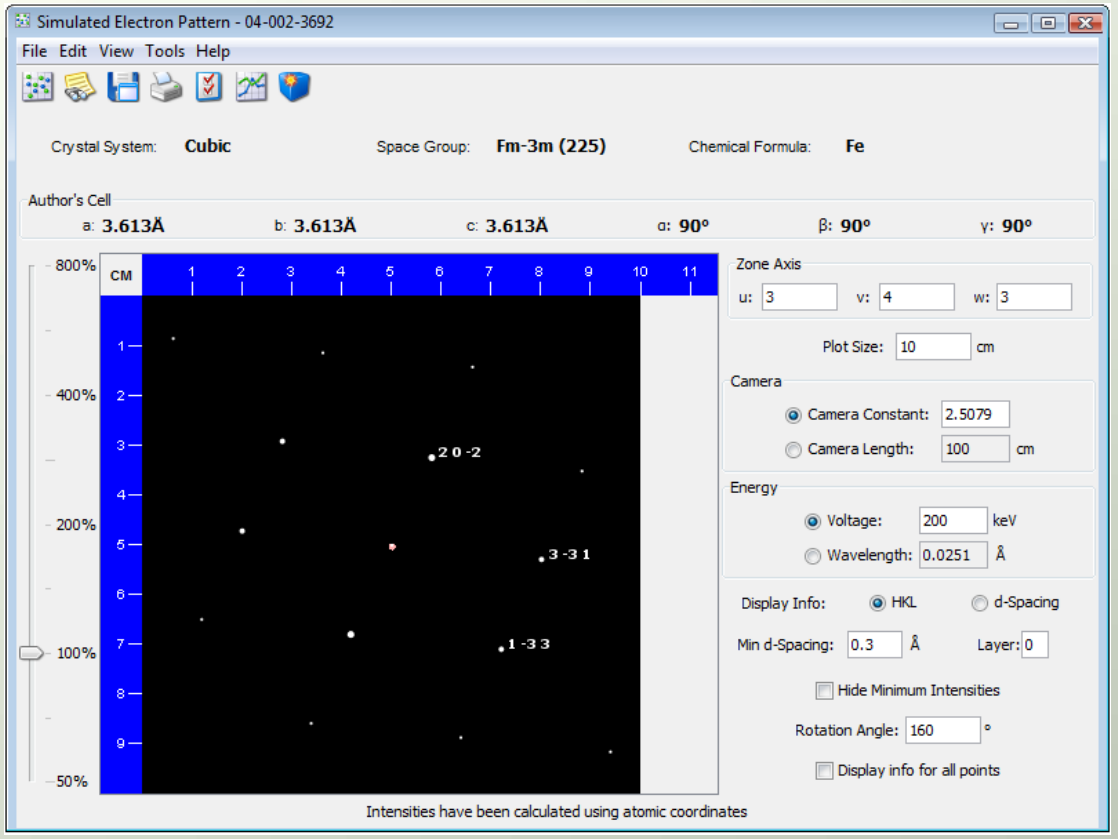


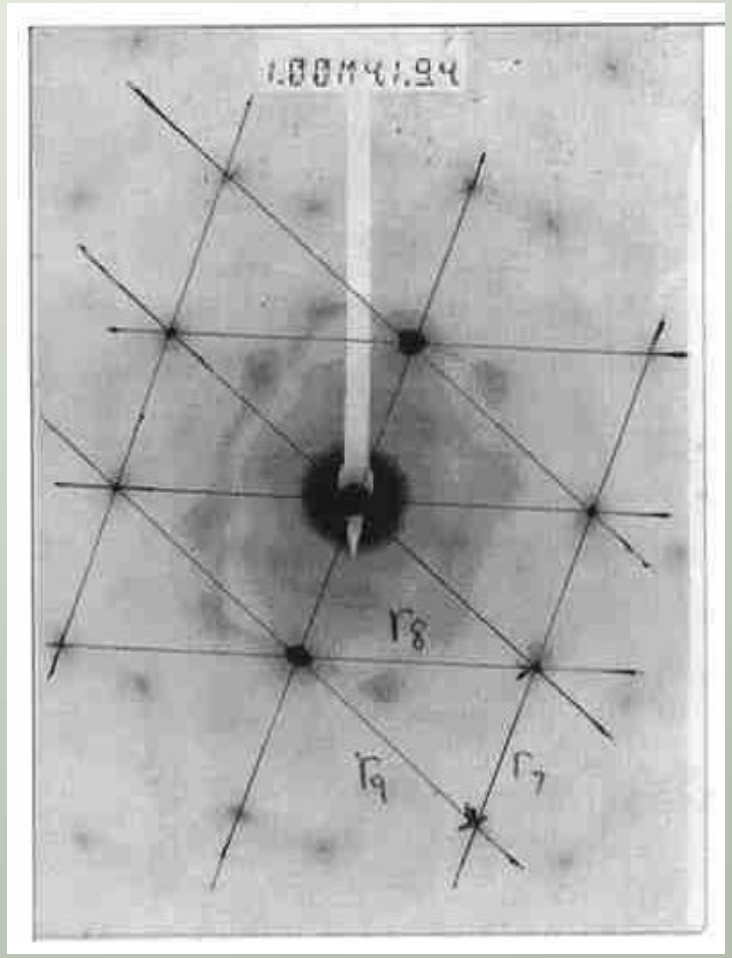
FCC Iron (Fe, Fm-3m)
[121] Zone Axis





FCC Iron (Fe, Fm-3m)
[343] Zone Axis





SAED Patterns – Summary

- The simulated FCC Iron SAED patterns match closely with the experimental patterns.

- PDF-4+ 2009 generates SAED patterns with intensities calculated from atomic coordinates based on atomic scattering factors for electrons when a structural model is available, and SAED patterns with intensities approximated using the D-I list for entries without atomic coordinates.

Thank you for viewing our tutorial.
Additional tutorials are available at the ICDD website (www.icdd.com).

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