Electron Diffraction Search and Identification Strategies

Search Strategies for Electron Diffraction Historical

The use of the Powder Diffraction File (PDF) for electron diffraction applications has a decades' long history. Several products have been developed, by researchers in the field, as aids to phase identification by electron diffraction. Many of these have been produced or published by the ICDD.

These products include:

Product	Published
Fink Index	1963
Matthews Index	1965
Elemental and Interplanar Spacing Index (EISI)	1989
The ICDD-NIST-Sandia Electron Diffraction Database	1994, 1997
PDF-4+	2005-current

Electron Diffraction Searches

The Fink method (1963) introduced the concept of using an eight-line search index with an emphasis on low angle interplanar spacings of high intensity. The Matthews index (1965) was based on IBM keypunch cards and allowed users the ability to search interplanar spacing and chemistry, at the same time. These two methods took advantage of two known strengths of electron diffraction analysis, the frequent use of accompanying elemental data from a microscope (EDS), and the emphasis on low angle data in electron diffraction analysis.

These initial two products were computationally complex, especially for the limitations on computer memory and speed, at the time of introduction.

The EISI Index and the Electron Diffraction Database were computer-based methods based upon the best of both of the above principles, and the power of computers in the late 1980's. The **EISI Index** (1989) introduced **elemental permutations and light element limitations** that are based on practical considerations of the basic detection capabilities **of energy dispersive spectrometers**. This product also introduced effective searches that were based on unit cell parameters, space groups, chemical names and formulas. These products were co-developed by researchers at the ICDD, NIST and Sandia National Laboratories, with input from ICDD users and members. The last release of the Electron Diffraction Database in 1997 contained 87,200 entries.

PDF-4+

Search strategies for PDF-4+ have been developed by combining the knowledge gained from decades of use from prior electron diffraction products, with the power of a relational database equipped with JAVA interfaces.

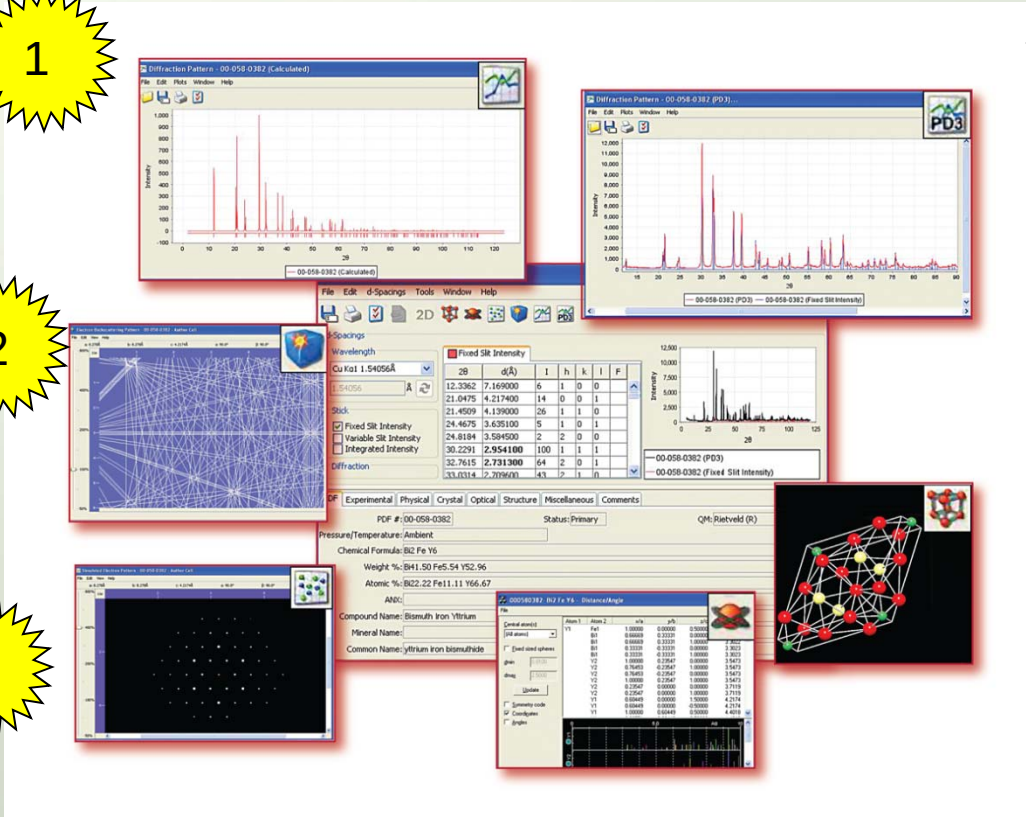
Data – The relational database format allows data to be added annually from international sources. In Release 2008, the database contained 285,000 entries and is continuously growing.

Custom Data Fields – All empirical formulae have been converted to atom % and weight %'s to facilitate composition searches. For every data set, a Fink Index Table entry and a Long 8 Index Table entry has been generated.

Designed Searches – There are a variety of elemental and composition searches, including weight % and atomic %. With the plug-in SIeve+, users can also use Hanawalt, Fink and Long 8 Searches. Unit cells can be searched by author cells, crystal cells or reduced cells. There are a total of 48 searches that can be combined and permuted.

Custom Data Simulations – Electron Diffraction Patterns, Spot Patterns, and Electron Backscatter Patterns – each pattern can be custom adjusted for instrumental and specimen parameters.

Custom Simulations for Electron Diffraction



1. 2D pattern, intensity versus 1/d or two theta
2. EBSD pattern uses author cell, crystal cell or reduced cell
3. Spot pattern, 3-axes, x,y orientation and intensity

Custom simulations will not be a focus of this tutorial.
Please see the tutorials on these subjects.

Electron Diffraction versus X-ray Diffraction Search Strategies

Precision and accuracy in powder x-ray diffraction experiments, for either interplanar spacings or lattice constants, approach 1-100 *parts per million* with calibrated instrumentation and standard methods. As a consequence, most search strategies for XRD are based on searching lattice parameters or d-spacings. Elemental analysis is used as a confirmation of correct identification and is often not used as part of the search strategy.

Precision and accuracy in electron diffraction experiments, for either interplanar spacings or lattice constants approach 1-100 *parts per thousand.* The lack of accuracy means that additional data is required for unambiguous identification. Fortunately, many ED experiments are routinely performed using accompanying chemical analysis from energy dispersive spectroscopy. Elemental analysis, or use of additional physical properties, is an essential part of an electron diffraction search and is a requirement for a correct identification.

Note: Modern EBSD, SAED and/or precession electron diffraction methods can improve precision and accuracy by ~10X over traditional ED analyses and represent an intermediate case.

Using Elemental Analysis for Electron Diffraction Searches

Interplanar Spacing (ESD)	Number of "hits" PDF-4+ No Chemistry	Contains Ca	Contains Si and Ca
3.2(1)	28,663	1,575	322
3.02(1)	3,434	139	20
3.002(1)	255	7	0
3.0002(1)	18	0	0

Results based on a *long line search*,* with and without chemistry, using PDF-4+ 2008.

*Searches of the longest (lowest angle) 8 d-spacings of a reference material using the cited constraints.

Search Strategies

The fundamental basis of most current commercial and public data analysis programs, available for phase identification by electron diffraction methods (ED, SAED, EBSD), is to combine measured d-spacings, or lattice parameters, with elemental analysis, to get a select small number of candidate materials (typically less than 20) to match with the unknown.

This is taking advantage of the statistics shown on the prior page.

Using Physical Properties for Electron Diffraction Searches

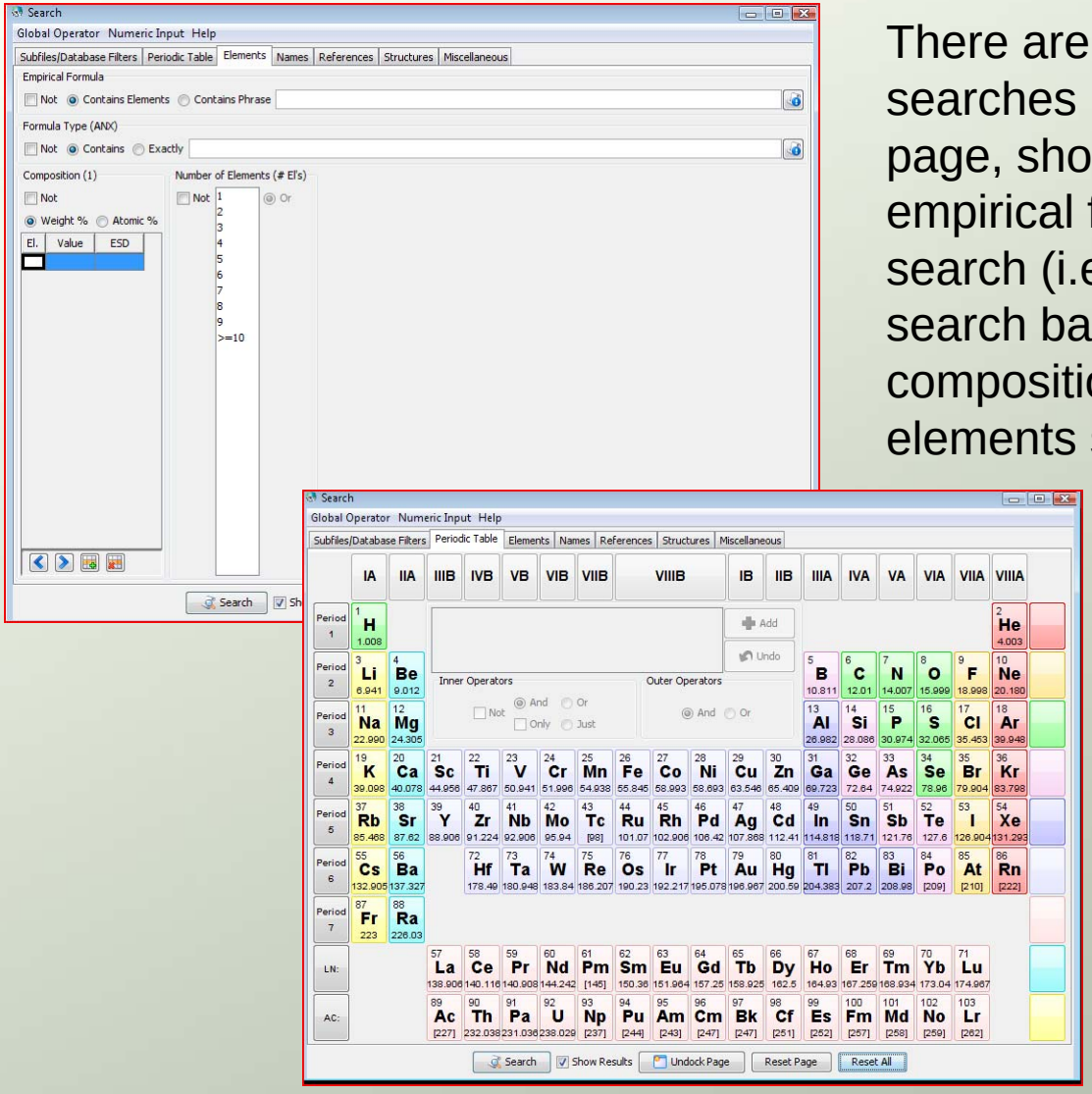
Similar correlations can be found with physical properties

Interplanar Spacing (ESD)	No Chemistry	Density 2.0(3)	Color Blue
3.2(1)	28,663	507	123
3.02(1)	3,434	56	11
3.002(1)	255	1	0
3.0002(1)	18	0	0

Results based on a *long line search*,* with and without chemistry, using PDF-4+ 2008.

* Searches of the longest (lowest angle) 8 d-spacings of a reference material using the cited constraints.

Elemental Searches in PDF-4+



There are several types of composition searches in PDF-4+. On the “Element” page, shown on the left, there is an empirical formula search, a formula type search (i.e. NaCl), and a composition search based on atomic % or weight % composition. There is also a number of elements search.

The periodic table search has a point and click interface to add elements or groups of elements in combination.

Boolean operators “Only, Just, And, Or” can be applied to the search sequence

Example

Several ways to search for carbon steel

Search by Mineral Name – Austenite, Martensite
Search by Empirical Formula – i.e. $Fe_{15}C$

Search by Composition (results below)
Carbon 5 atomic % with esd of 4
Iron 95 atomic % with esd of 4

PDF #	Status	QM	Atomic %	Common Name	RedCell-a	RedCell-b	RedCell-c
00-023-0298	D	O	C5.00 Fe95.00	Austenite	2.546	2.546	2.546
00-044-1289	P	C	C7.00 Fe93.00	martensite	2.526	2.526	2.526
00-044-1290	P	C	C2.50 Fe97.50	martensite	2.499	2.499	2.499
00-044-1291	P	C	C3.50 Fe96.50	martensite	2.504	2.504	2.504
00-044-1292	P	C	C4.50 Fe95.50	martensite	2.509	2.509	2.509
00-044-1293	P	C	C6.00 Fe94.00	martensite	2.516	2.516	2.516
00-052-0512	P	C	C6.21 Fe93.79	austenite	2.558	2.558	2.558
01-074-5520	P	I	C6.00 Fe94.00		2.558	2.558	2.558
01-074-5521	P	B	C1.00 Fe96.00 Sn3.00		2.502	2.502	2.502
04-007-2377	P	B	C8.26 Fe91.74		4.020	4.020	36.990
04-007-2490	P	B	C4.31 Fe95.69		2.511	2.511	2.511

Note: Searching by composition gets some austenites, but also finds martensite, and also finds some that are not identified.

Sort the Results

PDF #	Status	QM	Atomic %	Common Name	RedCell-a	RedCell-b	RedCell-c	RedCellVol	SG # ▲	SYS
04-007-2377	P	B	C8.26 Fe91.74		4.020	4.020	36.990	597.77	53	O
00-044-1289	P	C	C7.00 Fe93.00	martensite	2.526	2.526	2.526	12.36	139	T
00-044-1290	P	C	C2.50 Fe97.50	martensite	2.499	2.499	2.499	12.00	139	T
00-044-1291	P	C	C3.50 Fe96.50	martensite	2.504	2.504	2.504	12.07	139	T
00-044-1292	P	C	C4.50 Fe95.50	martensite	2.509	2.509	2.509	12.15	139	T
00-044-1293	P	C	C6.00 Fe94.00	martensite	2.516	2.516	2.516	12.23	139	T
04-007-2490	P	B	C4.31 Fe95.69		2.511	2.511	2.511	12.17	139	T
00-023-0298	D	O	C5.00 Fe95.00	Austenite	2.546	2.546	2.546	11.66	225	C
00-052-0512	P	C	C6.21 Fe93.79	austenite	2.558	2.558	2.558	11.84	225	C
01-074-5520	P	I	C6.00 Fe94.00		2.558	2.558	2.558	11.84	225	C
01-074-5521	P	B	C1.00 Fe96.00 Sn3.00		2.502	2.502	2.502	12.06	229	C

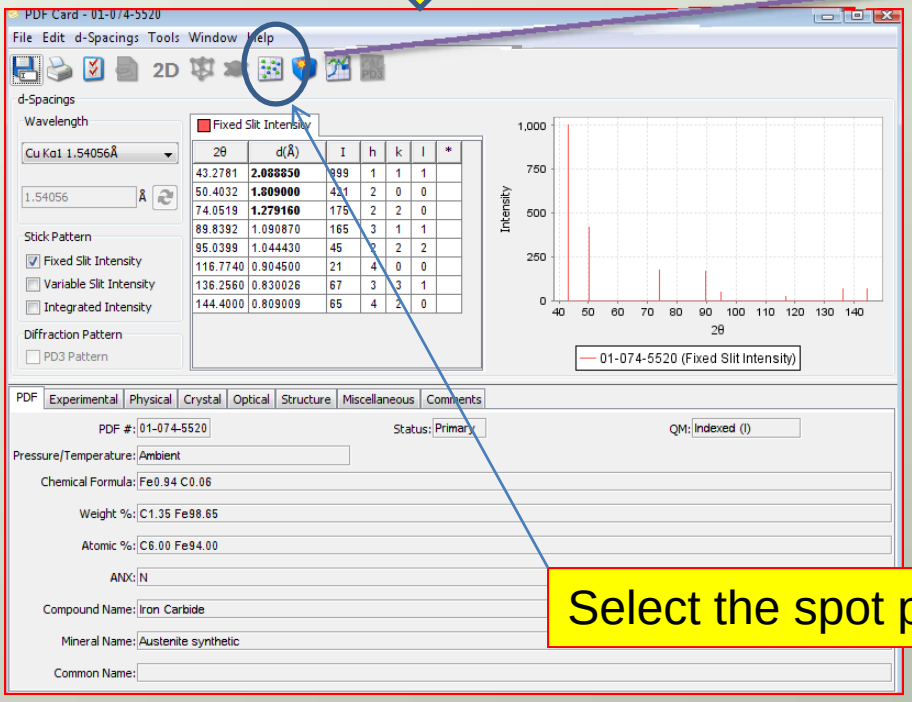
The results are sorted by space group, by clicking with the mouse at the column heading. The space group indicates 4 different structures, space group numbers 53,139,225 and 229.

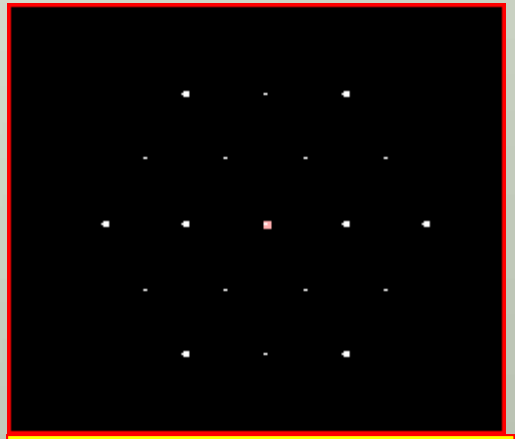
Examine an entry candidate

PDF #	Status	QM	Atomic %	Common Name	RedCell-a	RedCell-b	RedCell-c	RedCellVol	SG # ▲	SYS
04-007-2377	P	B	C8.26 Fe91.74		4.020	4.020	36.990	597.77	53	O
00-044-1289	P	C	C7.00 Fe93.00	martensite	2.526	2.526	2.526	12.36	139	T
00-044-1290	P	C	C2.50 Fe97.50	martensite	2.499	2.499	2.499	12.00	139	T
00-044-1291	P	C	C3.50 Fe96.50	martensite	2.504	2.504	2.504	12.07	139	T
00-044-1292	P	C	C4.50 Fe95.50	martensite	2.509	2.509	2.509	12.15	139	T
00-044-1293	P	C	C6.00 Fe94.00	martensite	2.516	2.516	2.516	12.23	139	T
04-007-2490	P	B	C4.31 Fe95.69		2.511	2.511	2.511	12.17	139	T
00-023-0298	D	O	C5.00 Fe95.00	Austenite	2.546	2.546	2.546	11.66	225	C
00-052-0512	P	C	C6.21 Fe93.79	austenite	2.558	2.558	2.558	11.84	225	C
01-074-5520	P	I	C6.00 Fe94.00		2.558	2.558	2.558	11.84	225	C
01-074-5521	P	B	C1.00 Fe96.00 Sn3.00		2.502	2.502	2.502	12.06	229	C

1

Highlight an entry



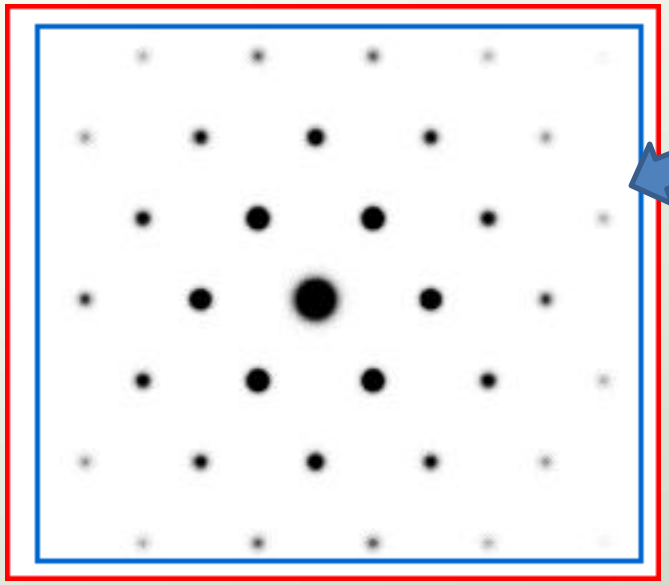


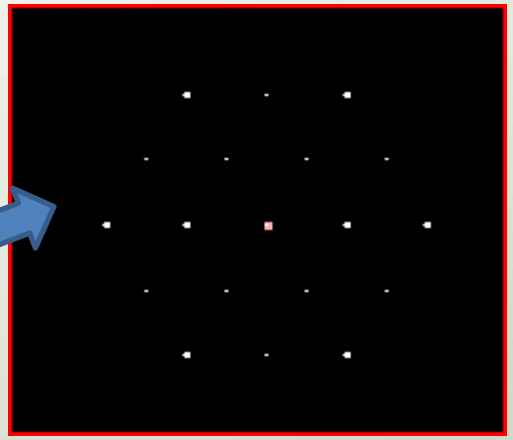
3

Generate spot pattern

Select the spot pattern option

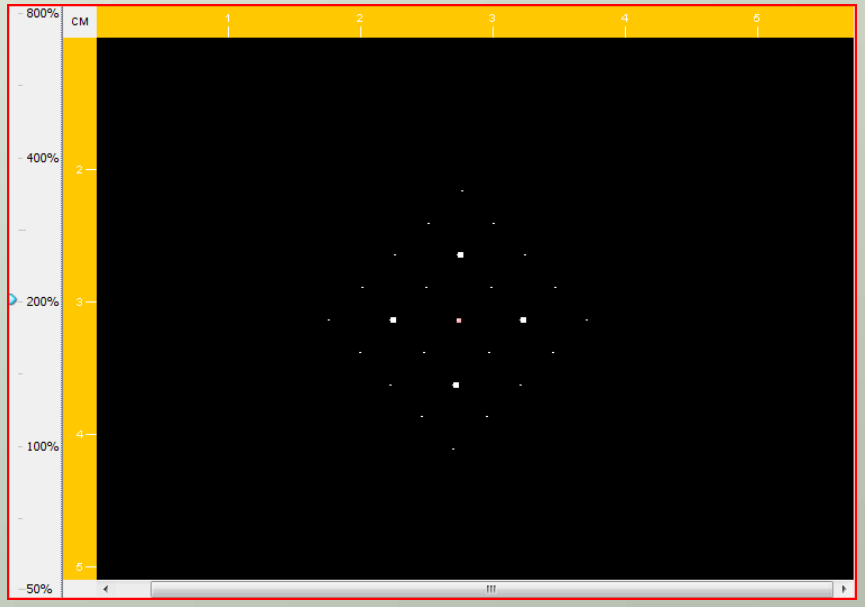
2





PDF 01-074-5520, Austenite

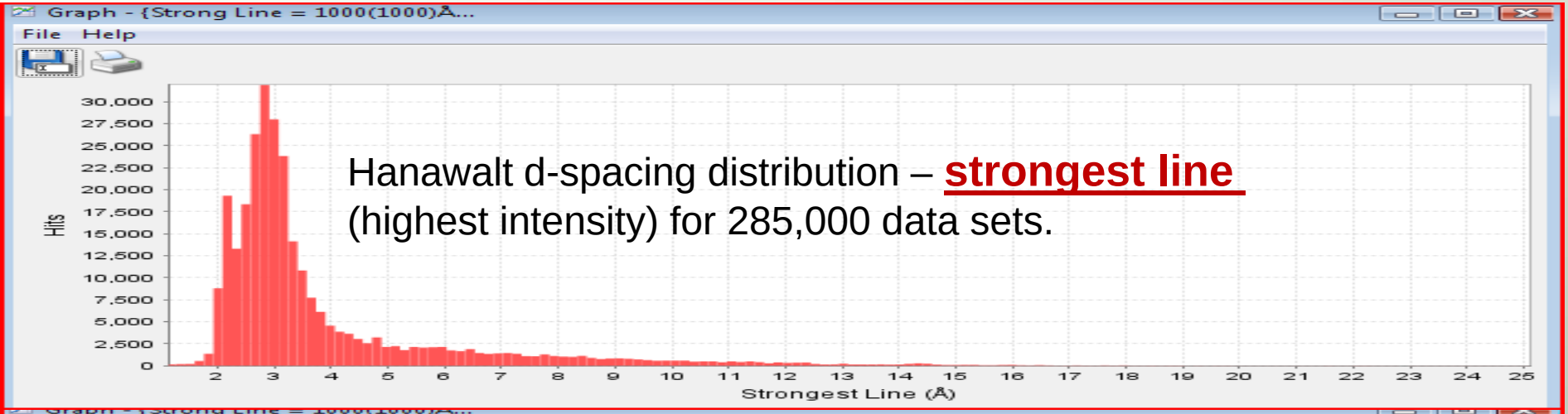
Experimental Data
[110] zone axis



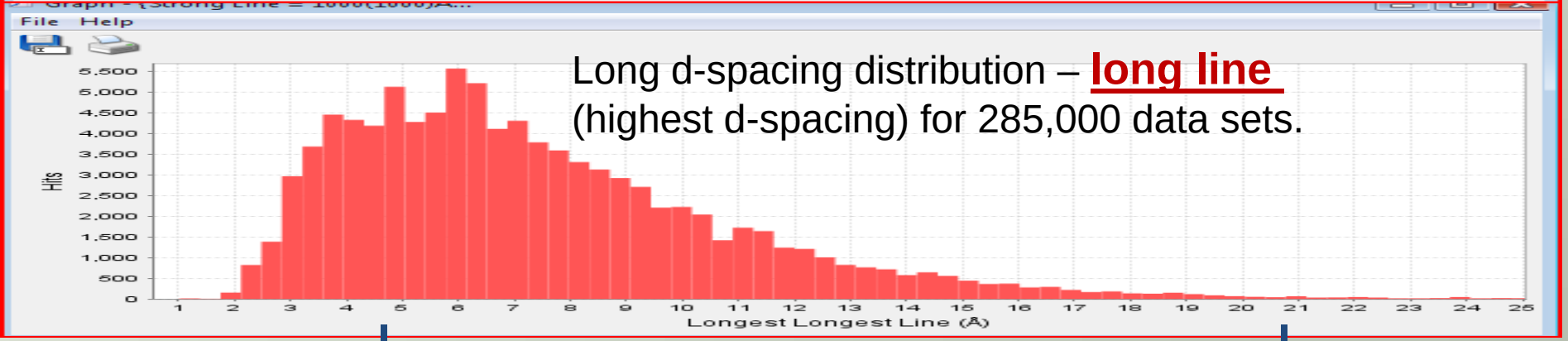
PDF 00-044-1291, Martensite

In this particular case, one can compare the experimental spot pattern to a small set of candidates that match the chemistry, to identify austenite.

Long Searches, Long 8 and Fink Searches



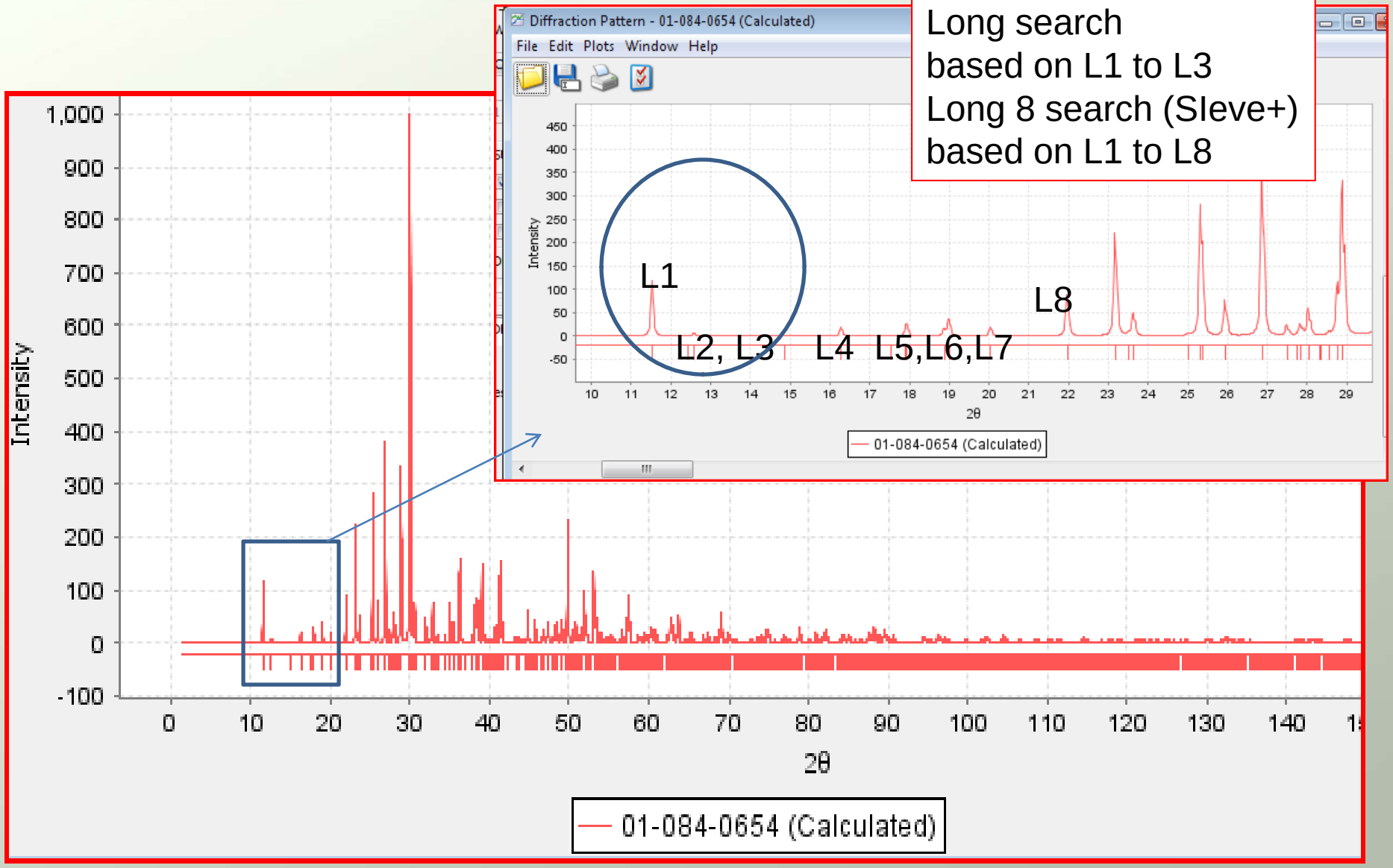
Hanawalt d-spacing distribution – **strongest line** (highest intensity) for 285,000 data sets.

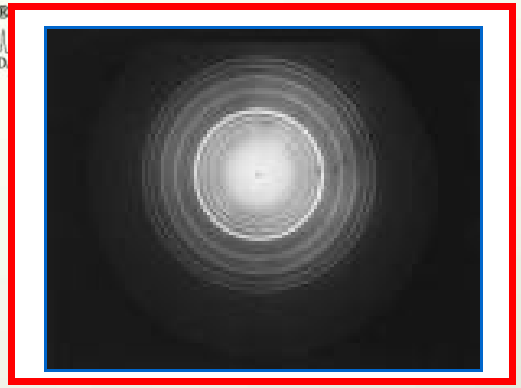


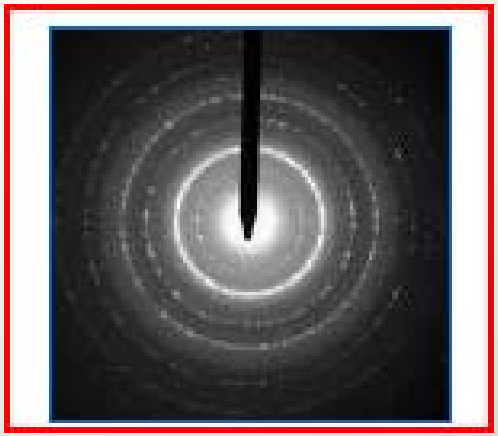
Long d-spacing distribution – **long line** (highest d-spacing) for 285,000 data sets.

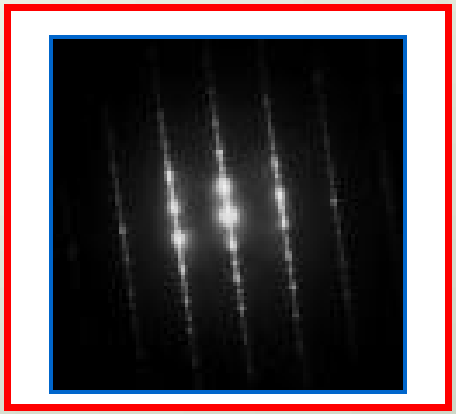
The long search, long 8 and Fink searches are all based on the above interplanar distance distribution statistics. Long lines have a much broader distribution than strong lines.

Long Search and Long 8



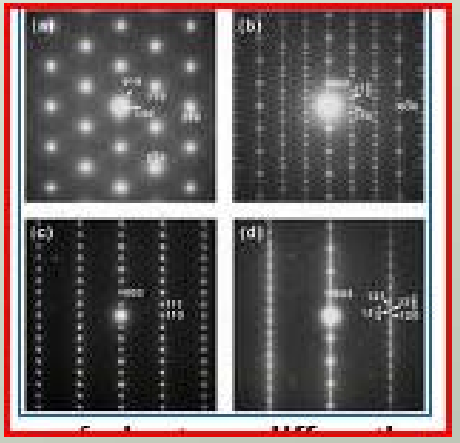


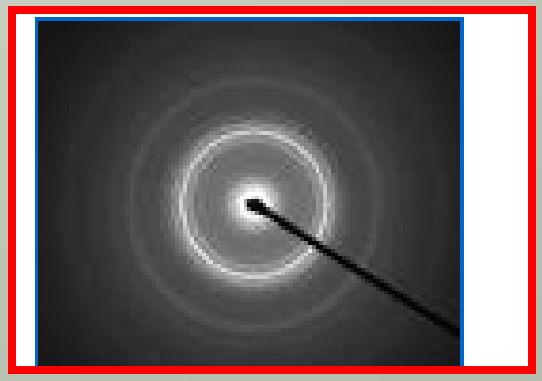


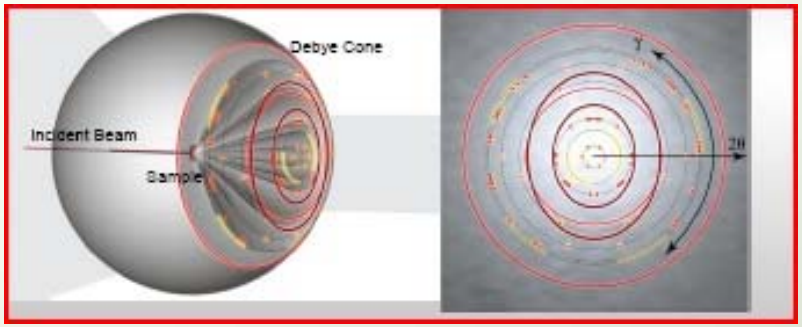


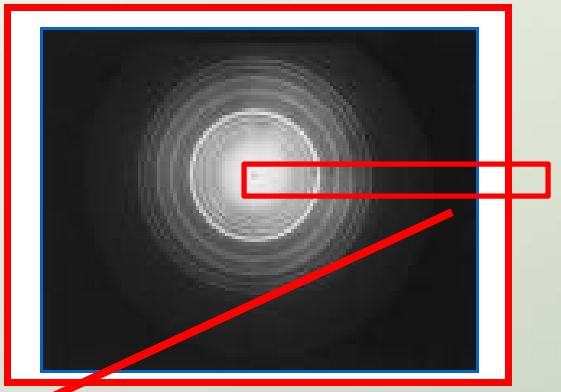
Various electron diffraction ring and spot patterns taken from the Internet.

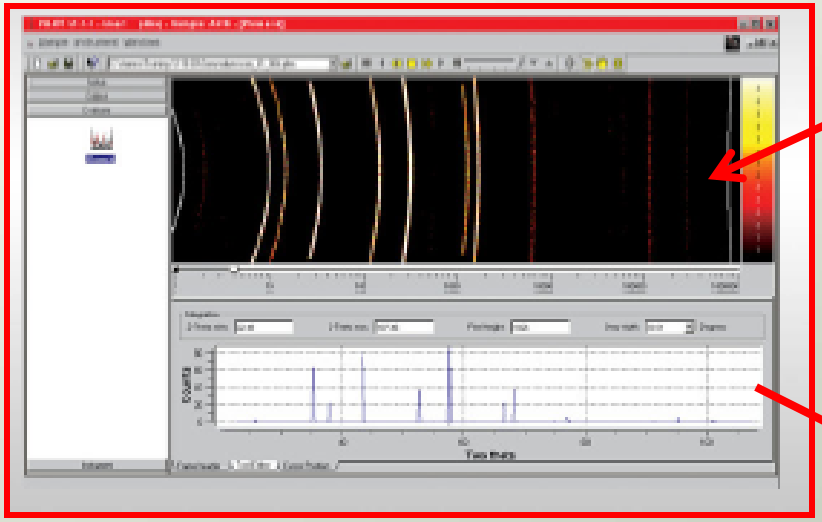
Strong lines (or spots) have the highest intensity, long lines (or spots) are those closest to the center of the image – both can be used to identify a material. The exact center of the image, in many cases, is the direct Beam. The shadow of a beam stop is shown in two of the images.



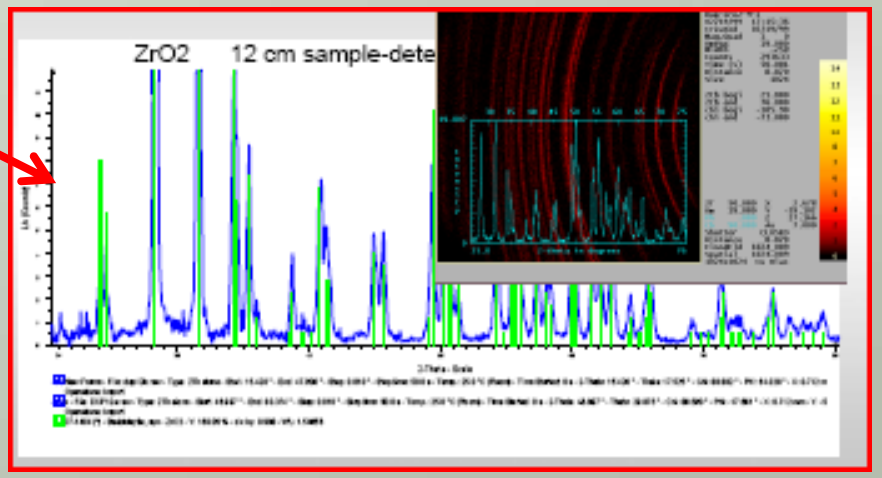








Relationship from 3D Debye cones to a 2D diffraction pattern and phase Identification.



Schematics and photo courtesy of Bruker-AXS. Identification by EVA.

Searches

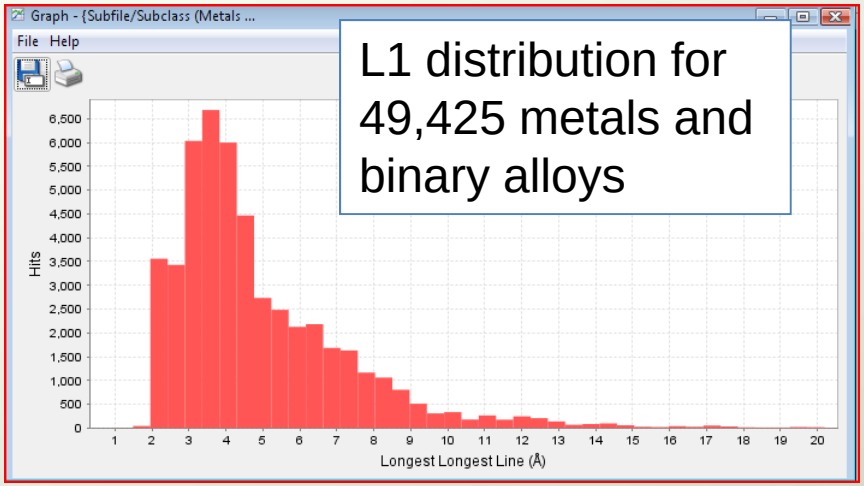
Strong Line Searches have the advantage in that the best counting statistics are based on the strong lines. These are the easiest interplanar spacings to detect in an experiment.

Long Line Searches take advantage of the broader distribution and shifted population of interplanar spacings to low angles (longer interplanar spacings).

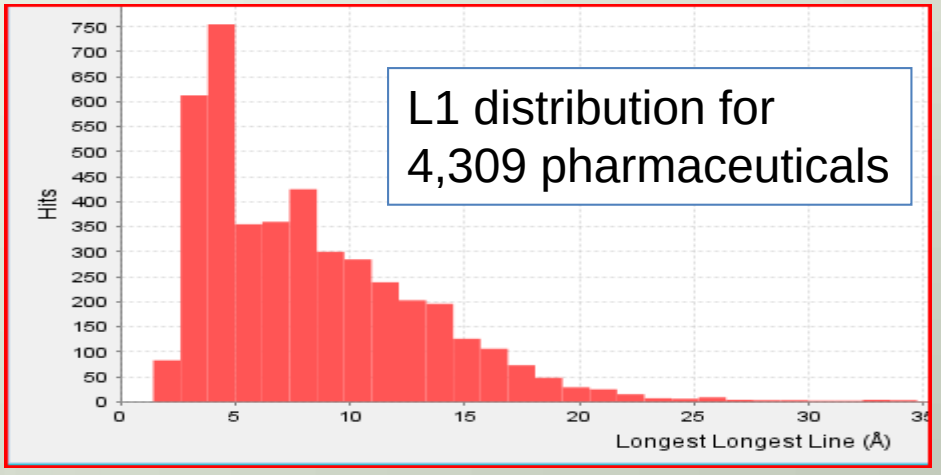
Many classes of materials (i.e. clays, zeolites) have characteristic peaks at long d-spacings (next slide).

Note: Since d-spacings are a reflection of the size of the unit cell, similar statistics can be generated for unit cell dimensions. Longer dimensions are more characteristic due to a low population distribution.

Material Characteristics

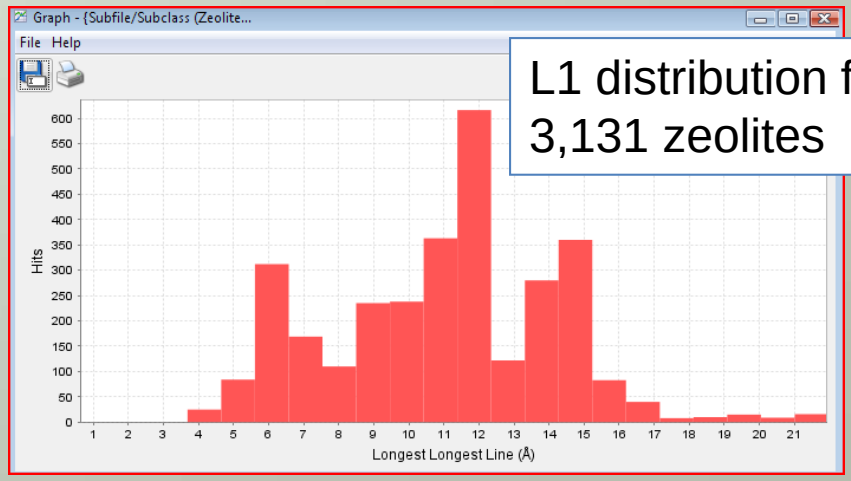


L1 distribution for 49,425 metals and binary alloys



L1 distribution for 4,309 pharmaceuticals

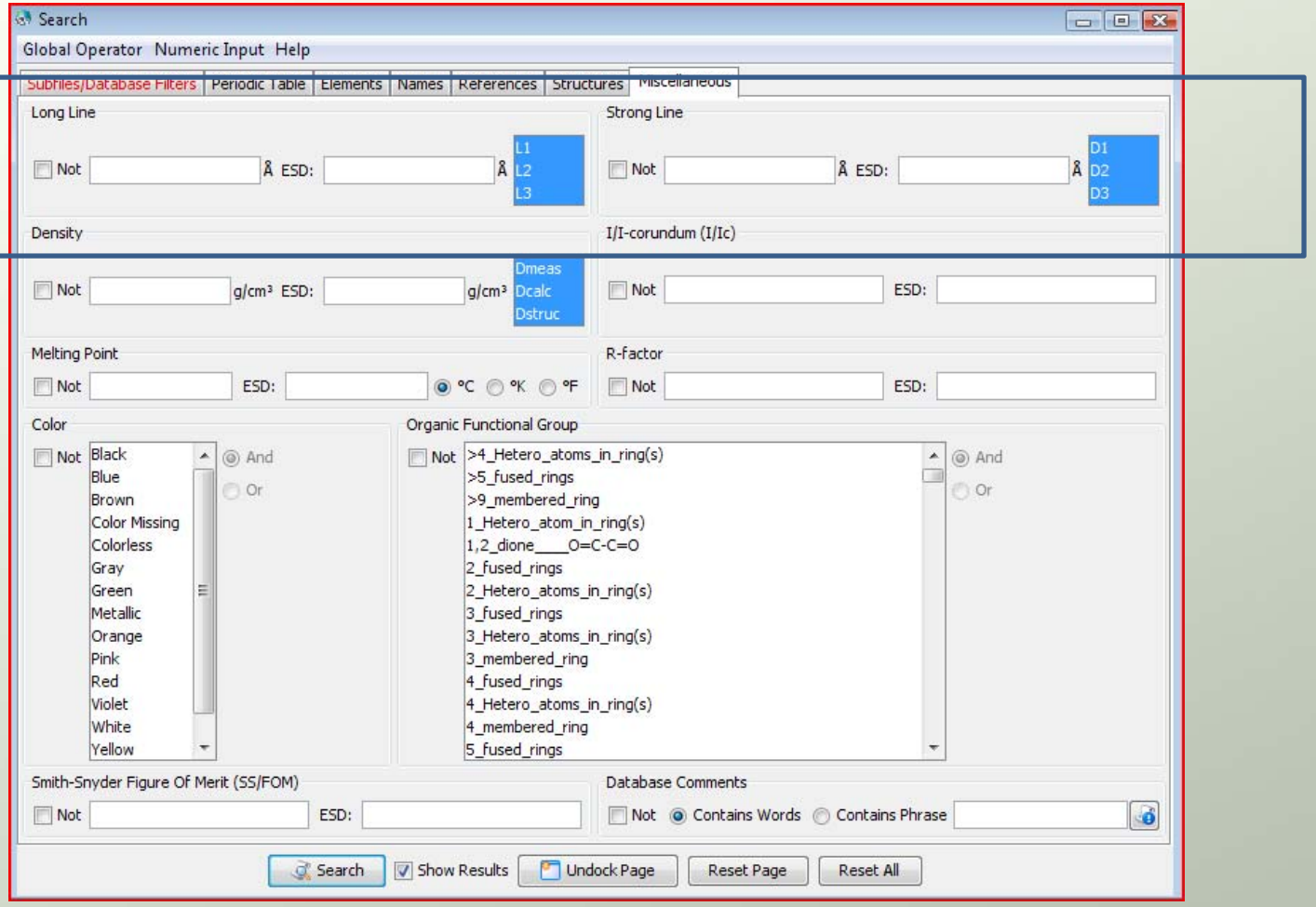
Long searches would be expected to be more effective for zeolites than for metals and alloys.



L1 distribution for 3,131 zeolites

Long and strong line searches in PDF-4+.

Searches can be combined.



This search page, entitled “Miscellaneous” Searches, contains both long and strong searches. It also contains physical property searches that make an effective combination with either interplanar spacing search.

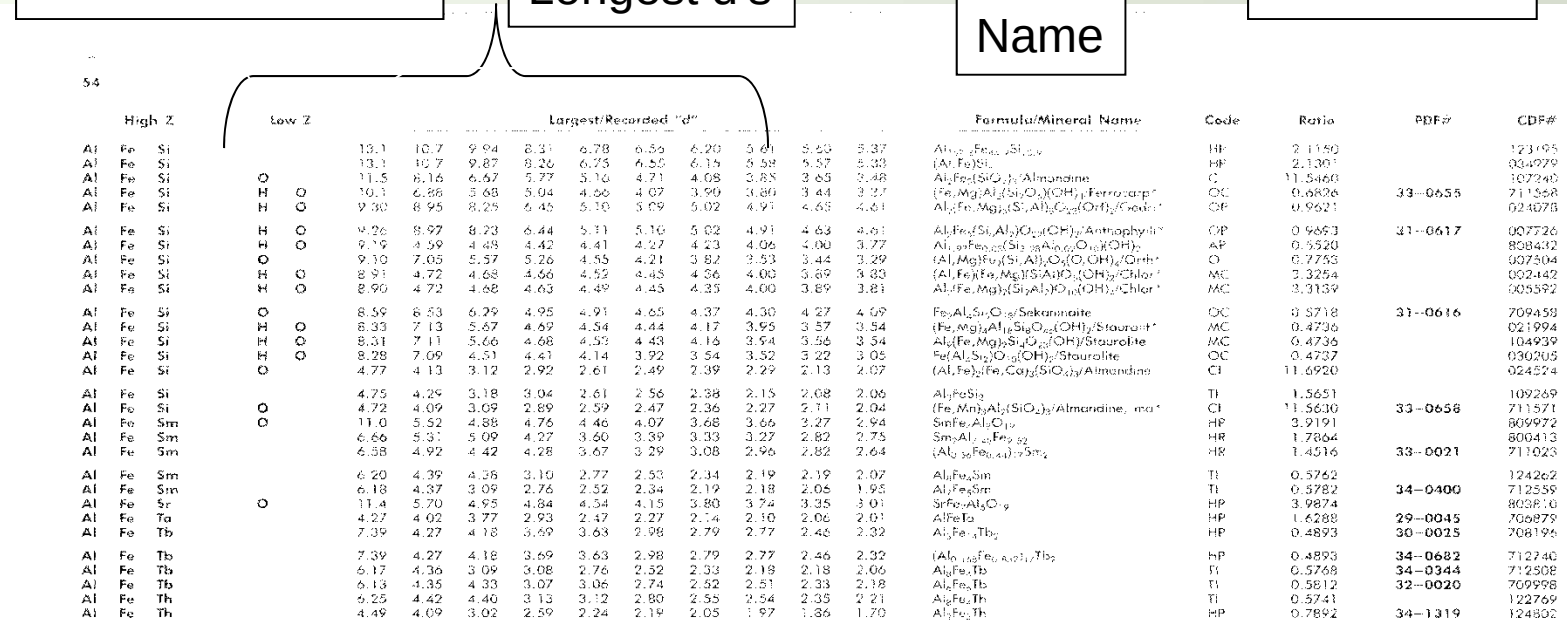
Elemental and Interplanar Spacing Index (EISI)

Element Selection

Longest d's

Name

Cross Ref's



54

High Z			Low Z			Largest/Recorded "d"									Formula/Mineral Name	Code	Ratio	PDF#	CDF#
Al	Fe	Si				13.1	10.7	9.94	8.31	6.78	6.56	6.20	5.61	5.55	5.37	$Al_{1.5}Fe_{0.5}Si_{0.5}$	HP	2.1150		123695
Al	Fe	Si				13.1	10.7	9.87	8.26	6.75	6.55	6.15	5.59	5.57	5.33	$(Al,Fe)Si_2$	HP	2.1307		034929
Al	Fe	Si	O			11.5	8.16	6.67	5.77	5.16	4.71	4.08	3.85	3.65	3.48	$Al_2Fe_3(SiO_4)_3$ Almandine	C	11.5460		307240
Al	Fe	Si	H	O		10.1	6.86	5.68	5.04	4.66	4.07	3.90	3.80	3.44	3.27	$(Fe,Mg)Al_2(Si_2O_5)(OH)_4$ Ferrosaponite*	OC	0.6826	33--0655	711558
Al	Fe	Si	H	O		9.30	8.95	8.25	6.45	5.10	5.09	5.02	4.91	4.65	4.61	$Al_2Fe_2Mg_3(Si_2Al_2)O_{20}(OH)_4$ Cookeite*	OP	0.9621		024078
Al	Fe	Si	H	O		9.26	8.97	8.23	6.44	5.11	5.10	5.02	4.91	4.63	4.61	$Al_2Fe_2(Si_4Al_2)O_{20}(OH)_4$ Anthophyllite*	OP	0.9663	31--0617	007726
Al	Fe	Si	H	O		9.19	4.59	4.48	4.42	4.41	4.27	4.23	4.06	4.00	3.77	$Al_{1.5}Fe_{0.5}(Si_{3.5}Al_{0.5})O_{10}(OH)_2$	AP	0.5520		808432
Al	Fe	Si	O			9.10	7.05	5.57	5.26	4.55	4.21	3.82	3.53	3.44	3.29	$(Al,Mg)Fe_2(Si,Al)_2O_6(O,OH)_2$ Orthopyroxene*	O	0.7753		007504
Al	Fe	Si	H	O		8.93	4.72	4.68	4.66	4.52	4.45	4.36	4.00	3.89	3.83	$(Al,Fe)(Fe,Mg)_5(Si,Al)_4O_{10}(OH)_8$ Chlorite*	MC	3.3254		002442
Al	Fe	Si	H	O		8.90	4.72	4.68	4.63	4.49	4.45	4.35	4.00	3.89	3.81	$Al_2(Fe,Mg)_5(Si_3Al)O_{10}(OH)_8$ Chlorite*	MC	3.3139		005592
Al	Fe	Si	O			8.59	8.53	6.29	4.95	4.91	4.65	4.37	4.30	4.27	4.09	$Fe_2Al_2Si_2O_{10}$ Sekaninaite	OC	0.5718	31--0616	709458
Al	Fe	Si	H	O		8.33	7.13	5.67	4.69	4.54	4.44	4.17	3.95	3.57	3.54	$(Fe,Mg)_2Al_{18}Si_8O_{46}(OH)_2$ Staurolite*	MC	0.4736		021994
Al	Fe	Si	H	O		8.31	7.11	5.66	4.68	4.53	4.43	4.16	3.94	3.56	3.54	$Al_2(Fe,Mg)_2Si_4O_{22}(OH)$ Staurolite	MC	0.4736		104939
Al	Fe	Si	H	O		8.28	7.09	4.51	4.41	4.14	3.92	3.54	3.52	3.22	3.05	$Fe(Al_2Si_2)O_{10}(OH)_2$ Staurolite	OC	0.4737		030205
Al	Fe	Si	O			4.77	4.13	3.12	2.92	2.61	2.49	2.39	2.29	2.13	2.07	$(Al,Fe)_2(Fe,Ca)_3(SiO_4)_3$ Almandine	CI	11.6920		024524
Al	Fe	Si				4.75	4.29	3.18	3.04	2.61	2.56	2.38	2.15	2.08	2.06	Al_2FeSi_2	TI	1.5651		109269
Al	Fe	Si	O			4.72	4.09	3.09	2.89	2.59	2.47	2.36	2.27	2.11	2.04	$(Fe,Mn)_3Al_2(SiO_4)_3$ Almandine, ma*	CI	11.5630	33--0658	711571
Al	Fe	Sm	O			11.0	5.52	4.88	4.76	4.46	4.07	3.68	3.66	3.27	2.94	$SmFe_2Al_2O_{10}$	HP	3.9191		809972
Al	Fe	Sm				6.66	5.31	5.09	4.27	3.60	3.39	3.33	3.27	2.82	2.75	$Sm_2Al_{1.48}Fe_{9.52}$	HR	1.7864		600413
Al	Fe	Sm				6.58	4.92	4.42	4.28	3.67	3.29	3.08	2.96	2.82	2.64	$(Al_{0.56}Fe_{0.44})_7Sm_4$	HR	1.4516	33--0021	711023
Al	Fe	Sm				6.20	4.39	4.36	3.10	2.77	2.53	2.44	2.19	2.19	2.07	Al_2Fe_4Sm	TI	0.5762		1242e2
Al	Fe	Sm				6.18	4.37	3.09	2.76	2.52	2.34	2.19	2.18	2.05	1.95	Al_2Fe_4Sm	TI	0.5782	34--0400	712559
Al	Fe	Sr	O			11.4	5.70	4.95	4.84	4.54	4.15	3.80	3.74	3.35	3.01	$SrFe_2Al_8O_{19}$	HP	3.9874		803810
Al	Fe	Ta				4.27	4.02	3.77	2.93	2.47	2.27	2.14	2.10	2.06	2.01	$AlFeTa$	HP	1.6288	29--0045	706879
Al	Fe	Tb				7.39	4.27	4.18	3.69	3.63	2.98	2.79	2.77	2.46	2.32	$Al_2Fe_{-4}Tb_2$	HP	0.4893	30--0025	708196
Al	Fe	Tb				7.39	4.27	4.18	3.69	3.63	2.98	2.79	2.77	2.46	2.32	$(Al_{0.158}Fe_{0.842})_2Tb_2$	HP	0.4893	34--0682	712240
Al	Fe	Tb				6.17	4.36	3.09	3.08	2.76	2.52	2.33	2.18	2.18	2.06	Al_8Fe_4Tb	TI	0.5768	34--0344	712508
Al	Fe	Tb				6.13	4.35	4.33	3.07	3.06	2.74	2.52	2.51	2.33	2.18	Al_2Fe_4Tb	TI	0.5812	32--0020	709998
Al	Fe	Th				6.25	4.42	4.40	3.13	3.12	2.80	2.55	2.54	2.35	2.21	Al_8Fe_4Th	TI	0.5741		122769
Al	Fe	Th				4.49	4.09	3.02	2.59	2.24	2.19	2.05	1.97	1.86	1.70	Al_2Fe_2Th	HP	0.7892	34--1319	124802

This is a page from the EISI Index, published in 1989. It combines elemental analysis selection, shown on the left, with long d-spacing searches, shown in the middle. From the statistics shown on the prior pages, *this combination* will frequently produce a unique identification. As a printed product, permutation of the elements with >100,000 material choices created practical limitations in size and fonts. The challenge in PDF-4+ was to duplicate the logic, without the space requirement.

Effective Search Strategies with Electron Diffraction Data

- Combining elemental analysis with a search on the experimental data

PDF-4+

General Method – Unknown Identification

Method 1

- Use element and composition searches

  (unlimited types and numbers of elements)
- Use 3 most intense d-spacings and 3 longest d-spacings to match
- Point and click on the matching entry to compare a full pattern to your data

PDF-4+

General Method – Unknown Identification

Method 2

- Use element and composition searches (unlimited types and numbers of elements)
- Import experimental data into Sleve+
- Automatically match data to the composition search using any of 4 algorithms (long lines, strong lines, strong & long)

General Method

Collect ED Pattern

Collect EDS Data

Search PDF-4+ Using Elemental Data and d-spacings

Produce Candidate List from Search Results

Match Candidate Simulated ED Pattern to Experimental Pattern

Options

1) Replace ED pattern with a) EBSD pattern, b) d,I listing, c) Integrated data from a ring scan (photo or CCD), measured unit cell parameters

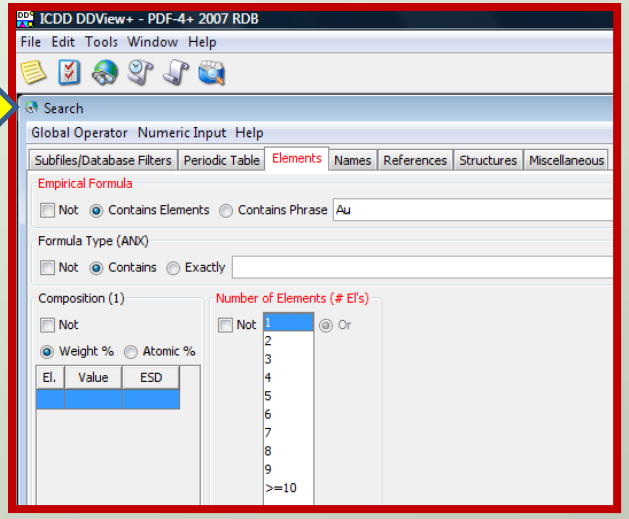
2) Replace EDS data with a) density, b) composition analysis, c) chemical analysis (use nomenclature search)

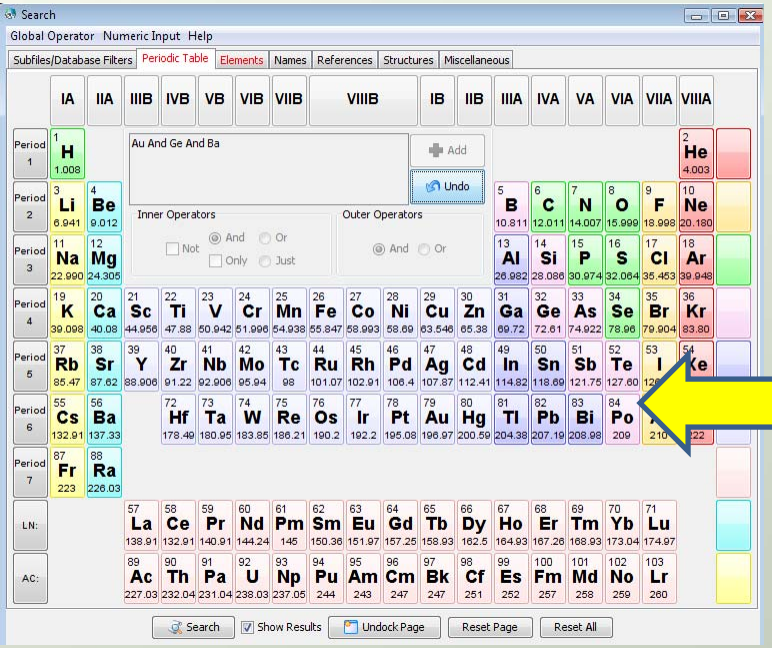
3) Replace candidate simulation pattern with candidate EBSD patterns, or 1/d plot

4) Match by candidate comparison to data simulations or use Sieve+ (Hanawalt, Long 8 and Fink searches)

Search by Elemental Composition

Use the Elemental Composition Search





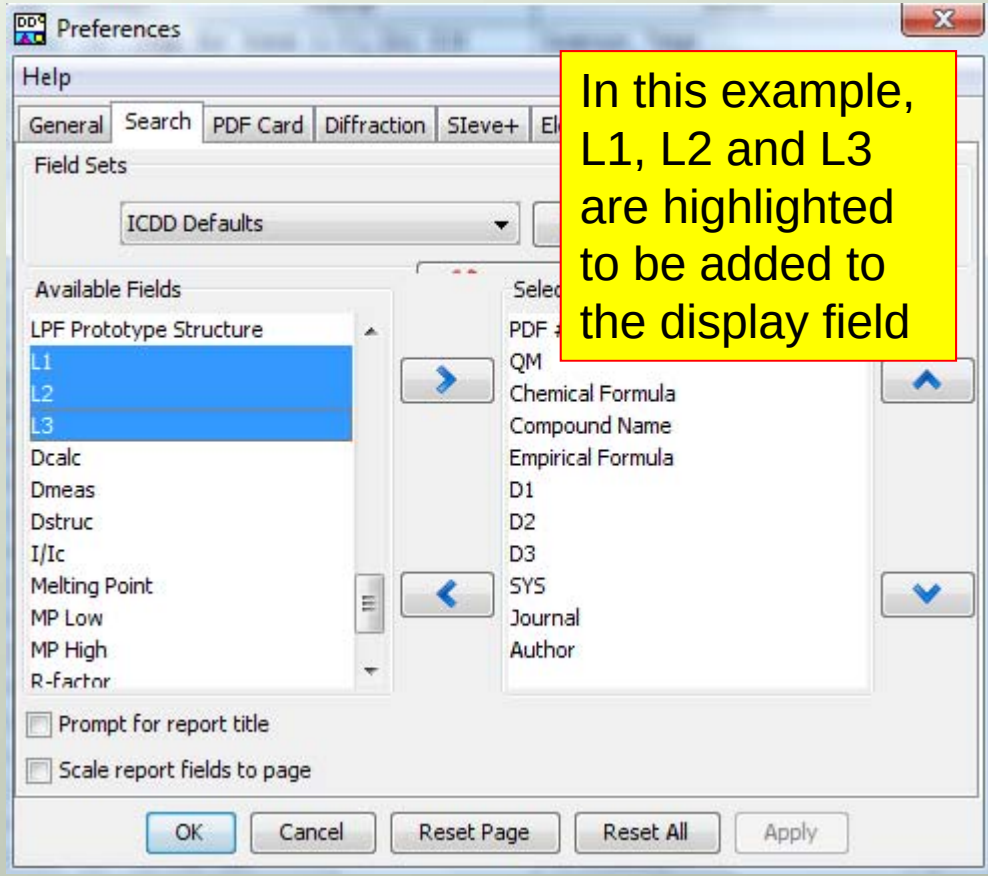
or a Point and Click Elemental Table Search

Get Results!

Empirical Formula ▲	L1	L2	L3	D1	D2	D3	ound Name	SYS	XtlC...	Pearson	QM	PDF #
Au3.16 Ba Ge0.84	5.280000	4.255680	3.288050	2.791090	2.325000	2.806560	Bar[illegible] Germanium	T	4.650	tI10.00	B	01-074-0014
Au6.32 Ba2 Ge1.68	5.279000	4.255000	2.804900	2.791200	2.324800	2.804900	Barium [illegible]manium Gold	T	4.650	tI10.00	C	00-031-0143
Au6.32 Ba2 Ge1.68	5.280000	4.255680	3.288050	2.791090	2.325000	2.806560	Gold Barium Germanium	T	4.650	tI10.00	I	03-065-2687
Au3 Ba4 Ge20	7.635830	5.399350	4.829330	2.886070	3.117320	1.751780	Barium Gold Germanium	C	10.799	cP54.00	I	04-005-3081

PDF-4+
Change the Display Fields

Use the preferences icon to add, delete, or sort display fields

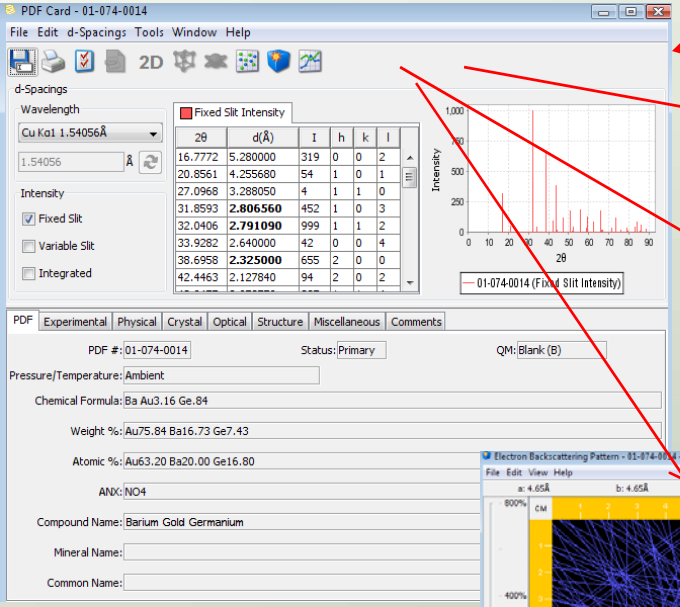


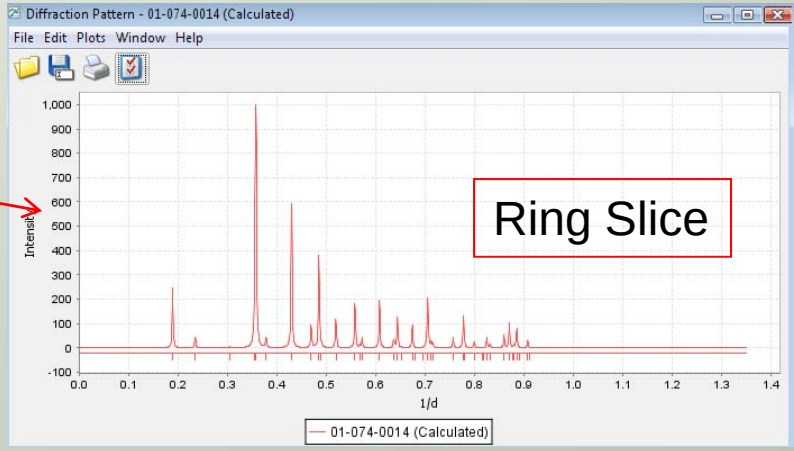
In this example, L1, L2 and L3 are highlighted to be added to the display field

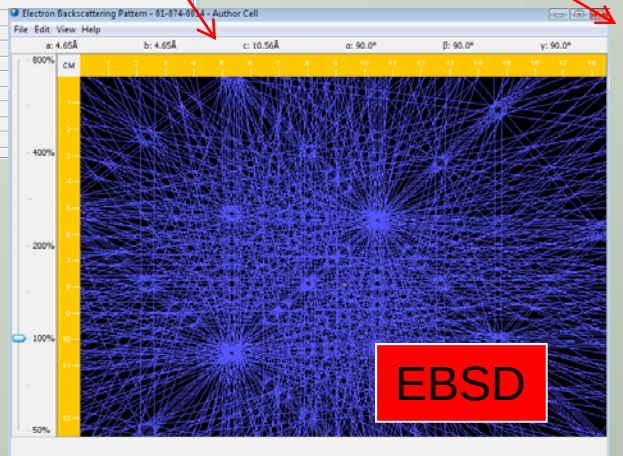
70 Fields to Choose From!

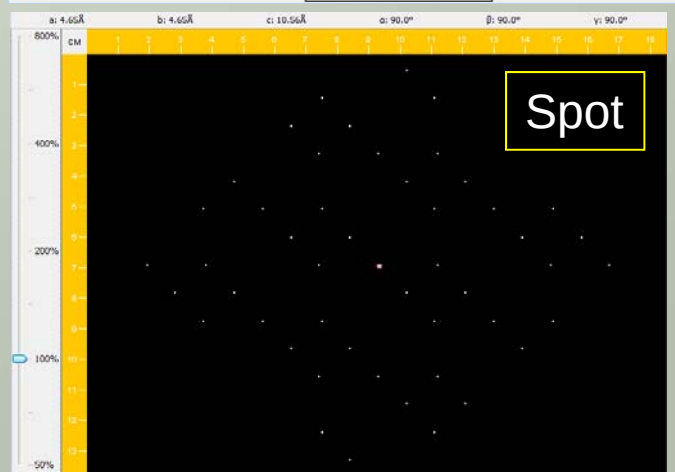
PDF-4+
Results to Data Entry to Simulations

Empirical Formula ▲	L1	L2	L3	D1	D2	D3	Compound Name	SYS	XtlC...	Pearson	QM	PDF #
Au3.16 Ba Ge0.84	5.280000	4.255680	3.288050	2.791090	2.325000	2.806560	Barium Gold Germanium	T	4.650	tI10.00	B	01-074-0014
Au6.32 Ba2 Ge1.68	5.279000	4.255000	2.804900	2.791200	2.324800	2.804900	Barium Germanium Gold	T	4.650	tI10.00	C	00-031-0143
Au6.32 Ba2 Ge1.68	5.280000	4.255680	3.288050	2.791090	2.325000	2.806560	Gold Barium Germanium	T	4.650	tI10.00	I	03-065-2687
Au3 Ba4 Ge20	7.635830	5.399350	4.829330	2.886070	3.117320	1.751780	Barium Gold Germanium	C	10.799	cP54.00	I	04-005-3081









Custom Design Display

EISI Index Simulation with PDF-4+

Element 3 Long Lines 3 Strong Lines Name Cell Edge Pearson Symbol QM PDF

Emp...	L1	L2	L3	D1	D2	D3	Comp...	SYS	Xt... ▲	Pearson	QM	PDF #
Au	2.350000	2.030000	1.440000	2.350000	1.230000	2.030000	Gold	C	4.064	cF4.00	B	00-001-1174
Au	2.360000	2.040000	1.440000	2.360000	2.040000	1.230000	Gold	C	4.068	cF4.00	B	00-002-1095
Au	2.350000	2.030000	1.440000	2.350000	2.030000	1.230000	Gold	C	4.070	cF4.00	B	00-001-1172
Au	2.349820	2.035000	1.438960	2.349820	2.035000	1.227150	Gold	C	4.070	cF4.00	I	04-003-5615
Au	2.349820	2.035000	1.438960	2.349820	2.035000	1.227150	Gold	C	4.070	cF4.00	I	04-003-7037
Au	2.349870	2.035050	1.439000	2.349870	2.035050	1.227180	Gold	C	4.070	cF4.00	I	04-004-5106
Au	2.349820	2.035000	1.438960	2.349820	2.035000	1.227150	Gold	C	4.070	cF4.00	I	04-004-8456
Au	2.350970	2.036000	1.439670	2.350970	2.036000	1.227750	Gold	C	4.072	cF4.00	I	03-065-8601
Au	2.351550	2.036500	1.440020	2.351550	2.036500	1.228060	Gold	C	4.073	cF4.00	I	01-071-4615
Au	2.354030	2.038650	1.441540	2.354030	2.038650	1.229350	Gold	C	4.077	cF4.00	I	04-001-2616
Au	2.354490	2.039050	1.441830	2.354490	2.039050	1.229590	Gold	C	4.078	cF4.00	I	01-071-3755
Au	2.354430	2.039000	1.441790	2.354430	2.039000	1.229560	Gold	C	4.078	cF4.00	I	04-001-3179
Au	2.354380	2.038950	1.441760	2.354380	2.038950	1.229530	Gold	C	4.078	cF4.00	I	04-002-1170
Au	2.354670	2.039200	1.441930	2.354670	2.039200	1.229680	Gold	C	4.078	cF4.00	I	04-003-2942
Au	2.354550	2.039100	1.441860	2.354550	2.039100	1.229620	Gold	C	4.078	cF4.00	I	04-003-3089
Au	2.354490	2.039050	1.441830	2.354490	2.039050	1.229590	Gold	C	4.078	cF4.00	I	04-003-3368
Au	2.354430	2.039000	1.441790	2.354430	2.039000	1.229560	Gold	C	4.078	cF4.00	I	04-003-7284
Au	2.354320	2.038900	1.441720	2.354320	2.038900	1.229500	Gold	C	4.078	cF4.00	I	04-004-4643
Au	2.354430	2.039000	1.441790	2.354430	2.039000	1.229560	Gold	C	4.078	cF4.00	I	04-004-8502
Au	2.354430	2.039000	1.441790	2.354430	2.039000	1.229560	Gold	C	4.078	cF4.00	I	04-004-9166
Au	2.354430	2.039000	1.441790	2.354430	2.039000	1.229560	Gold	C	4.078	cF4.00	I	04-004-9181
Au	2.354670	2.039200	1.441930	2.354670	2.039200	1.229680	Gold	C	4.078	cF4.00	I	04-005-1700
Au	2.355000	2.039000	1.442000	2.355000	2.039000	1.230000	Gold	C	4.079	cF4.00	S	00-004-0784
Au	2.354980	2.039470	1.442120	2.354980	2.039470	1.229850	Gold	C	4.079	cF4.00	I	01-071-4073

This is an example, using gold, where an “EISI” Index was generated using PDF-4+ and selecting display field preferences. In comparison to the EISI index, the long 8 display has been replaced by a long 3 and strong 3 display. PDF-4+ has an advantage in that any of 70 fields can be displayed and sorted for all entries.

Additional Information

- More examples on how to search using elemental data are given in the tutorial "*XRF and SEM-EDS*"
- Examples of how to use electron diffraction data simulations and simulation variables are given in the tutorial, "*Electron Diffraction*"
- Examples of how to use Sleve+ for Long 8 and Fink Searches are given in the tutorials, *"Advanced Identification Tools"* and *"Identification PDF-4+ Sleve+"*

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

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