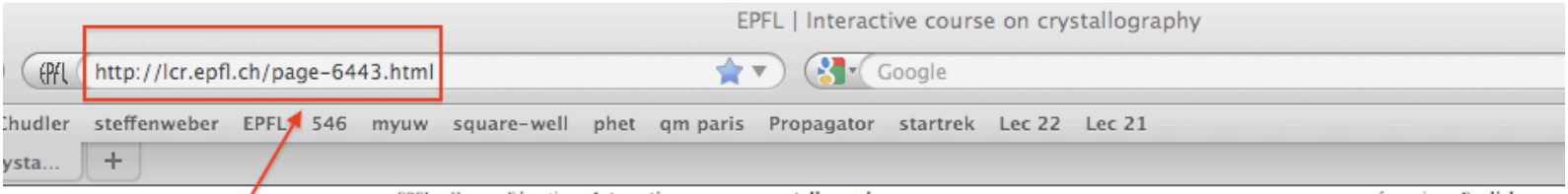


Go to this webpage

LABORATORY OF CRYSTALLOGRAPHY LCR

Interactive course of Crystallography

This course introduces the basic concepts of crystallography and is freely available on the web for everyone. The symmetry of crystalline material and the properties of diffraction are presented by means of interactive applets. The description of structures is greatly facilitated by the combination of drawing tools and easy access to databases.

More specifically, the following applets are available :

- **cellConverter**
  An applet to transform a unit cell ant its content to another cell. Based on the originial CIF file, the applet generates a new CIF file resulting from the transformation specified by the user.

- **Charge flipping**
  An applet to solve the phase problem in diffraction by the charge flipping algorithm. The user can create a 2D crystalline structure and follow the evolution of the algorithm in solving the structure.

- **Crystal symmetry environment (CSE)**
  An applet to represent (among others) the general and special positions of the 230 space groups.

- **crystalOgraph**
  An applet to represent any type of crystalline structure given the lattice parameters, the space group and the atomic coordinates of symmetry independent atoms. It is also possible to import directly a structure from the ICSD database or from a CIF file.

- **Diffraction and Fourier Transform**
  An applet to calculate the Fourrier Transform of a density function ρ(**x**) yielding the complex magnitude G(**S**). The applet is also able to calculate the inverse Fourier transform of G(**S**). The density function can be either periodic or non-periodic. Numerous tools can be applied in order to understand the role of amplitudes and phases which are of particular importance in diffraction phenomena.

- **diffractOgram**
  An applet to simulate any type of diffraction pattern based on the Ewald sphere and the reciprocal lattice. In particular, Laue patterns, Debye Scherrer diagrams, rotating crystals and even precession photographs can be generated.

- **Escher Web Sketch 2**
  An applet to simulate any symmetry decoration of the plane (17 two-dimensional planar groups).

- **Ewald sphere animation**
  Mpeg: 5.1 MB - 2.8 MB
  QuickTime: 4.7 MB - 2.3 MB
  Video sequence illustrating the diffraction phenomenon based on the Ewald sphere.

- **Initiation to the discovery of symmetry**
  An applet to discover the point group symmetry of platonic and other polyhedra. In particular, rotations, inversion and combinations of them can be simulated.

- **Powder diffraction files** (For license reason, this applet is only available at the EPFL campus)
  An applet to extract the powder diffraction patterns from a database. Each pattern can be retrieved by specifying some characteristics, e.g. its element contents and number, the name of the compound, the pdf number of the compound or the d-values of the most intensive lines.

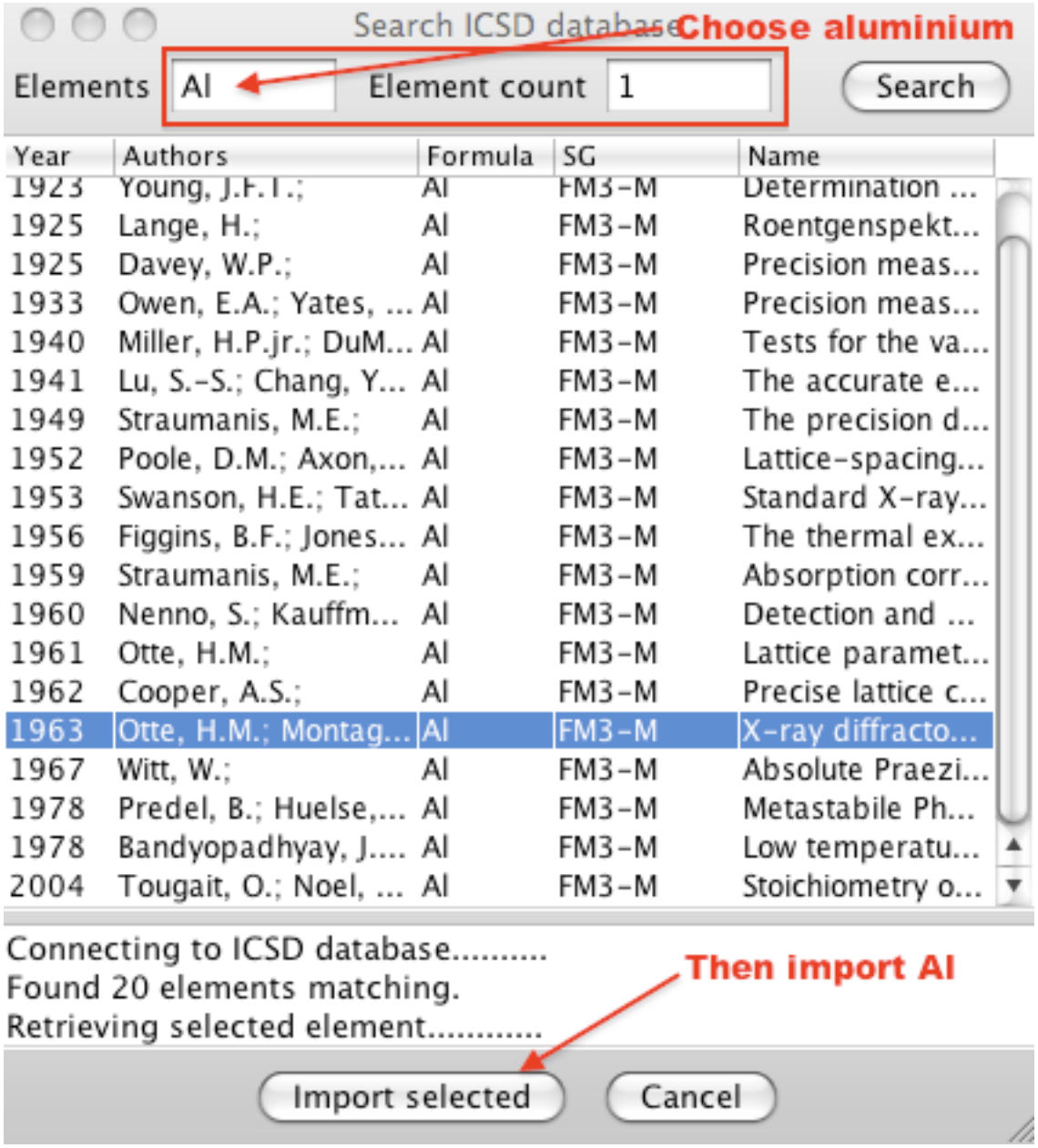
- **Reciprocal lattice generator**
  From a periodic diagram generated by EWS, the user is guided step by step by the applet in order to create the reciprocal lattice corresponding to the periodicity of the initial periodic pattern.

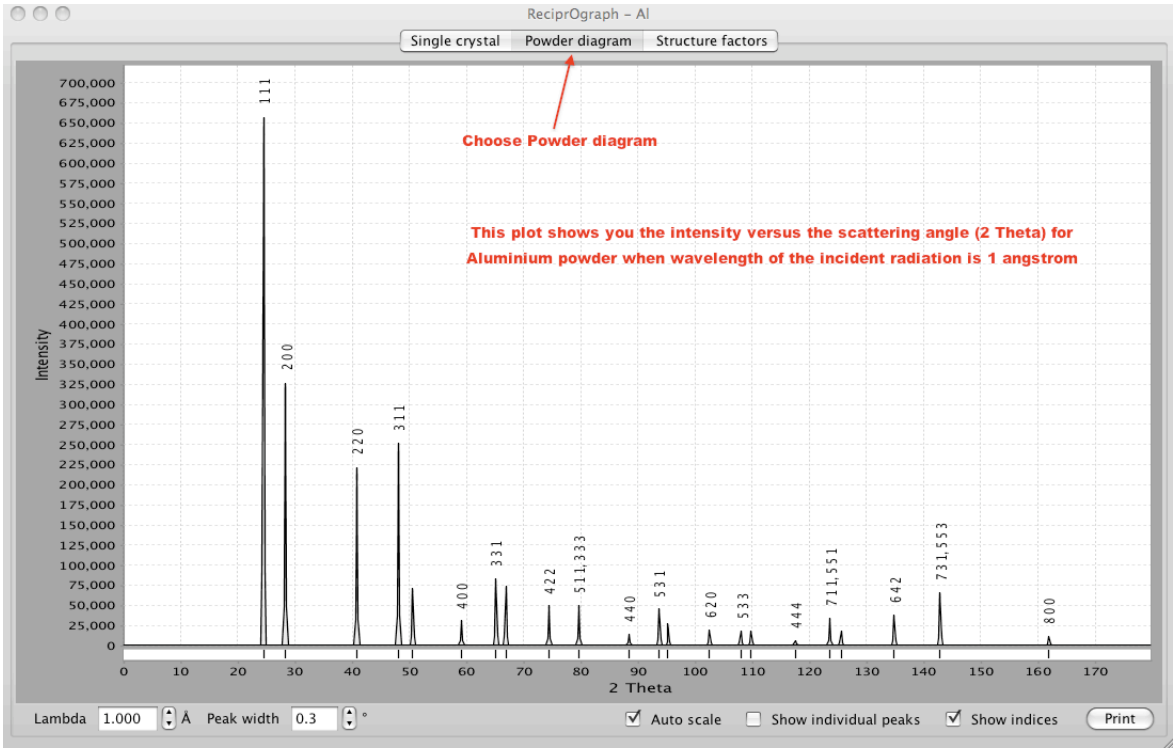
Open this applet

- **reciprOgraph**
  An applet to simulate the X-ray diffraction intensities for single crystal in reciprocal space and powder diffraction patterns. Structures can be selected from the ICSD database or from CIF files.

Additional resources:

The website of the International Union of crystallography (IUCr) maintains a list of public resources dedicated to crystallography education available at this link.


Search ICSD database
Choose aluminium
Elements
Al
Element count
1
Search
Year
Authors
Formula
SG
Name
1923 Young, J.F.T.; Al FM3-M Determination ...
1925 Lange, H.; Al FM3-M Roentgenspekt...
1925 Davey, W.P.; Al FM3-M Precision meas...
1933 Owen, E.A.; Yates, ... Al FM3-M Precision meas...
1940 Miller, H.P.jr.; DuM... Al FM3-M Tests for the va...
1941 Lu, S.-S.; Chang, Y... Al FM3-M The accurate e...
1949 Straumanis, M.E.; Al FM3-M The precision d...
1952 Poole, D.M.; Axon,... Al FM3-M Lattice-spacing...
1953 Swanson, H.E.; Tat... Al FM3-M Standard X-ray...
1956 Figgins, B.F.; Jones... Al FM3-M The thermal ex...
1959 Straumanis, M.E.; Al FM3-M Absorption corr...
1960 Nenno, S.; Kauffm... Al FM3-M Detection and ...
1961 Otte, H.M.; Al FM3-M Lattice paramet...
1962 Cooper, A.S.; Al FM3-M Precise lattice c...
1963 Otte, H.M.; Montag... Al FM3-M X-ray diffracto...
1967 Witt, W.; Al FM3-M Absolute Praezi...
1978 Predel, B.; Huelse,... Al FM3-M Metastabile Ph...
1978 Bandyopadhyay, J.... Al FM3-M Low temperatu...
2004 Tougait, O.; Noel, ... Al FM3-M Stoichiometry o...
Connecting to ICSD database.....
Found 20 elements matching.
Retrieving selected element.....
Then import Al
Import selected
Cancel


ReciprOgraph – Al
Single crystal
Powder diagram
Structure factors
Choose Powder diagram
This plot shows you the intensity versus the scattering angle (2 Theta) for
Aluminium powder when wavelength of the incident radiation is 1 angstrom
Intensity
2 Theta
111
200
220
311
400
331
422
511,333
440
531
620
533
444
711,551
642
731,553
800
Lambda
1.000
Å
Peak width
0.3
°
Auto scale
Show individual peaks
Show indices
Print

ReciprOgraph – Al

the program also gives you d(hkl)

Single crystal | Powder diagram | Structure factors

and the Structure Factor

h	k	l	d(hkl)	2-Theta	F(re)	F(Im)	$\|F\|^2$
3	3	3	0.7793	79.825	17.41	0.00	303.10
3	3	1	0.9290	65.127	21.24	0.00	451.11
3	3	-1	0.9290	65.127	21.24	0.00	451.11
3	3	-3	0.7793	79.825	17.41	0.00	303.10
3	1	3	0.9290	65.127	21.24	0.00	451.11
3	1	1	1.2209	48.351	26.63	0.00	709.15
3	1	-1	1.2209	48.351	26.63	0.00	709.15
3	1	-3	0.9290	65.127	21.24	0.00	451.11
3	-1	3	0.9290	65.127	21.24	0.00	451.11
3	-1	1	1.2209	48.351	26.63	0.00	709.15
3	-1	-1	1.2209	48.351	26.63	0.00	709.15
3	-1	-3	0.9290	65.127	21.24	0.00	451.11
3	-3	3	0.7793	79.825	17.41	0.00	303.10
3	-3	1	0.9290	65.127	21.24	0.00	451.11
3	-3	-1	0.9290	65.127	21.24	0.00	451.11
3	-3	-3	0.7793	79.825	17.41	0.00	303.10
2	2	2	1.1689	50.649	25.84	0.00	667.89
2	2	0	1.4316	40.883	29.27	0.00	856.51
2	2	-2	1.1689	50.649	25.84	0.00	667.89
2	0	2	1.4316	40.883	29.27	0.00	856.51
2	0	0	2.0246	28.595	34.04	0.00	1158.43
2	0	-2	1.4316	40.883	29.27	0.00	856.51
2	-2	2	1.1689	50.649	25.84	0.00	667.89
2	-2	0	1.4316	40.883	29.27	0.00	856.51
2	-2	-2	1.1689	50.649	25.84	0.00	667.89
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1	3	1	1.2209	48.351	26.63	0.00	709.15
1	3	-1	1.2209	48.351	26.63	0.00	709.15
1	3	-3	0.9290	65.127	21.24	0.00	451.11
1	1	3	1.2209	48.351	26.63	0.00	709.15
1	1	1	2.3378	24.699	35.82	0.00	1283.19
1	1	-1	2.3378	24.699	35.82	0.00	1283.19
1	1	-3	1.2209	48.351	26.63	0.00	709.15
1	-1	3	1.2209	48.351	26.63	0.00	709.15
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1	-1	-1	2.3378	24.699	35.82	0.00	1283.19
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1	-3	1	1.2209	48.351	26.63	0.00	709.15
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1	-3	-3	0.9290	65.127	21.24	0.00	451.11
0	2	2	1.4316	40.883	29.27	0.00	856.51
0	2	0	2.0246	28.595	34.04	0.00	1158.43
0	2	-2	1.4316	40.883	29.27	0.00	856.51
0	0	2	2.0246	28.595	34.04	0.00	1158.43
0	0	-2	2.0246	28.595	34.04	0.00	1158.43
0	-2	2	1.4316	40.883	29.27	0.00	856.51
0	-2	0	2.0246	28.595	34.04	0.00	1158.43
0	-2	-2	1.4316	40.883	29.27	0.00	856.51
-1	3	3	0.9290	65.127	21.24	0.00	451.11
-1	3	1	1.2209	48.351	26.63	0.00	709.15
-1	3	-1	1.2209	48.351	26.63	0.00	709.15
-1	3	-3	0.9290	65.127	21.24	0.00	451.11
-1	1	3	1.2209	48.351	26.63	0.00	709.15
-1	1	1	2.3378	24.699	35.82	0.00	1283.19
-1	1	-1	2.3378	24.699	35.82	0.00	1283.19
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