- User's Guide -

(for version 1511)

Author: **Oriol Vallcorba**
Experiments Division - MSPD Beamline (BL04)
ALBA Synchrotron Light Source - CELLS (www.cells.es)

Collaborator: **Jordi Rius**
Institut de Ciència de Materials de Barcelona (ICMAB)
Consejo Superior de Investigaciones Científicas (CSIC)

For comments/complaints/errors/suggestions, please contact to: **ovallcorba@cells.es**

Conditions of use

This software can be used free of charge for non-commercial academic purposes only. For any other purpose, please contact directly with the author. Further distribution of this software is not allowed.

Citation of the author/program/affiliation would be greatly appreciated when this program helped to your work.

Disclaimer

This software is distributed WITHOUT ANY WARRANTY. The authors (or their institutions) have no liabilities in respect of errors in the software, in the documentation and in any consequence of erroneous results or damages arising out of the use or inability to use this software. Use it at your own risk.

d2Dplot is programmed with Java™

Acknowledgements

Thanks are due the Spanish "Ministerio de Ciencia e Innovación" and to the "Generalitat the Catalunya" for continued financial support.

Contents

1. Installation and use of *d2Dplot*

No installation of the program is required. Only extract the files and folders of the zip file into the desired folder in your hard drive and run the executable file (`d2Dplot.exe` in Windows and `d2Dplot` in Linux). In most of the recent Linux distributions, the executable files can be executed by double click from the file explorer but alternatively you can also run it from the command line with `./d2Dplot`. If the execute flag of the file is turned off, turn it on with: `chmod +x d2Dplot`

Tip: Running it from the command line has the advantage that you can give an image file as the argument and it will be automatically opened.

Note: JAVA is required (version 1.6.0_18 or higher).

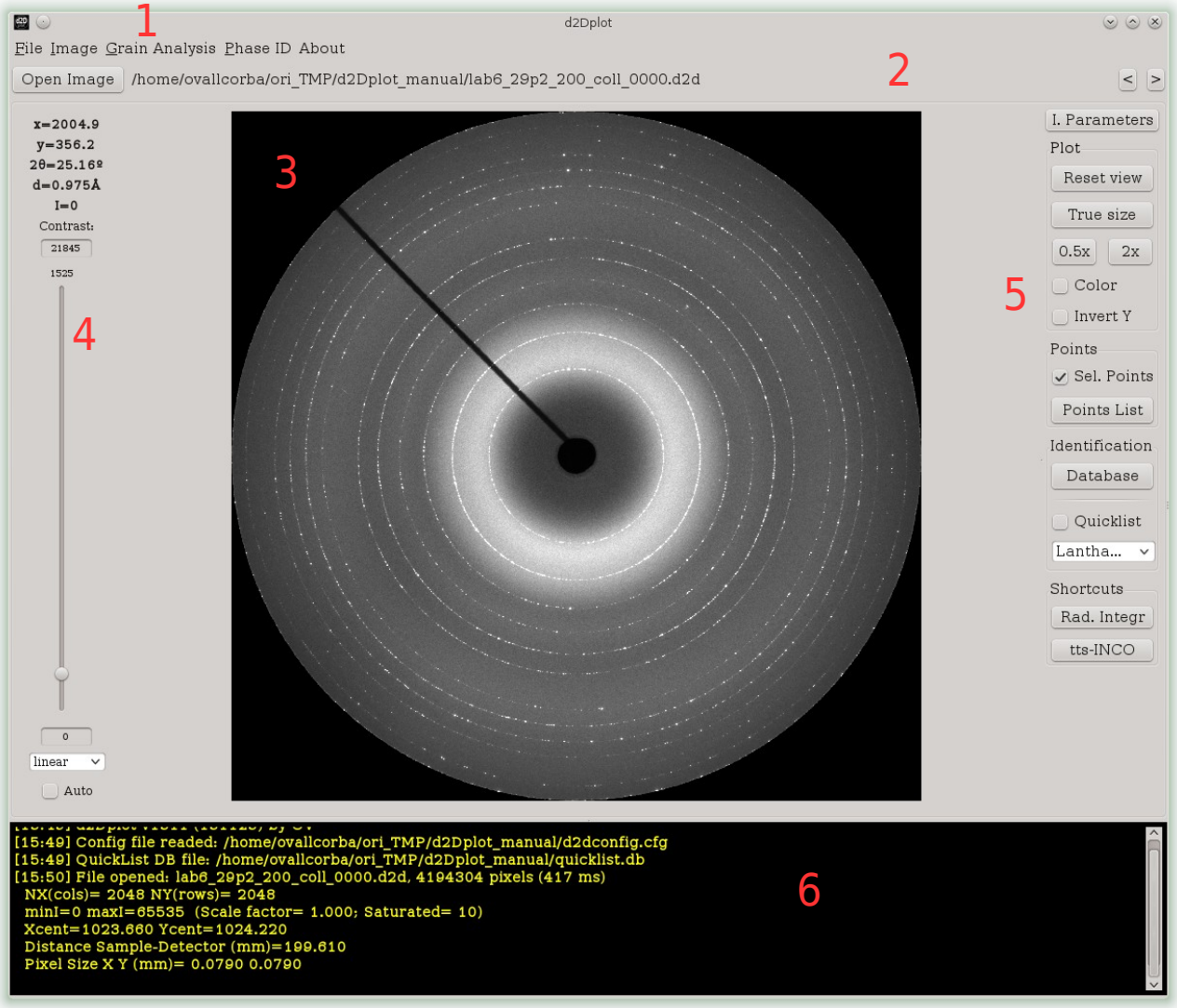
Configuration file

The first run, the program generates a plain text configuration file (`d2dconfig.cfg`) at the same folder where the program is installed. However, in some systems it can be created inside the user folder or somewhere else (the program will display the location of the file on the output panel located at the bottom part of the main window). Usually there is no need to change anything of this file but, if desired, the parameters are self-explanatory and their value can be modified.

The only two parameters worth mentioning are the default paths to the compound databases (`defQuickListDB` and `defCompoundDB`) which can be modified according to our preferences. Also, in the case the file `d2dconfig.cfg` is not created at the program folder, these paths may need to be corrected to the right paths wher these files are.

2. Overview

This is the aspect of the main window after opening an image (via menu `File-Open`) or clicking the button `Open Image`.



The main parts are (some of them are explained in detail at the corresponding sections of the guide):

1. **Menu bar**. To access all the program modules and options. It contains:
   - **`File`**
     - `Open Image`. Opens an image file.
     - `Save Image`. Save the image file (to any of the supported formats)

- `Export as PNG.` Save as a PNG file.
- `Sum Images`. To merge several images to a single one.
- `Subtract Images`. To subtract one image from another.
- `Batch Convert`. To convert a list of files to another file format.
- `Quit`. Exit the program

- **`Image`**
  - `Instrumental Parameters.` To introduce the instrumental parameters of the image.
  - `LaB6 Calibration`. Use the LaB6 rings to calibrate the sample-to-detector distance, the beam center and the tilt/rot of the detector.
  - `Excluded Zones`. To select zones of the image that have to be omitted in further calculations.
  - `Background Subtraction.` To subtract the background of the image. In the case there is some contribution of a holder (glass, etc...) and we want to get a background clean image.
  - `Radial Integration.` To get the 1D powder pattern corresponding to the radial integration of the image.
  - `HP Cu Pcalc`. To calculate the system pressure from two peaks of the Cu used as internal standard in high pressure experiments.
- **`Grain Analysis`**
  - `Load tts-INCO/REDUC files.` Open the files generated by tts-INCO or tts-REDUC programs to check the correctness of single grain orientations.
  - `Load XDS file.` Open a spot.xds file from XDS (**X**-ray **D**etector **S**oftware, CCP4) to show the position of the peaks.
  - `Find Peaks`. Locate diffraction peaks on the image.
  - `Clear all.` Remove all previous opened files for grain analysis.
- **`Phase ID`**
  - `Database`. Opens the compound database window. To plot theoretical rings from a compound database and search compounds from the image ring positions (more explained in the corresponding section of the guide).
- `About`. Some information about the program.

2. **Top bar**. It contains a button to quickly open an image file and also shows the path of the current displayed image. On the right part there are to arrow buttons which allow a quick navigation between consecutive images. Consecutive images are those which have the same filename followed by four sequential digits (e.g. `lab6_0000.d2d, lab6_0001.d2d, lab6_0002.d2d, lab6_0003.d2d`,...).

3. **Image panel**. Where the image is shown. The general interaction is:

- Left mouse button: Selection, peak addition, etc... (dependent on the module)
- Middle mouse button: Press and drag to move the image.
- Mouse wheel: Zoom.
- Right mouse button: Deletion. Pres and drag (UP and DOWN) for zoom.

4. **Image panel controls**. Information about the current pixel we are pointing is shown here. Also the contrast can be adjusted with the slide. The `auto` checkbox is to calculate automatically the contrast value for every opened image (it is done by default on the first one opened but if a consecutive images are opened it is often desired to have it disabled for comparison).

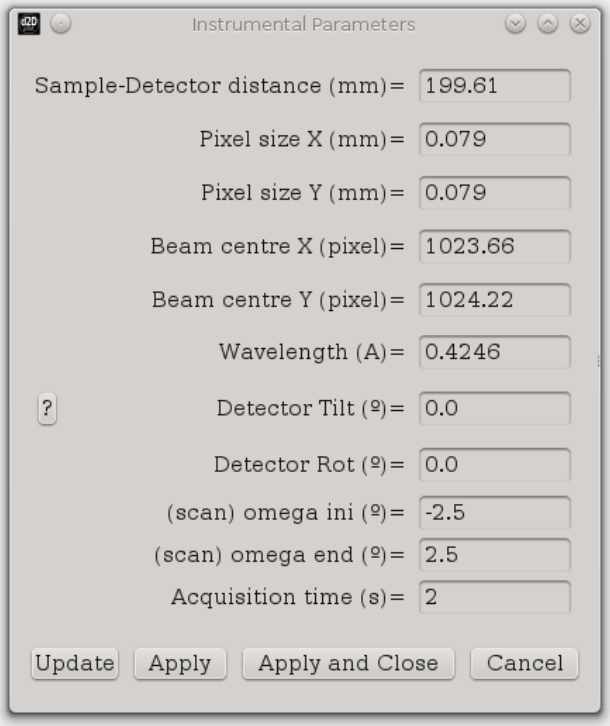
5. **Right panel**. Here, we have:

- Shortcuts for the instrumental parameters, radial integration, grain analysis and compound database.
- Plotting options regarding the image display (`true size` means that a pixel of the screen corresponds to a pixel of the image).
- Point selection tool. To select (by left mouse button clicking) points or rings of the image. The point list can be retrieved with the button Point List (and exported to a file if it wants to be used somewhere else). These points can be used later to search in the database (or calculate the pressure with Cu).
- Quicklist. It contains a selection of the compounds for quick display of the rings. More about the quicklist is explained in the corresponding section of the guide.

6. **Output panel**. Some messages of the program are displayed here.

3. Image menu modules

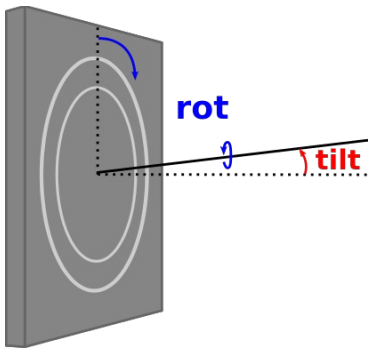
Instrumental parameters



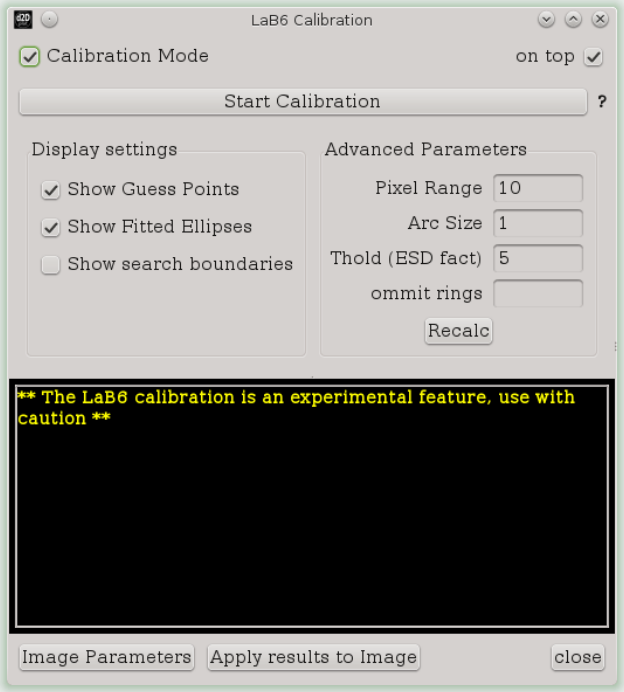
Instrumental and acquisition parameters are introduced here, names are self explanatory and the units are shown The Tilt/Rot convention used is:

- Tilt: Deviation (angle) of the orthogonality of the beam direction.
- Rot: Clockwise rotation (angle) of a perpendicular axis taking as “zero” the vertical (i.e. 12h on a clock...).

(Better a drawing...)



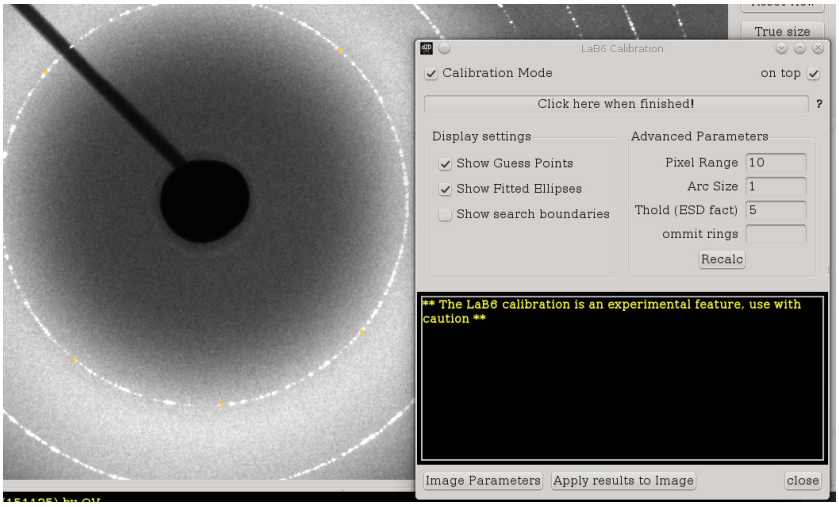
LaB6 calibration



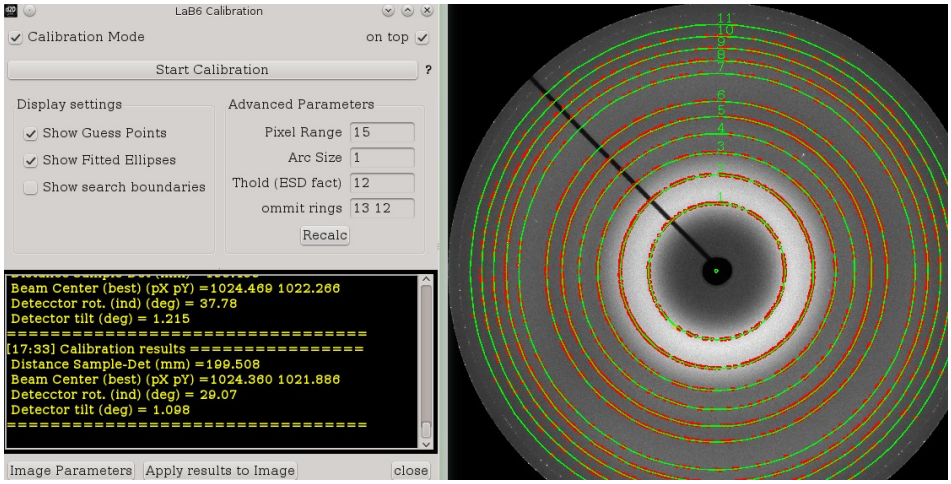
This module is still on development and may not be completely accurate... use with caution and check the obtained parameters.

It calibrates the sample-to-detector distance, the beam center and the detector tilt/rot angles. To do so from LaB6 rings we have to:

1. Click on `start calibration` button
2. Click >5 points on the inner LaB6 ring (do not need to be very accurate...)



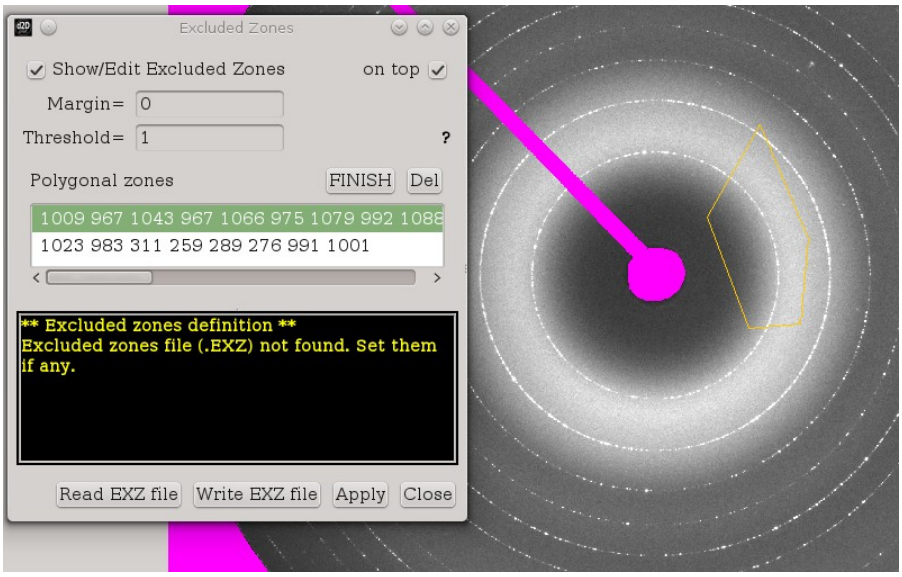
3. Click on the same button (now labeled `Click here when finished!`)
4. The rings and instrumental parameter values will be calculated



5. It can be repeated by clicking on the `Recalc` button (changing the parameters from the search rings if necessary).

The display settings show more info regarding the search of the lab6 rings.

Excluded zones



To select zones of the image to discard in further calculations, you can:

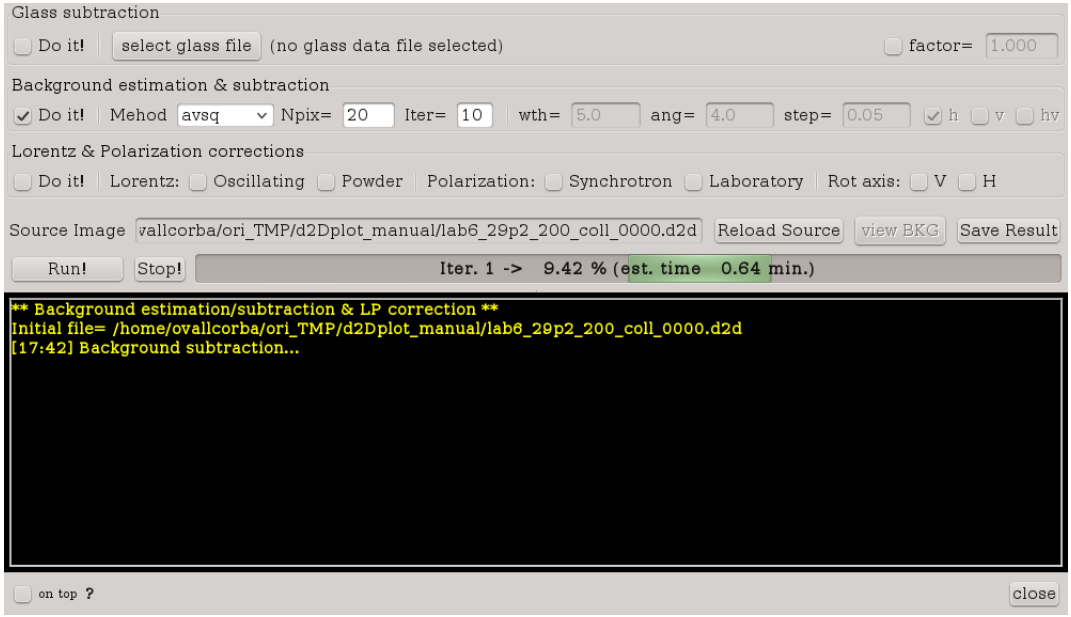
- Define a threshold such as if Y<Threshold the pixel will be excluded
- Add a polygonal excluded zone click ADD and click several points to define the zone

There are 2 options after defining excluded zones:

- Save in a format (D2D, BIN) that contain the information
- Save an Excluded Zones (ExZ) file to be loaded later.

Otherwise this information will be lost.

Background subtraction



There are 3 sections:

1. In the first one you can subtract a “glass” (or background) file by selecting it. A factor can be given (otherwise will be calculated in a conservative way and you can adjust it in next runs)
2. In the second one there are 5 methods to estimate the background, in summary:
   - `avsq`: Each iteration estimates the background by averaging square areas around each pixel from the previous iteration. Set the number of pixels for the side of the square (`Npix`) and the number of iterations (`Niter`). It is a slow process for high `Npix` and `Niter` values.
   - `avarc`: The same as previous option but using arc shaped areas (within 2-theta) around each pixel. Set the number of iterations (`Niter`) and the factors for the width (`wdt`) and angular aperture (`ang`) for the arcs. This is a very slow method.
   - `avcirc`: The background estimation for each pixel is the mean intensity from a radial integration (in the 2-theta circle containing each pixel). Set the stepsize for the 2-theta ranges (`step`).

- `minsq`: The background intensity value for each pixel (v0) is calculated as: Minimum (v0, v1, v2, v3) where v1, v2 and v3 are related pixels applying a reflection of the image (vertical, horizontal and both). Set which operations to use (`v,h,vh`), and the number of pixels (`Npix`) defining the square zone to be averaged after the operation (use 0 to consider only 1 pixel). It is a fast method but some peak intensity may be subtracted.
- `minarc`: The same as `minsq` but using an arc shaped zone for each pixel. Set the operations (`v,h,vh`) and the factors for width and angular aperture (`wdt,ang`).

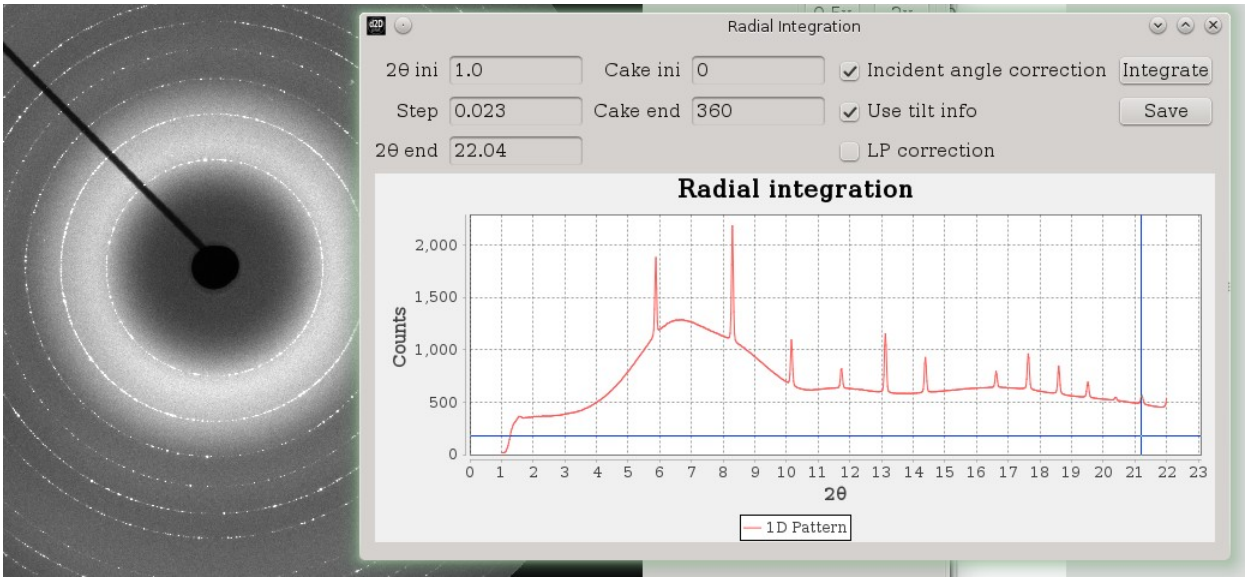
3. The third one is to apply the corrections for Lorentz & polarization to the image pixels. Select the proper conditions (single grain oscillating/powder, synchrotron/lab, oscillating axis horizontal/vertical).

When clicking on `Run!` the sections marked with the `do it` tick will be executed.

Visual inspection for residual peak intensity in the subtracted background can be done by clicking the [view BKG] button. Result images can be seen on the main window and source image can be reloaded if wanted. It is recommended to save the result to an image file before applying more corrections to the result file.

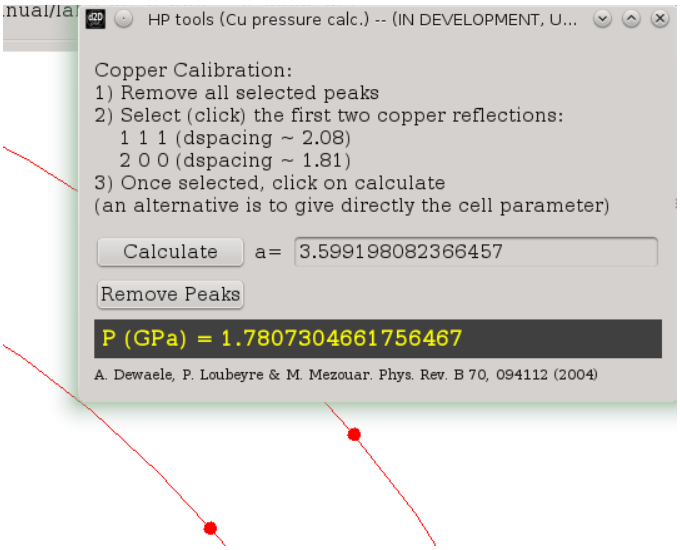
To subtract the background **it is very important to define previously the excluded zones**.

Radial Integration



Give the range and conditions (fields are self-explanatory) to integrate the image. You can save it in a two columns file (2-theta intensity). The cake ini/end units are degrees and starting from the vertical (12h. on a clock) going positive clockwise.

Copper pressure calculator (for High Pressure experiments)

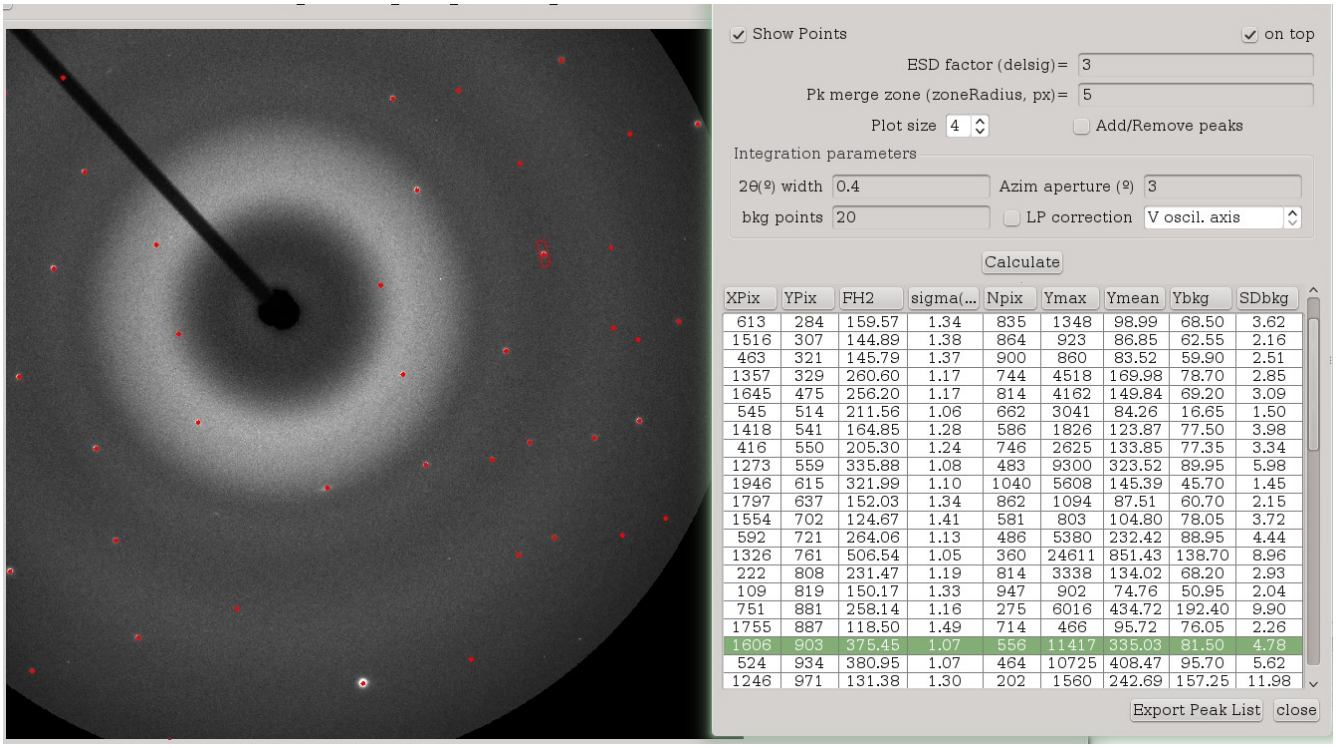


This module is still very preliminary and the only function it has implemented is the calculation of the pressure by the selection of two copper peaks (or alternatively directly from a given cell parameter).

4. Grain Analysis module

This module contains tools to work with images of single/few grains, but not powders.

Find Peaks



XPix	YPix	FH2	sigma(...	Npix	Ymax	Ymean	Ybkg	SDbkg
613	284	159.57	1.34	835	1348	98.99	68.50	3.62
1516	307	144.89	1.38	864	923	86.85	62.55	2.16
463	321	145.79	1.37	900	860	83.52	59.90	2.51
1357	329	260.60	1.17	744	4518	169.98	78.70	2.85
1645	475	256.20	1.17	814	4162	149.84	69.20	3.09
545	514	211.56	1.06	662	3041	84.26	16.65	1.50
1418	541	164.85	1.28	586	1826	123.87	77.50	3.98
416	550	205.30	1.24	746	2625	133.85	77.35	3.34
1273	559	335.88	1.08	483	9300	323.52	89.95	5.98
1946	615	321.99	1.10	1040	5608	145.39	45.70	1.45
1797	637	152.03	1.34	862	1094	87.51	60.70	2.15
1554	702	124.67	1.41	581	803	104.80	78.05	3.72
592	721	264.06	1.13	486	5380	232.42	88.95	4.44
1326	761	506.54	1.05	360	24611	851.43	138.70	8.96
222	808	231.47	1.19	814	3338	134.02	68.20	2.93
109	819	150.17	1.33	947	902	74.76	50.95	2.04
751	881	258.14	1.16	275	6016	434.72	192.40	9.90
1755	887	118.50	1.49	714	466	95.72	76.05	2.26
1606	903	375.45	1.07	556	11417	335.03	81.50	4.78
524	934	380.95	1.07	464	10725	408.47	95.70	5.62
1246	971	131.38	1.30	202	1560	242.69	157.25	11.98

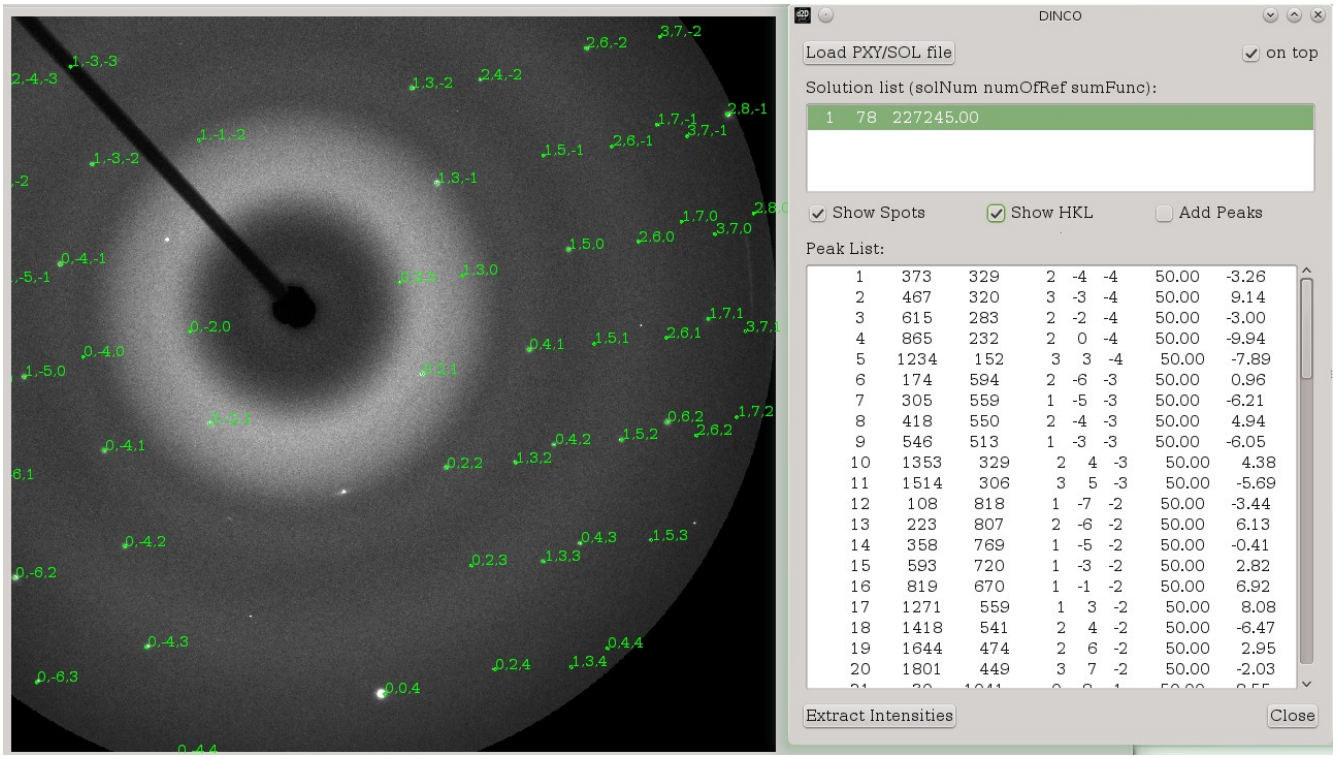
Here, giving a threshold (related to the intensity standard deviation) and a peak merge zone, this module find the diffraction peaks and performs the intensity integration. The results are shown on a table with multiple information: Peak location, Peak intensity and sigma, number of pixels of the integrated zone, max/mean intensities, background intensity that has been considered and its standard deviation.

By clicking on a peak the integration zone is shown on the image.

The peak list and intensity info can be exported as a text file.

Load tts-INCO/REDUC files

Here the output files from tts-REDUC or tts-INCO can be opened to display the reflections on the image for the multiple solutions. If there are more than one, can be selected simultaneously (painted in different colors) to check if there are multiple grains. HKL indexes can be shown, peaks can be added (activating the option add peaks to click on the image) or removed (delete from list or by right-clicking).



Also the peaks can be integrated by clicking `extract intensities` and a window equivalent as the one in find peaks will be opened.

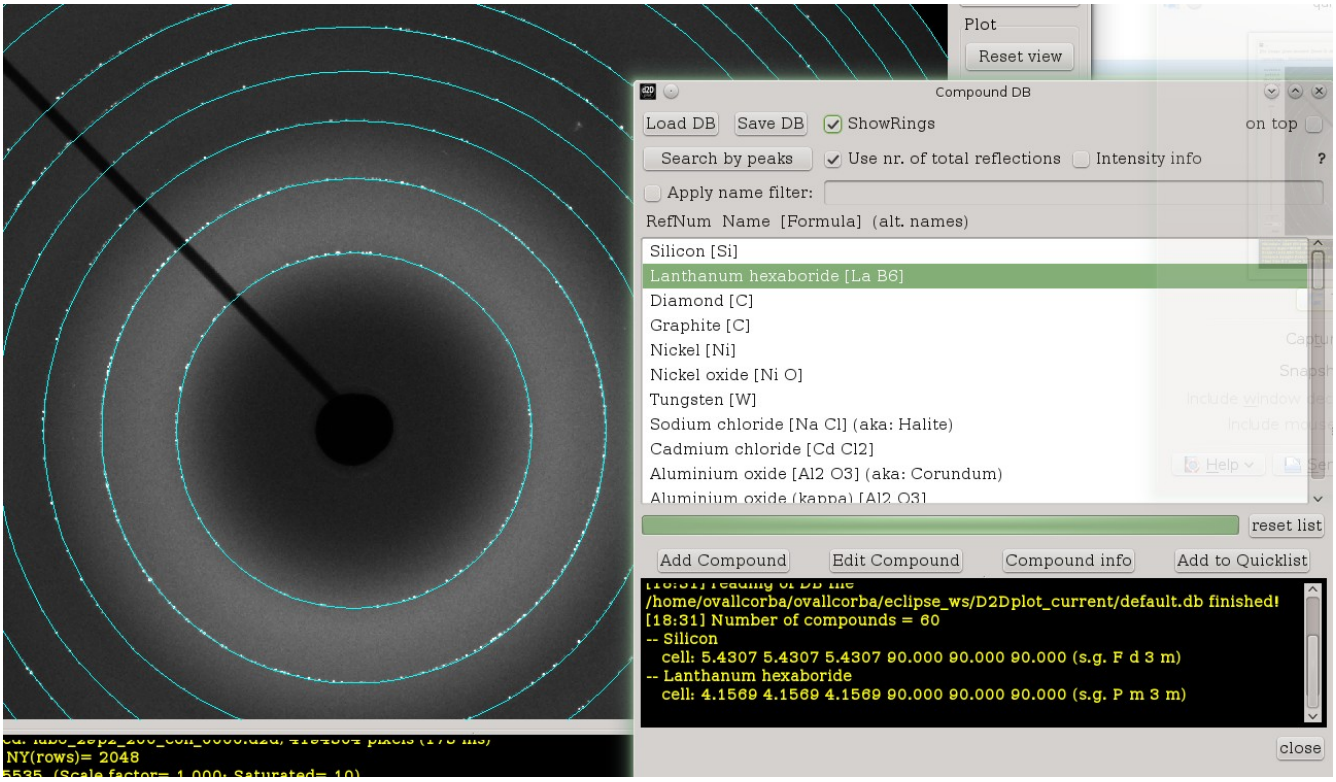
Load XDS file

This option is similar as the previous one but with a spot.xds file from XDS (**X**-ray **D**etector **S**oftware, CCP4).

5. Phase ID

There are two different “compound databases” considered in the program (actually lists will be the correct term to refer to them and not database...). The full database, which is accessed via `Phase_ID - Database` menu or the `Database` button in the main window, and the QuickList database which is intended to be a much smaller one (a selection of compounds from the full database) and that can be accessed directly from the main window. The “databases” (or lists) are stored in plain-text files and the paths for the default ones that are automatically considered by the program are given in the `d2dconfig.cfg` file.

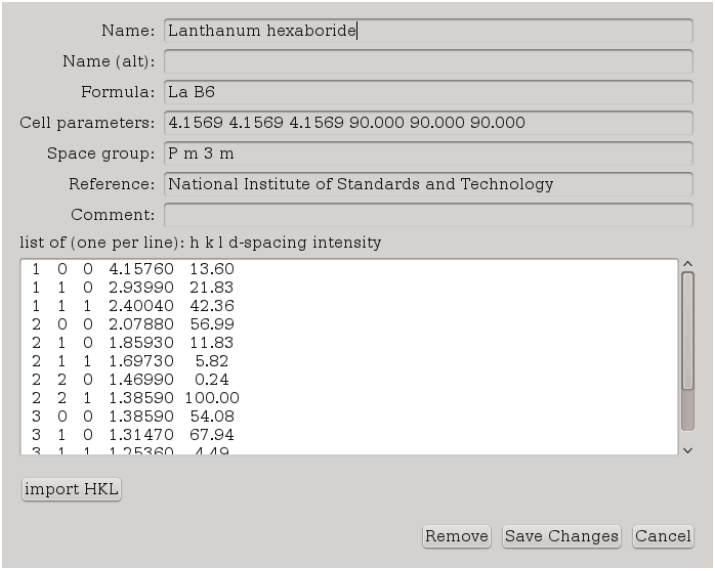
Database



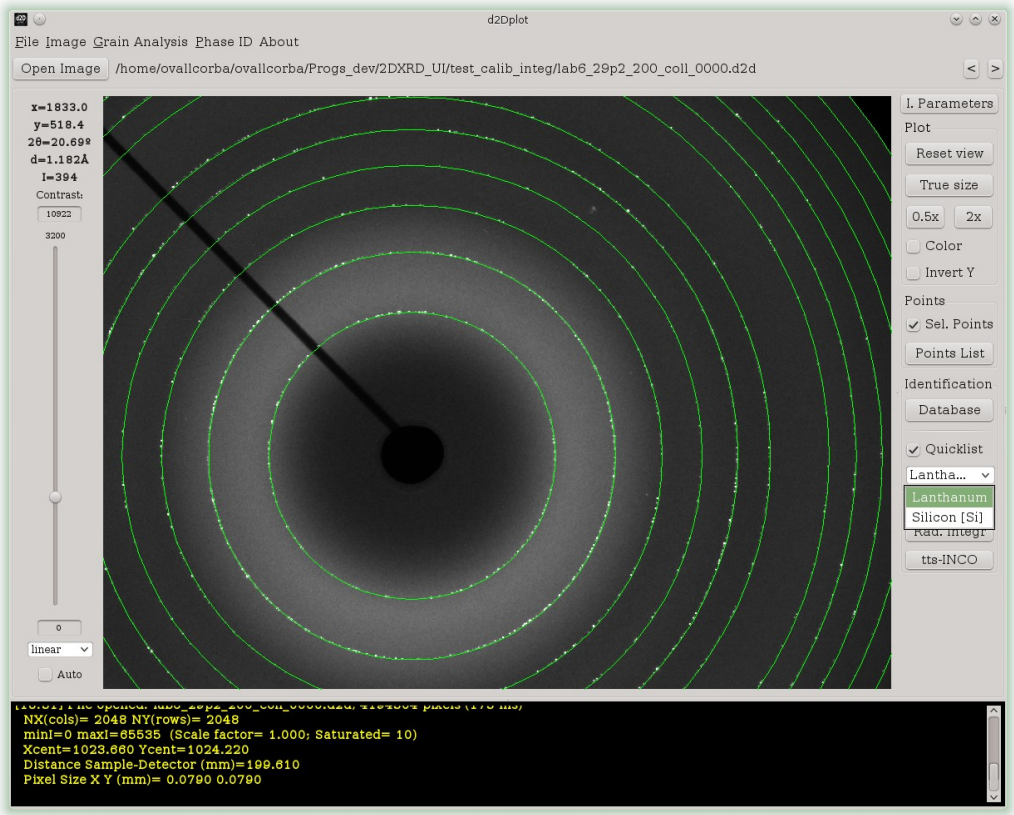
Here a plain-text DB file can be loaded. With the program it comes an example one that is taken by default at the beginning (a file called `default.db` which is in the program folder). Once loaded:

- Click on a compound to see the rings on the image (if `ShowRings` is selected)
- Check `apply name filter` and type to easily find the desired compound
- `Add/Edit compounds` by clicking the respective buttons and filling the info.

Alternatively you can edit manually the DB file (which is a simple self-explanatory text file). The format is explained in another section of this guide.

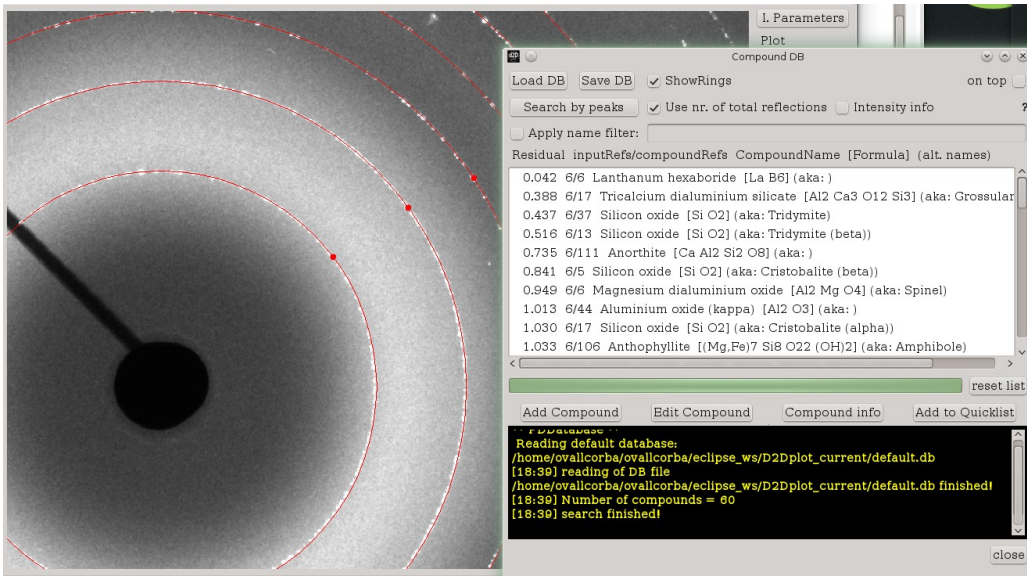


- `Add to QuickList` (QL) to be able to access the rings from the main window directly. Compounds in the QL are saved in a separate file with the same format as the DB file and can also be edited the same way



To search by peaks:

- On the main window click on the desired rings so that they are selected in the point list (`Sel.points` should be active)
- Click the button `search by peaks.` There are two options that affect the result of the search:
  - To consider the total number of reflections up to the d-spacing corresponding to the last input ring (recommended).
  - To consider the intensity of the rings (not recommended, only if the rings are well defined, the database contain intensity info and the first option did not gave good results).
- List will be updated by the best matching compounds (with respective residuals)
- Click on the compounds to see the rings on top of your image and check if they really match.



Note: The purpose of this database system in *d2Dplot* is to allow you (the user of the program) creating your own database with your choice of compounds (e.g. the family of compounds you are working with as possible candidates for phase identification, etc...). There are several compound databases where you can find X-ray diffraction information, including d-spacings to introduce to your *d2Dplot* database. These databases can be proprietary (ICDD, ICSD, CCDC,...) so that you need to purchase a license, or free (COD). The author of *d2Dplot* takes no responsibilities regarding where the final users of the program gets the x-ray diffraction information or its correctness.

The default DB is a small selection of 60 compounds taken from different sources. Each entry contains the reference from where it has been taken (with the respective authors) which can be retrieved by clicking `compound info` or by editing the compound. If any of these entries should be removed (for whatever reason) please contact the author and they will be removed immediately.

For any doubts/comments/complaints/suggestions, please contact the author

5. Image formats info

D2D format

This is a ASCII-header *d2Dplot* format followed by a binary data part using and encoding of unsigned shorts (2-byte little-endian unsigned integers), similar to EDF or IMG formats but with custom header items. It looks like this:

```
{
ByteOrder = LowByteFirst
DataType = UnsignedShort
DataSize = 8388608
Dim_1 = 2048
Dim_2 = 2048
Beam_center_x = 1023.66
Beam_center_y = 1024.22
Pixelsize_x = 79.00
Pixelsize_y = 79.00
Ref_distance = 199.61
Ref_wave = 0.4246
Det_tiltDeg = 0.000
Det_rotDeg = 0.000
Scan_omegaIni = 0.0
Scan_omegaFin = 0.0
Scan_acqTime = -1.0
EXZMargin =0
EXZThreshold =1
EXZpol1 =976 982 957 1013 964 1048 986 1073 1016 1081 1059 1075 1085 1039 1088 998 1057 969 1005 958 313 263 292 282
}
```

BIN format

This is a pure binary *d2Dplot* format. There are 60 bytes of header followed by the diffraction data (starting at byte 61) using an encoding of signed shorts (2-byte little-endian signed integers). The header info is:

```
Integer (4 bytes)  dimension X (image “columns”) in pixels
Integer (4 bytes)  dimension Y (image “rows”) in pixels
   Real (4 bytes)  Image scale factor
   Real (4 bytes)  Beam X (in pixels)
   Real (4 bytes)  Beam Y (in pixels)
   Real (4 bytes)  Pixel size X (microns)
   Real (4 bytes)  Pixel size X (microns)
   Real (4 bytes)  Sample-to-detector distance (mm)
   Real (4 bytes)  Wavelength (Angstrom)
   Real (4 bytes)  Omega initial (degrees)
   Real (4 bytes)  Omega final (degrees)
   Real (4 bytes)  Acquisition time (seconds)
```

EDF format

ESRF Data Format. (search the ESRF web page for more info, e.g. http://www.esrf.eu/computing/scientific/SAXS/doc/SaxsKeywords/SaxsKeywords.pdf). There are different implementations of the format, the one supported by *d2Dplot* looks like this:

```
{
HeaderID = EH:000001:000000:000000 ;
ByteOrder = LowByteFirst ;
DataType = UnsignedShort ;
Size = 8388608 ;
Dim_1 = 2048 ;
Dim_2 = 2048 ;
beam_center_x = 1023.66 ;
beam_center_y = 1024.22 ;
pixelsize_x = 79.00 ;
pixelsize_y = 79.00 ;
ref_distance = 199.61 ;
ref_wave = 0.4246 ;
scan_type = mar_ct (-1.0,) ;
}
(binary data)
```

IMG format

ADSC-style IMG files. The ones supported looks like this:

```
{
HEADER_BYTES= 512;
TYPE=unsigned_short ;
BYTE_ORDER=little_endian;
SIZE1=2048;
SIZE2=2048;
DISTANCE= 199.610 ;
PIXEL_SIZE= 0.079000 ;
WAVELENGTH=0.424600;
BEAM_CENTER_X=80.87;
BEAM_CENTER_Y=80.91;
}
(binary data)
```

GFRM format

Bruker Area Detector Frame Format (e.g. GADDS detector).

SPR format

“Spreadsheet” format. Table of intensities in ASCII format with the image pixel size (X Y) in the first line.

```
    2048    2048
1.78000E+02  1.61000E+02  1.73000E+02  1.86000E+02  2.23000E+02  2.57000E+02 ...  (... 2048 columns)
1.23000E+02  2.36000E+02  1.77000E+02  1.56000E+02  1.88000E+02  2.56000E+02 ... (... 2048 columns)
... (2048 rows).
```

6. Other file formats info

Database (DB) format

The database files (*.DB) contain crystallographic information of compounds. They are plain text files with an entry like this one for each of the compounds:

```
#COMP: Lanthanum hexaboride
#NAMEALT: here alternative names can be introduced (will be used in the name search filter)
#NAMEALT: there can be more than one line like this
#FORMULA: La B6
#CELL_PARAMETERS: 4.1569 4.1569 4.1569 90.000 90.000 90.000
#SPACE_GROUP: P m 3 m
#REF: National Institute of Standards and Technology
#COMMENT: Any comment regarding the entry (temperature, pressure, etc...) can be entered here.
#COMMENT: Also multiple comment fields can be added.
#LIST: H  K  L  dsp  Int
  1   0   0   4.15760   13.60
  1   1   0   2.93990   21.83
  1   1   1   2.40040   42.36
  2   0   0   2.07880   56.99
  2   1   0   1.85930   11.83
  2   1   1   1.69730    5.82
  2   2   0   1.46990    0.24
  2   2   1   1.38590  100.00
  3   0   0   1.38590   54.08
  3   1   0   1.31470   67.94
  3   1   1   1.25360    4.49
```

Different compounds are separated by a blank line.

Of all the fields, the only ones that are really required are the compound name (#COMP) and the d-spacing list (#LIST), which can be also introduced without intensities.

Compounds in the database can be added manually with a text editor or by using the database module of *d2Dplot* (add/edit compound).

Excluded zone (EXZ) format

The excluded zone file itself have comments explaining the three possible fields defining excluded zones. It looks like this:

```
! Excluded zones file for: /home/ovallcorba/lab6_29p2_200_coll_0000.edf
EXZmargin=0
EXZthreshold=1
EXZpol1=981 982 965 1016 969 1049 991 1073 1031 1080 1073 1055 1086 1020 1076 983 1038 963 1008 967
EXZpol2=288 288 991 991 1019 972 317 250

! EXZmargin     Margin of the image in pixels (if any)
! EXZthreshold  Pixels with Y<threshold will be excluded
! EXZpol#       Sequence of pixels (X1 Y1 X2 Y2 X3 Y3...) defining a polygonal shape to be
!               considered as excluded zone for the image
```

7. Miscellaneous

Release notes

Version 151125 (Nov 25, 2015). First release (public) version.

d2Dplot development started on 2013 as a tool to visualize the orientation search results of microvolumes (*tts*-INCO and related methodologies, Rius *et al*. IUCrJ. 2015; 2, 452-463) and as complement to its development. The reason for making it available is that it has grown a bit since then (although it has been programmed mainly during "free" times and never been a priority) and while it remains basically a tool to visualize diffraction images I find it useful and interesting for a general usage.

Known issues:

- LaB6 calibration is still on development and it needs to be improved, use with caution.
- Sometimes after opening different images during the same session some parts of the program may not be updated properly and it may be required to restart the program
- Only copper pressure calibration is implemented as a HP tool, and it has not been tested.

d2Dplot is completely programmed with Java™ (www.java.com) using jdk version 1.6. (Oracle License: http://www.oracle.com/technetwork/java/javase/downloads/jdk-6u21-license-159167.txt).

The following 3rd party libraries have been used:

- Commons Math. https://commons.apache.org/proper/commons-math/
  Apache License: http://www.apache.org/licenses/LICENSE-2.0
- MigLayout. http://www.miglayout.com
  BSD license: http://directory.fsf.org/wiki/License:BSD_4Clause
- JFreeChart. http://www.jfree.org/jfreechart
  LGPL license: http://www.gnu.org/licenses/old-licenses/lgpl-2.1.html

(No changes on the source codes of these libraries have been made, you can download the source codes for these libraries at their respective websites).

Contact information

Oriol Vallcorba
Experiments Division - MSPD Beamline (BL04)
ALBA Synchrotron Light Source - CELLS (www.cells.es)
Carrer de la Llum 2-26, 08290 Cerdanyola del Vallès, Barcelona (Spain)
Phone: +34 93 592 4363 e-mail: ovallcorba@cells.es

Conditions of use

This software can be used free of charge for non-commercial academic purposes only. For any other purpose, please contact directly with the author. Further distribution of this software is not allowed.

Citation of the author/program/affiliation would be greatly appreciated when this program helped to your work.

Disclaimer

This software is distributed WITHOUT ANY WARRANTY. The authors (or their institutions) have no liabilities in respect of errors in the software, in the documentation and in any consequence of erroneous results or damages arising out of the use or inability to use this software. Use it at your own risk.

The purpose of the database system implemented in the program is the creation of a personal compound database by the users. The authors of the program (or their institutions) take no responsibilities in respect of where the data is taken from or its correctness. The default DB is a small selection of 60 compounds coming from different sources. Each entry contains the reference from where it has been taken (with the respective authors). If any of these entries should be removed (for whatever reason) please contact the author and they will be removed immediately.

d2Dplot is programmed with Java™

Acknowledgements

Thanks are due the Spanish "Ministerio de Ciencia e Innovación" and to the "Generalitat the Catalunya" for continued financial support.

(document last revision on Nov 23, 2015)