



- User's Guide -

(for version 1611)

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 Economía y Competitividad", to the "Generalitat the Catalunya" and to ALBA Synchrotron for continued financial support (Project in course: MAT2015-67593P).

Contents

1. Installation and use of <i>d2Dplot</i>.....	4
Configuration file.....	4
2. Overview.....	5
3. Image menu modules.....	8
Instrumental parameters.....	8
LaB6 calibration.....	9
Excluded zones.....	10
Background subtraction.....	11
Radial Integration.....	13
Copper pressure calculator (for High Pressure experiments).....	13
4. Grain Analysis module.....	14
Find/Integrate Peaks.....	14
Load tts-INCO SOL/PCS files.....	15
Load XDS file.....	16
5. Phase ID.....	17
Database.....	17
6. Macro mode.....	21
7. Image formats info.....	23
D2D format.....	23
BIN format.....	23
EDF format.....	24
IMG format.....	24
GFRM format.....	24
SPR format.....	24
8. Other file formats info.....	25
Database (DB) format.....	25
Excluded zone (EXZ) format.....	25
9. Miscellaneous.....	26
Release notes.....	26
Contact information.....	26
Conditions of use.....	26
Disclaimer.....	27
Acknowledgments.....	27

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. Also you can use the *macro* mode to give instructions to operate the program through command line arguments (no GUI).

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

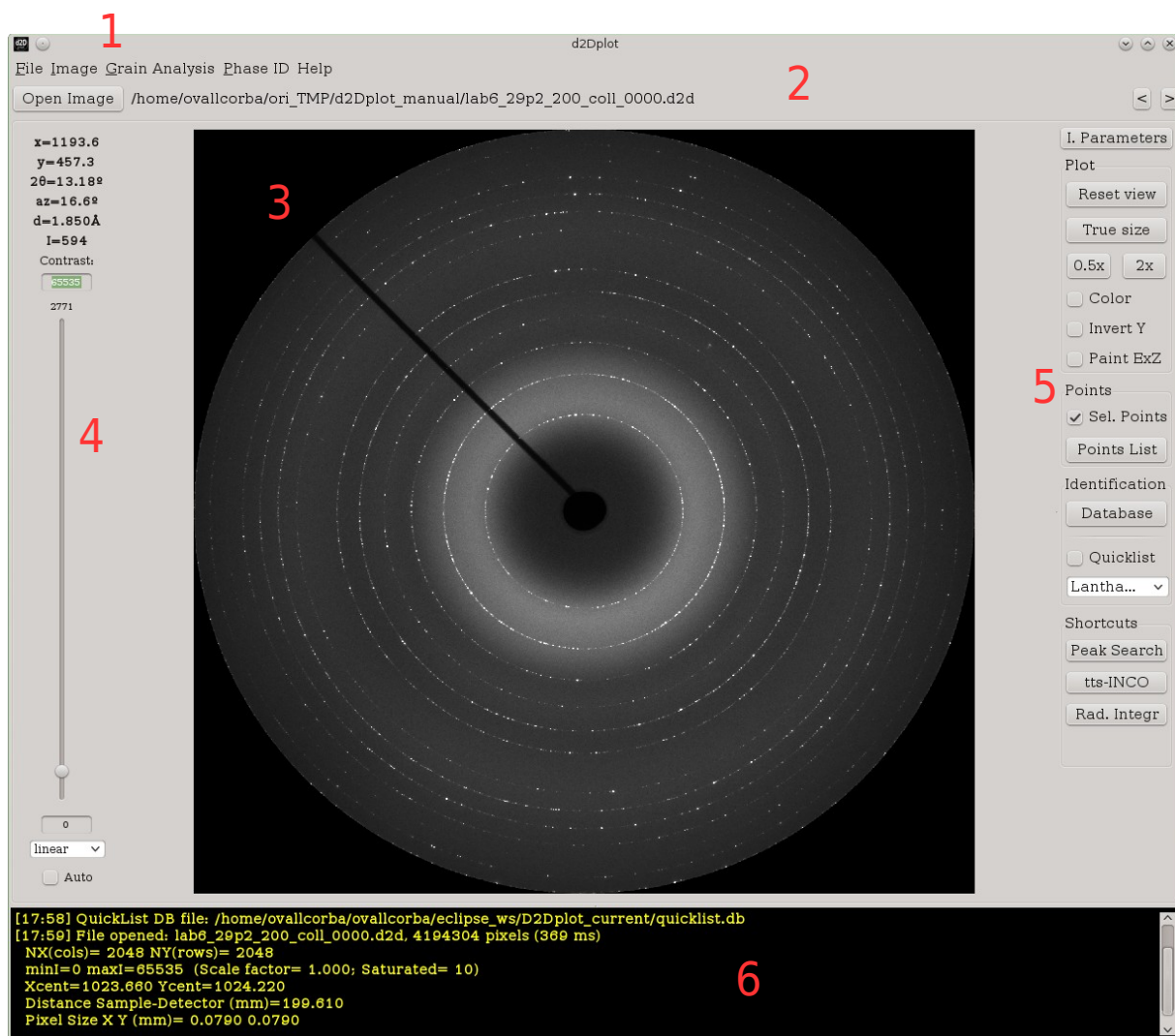
Configuration file

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 important parameters 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 where 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/Integrate 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).
- **Help**
 - **About.** Some information about the program.

- **Manual**. Link to this user's guide.

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 two 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... (depend on the opened module)
- Middle mouse button: Press and drag to move the image.
- Mouse wheel: Zoom.
- Right mouse button: Deletion. Press 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, peak search/integrate 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). **ExZ** = Excluded zones.
- 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.

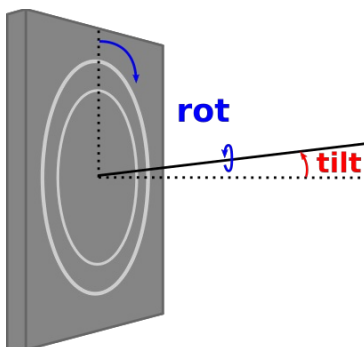
3. Image menu modules

Instrumental parameters

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

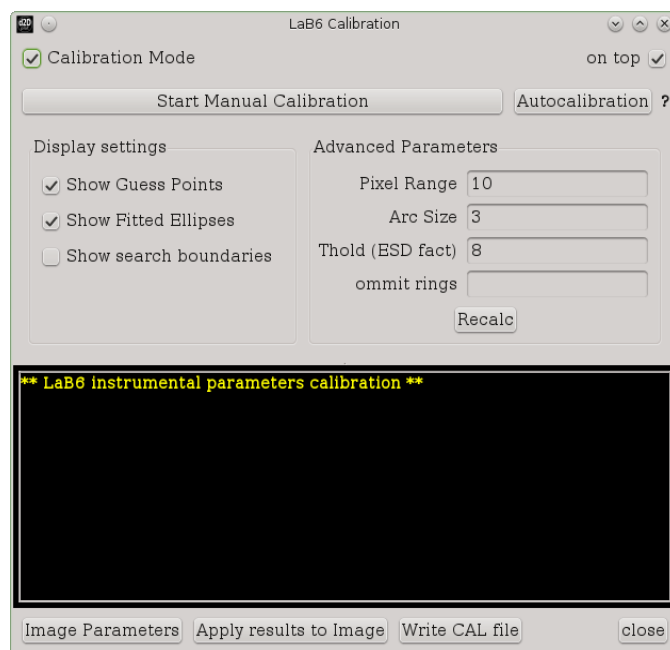
- Tilt: Deviation (angle) of the orthogonality of the beam direction.
- Rot: Clockwise rotation (angle) of a perpendicular axis taking as “zero” the vertical (i.e. 12h on a clock...).

(Better a drawing...)



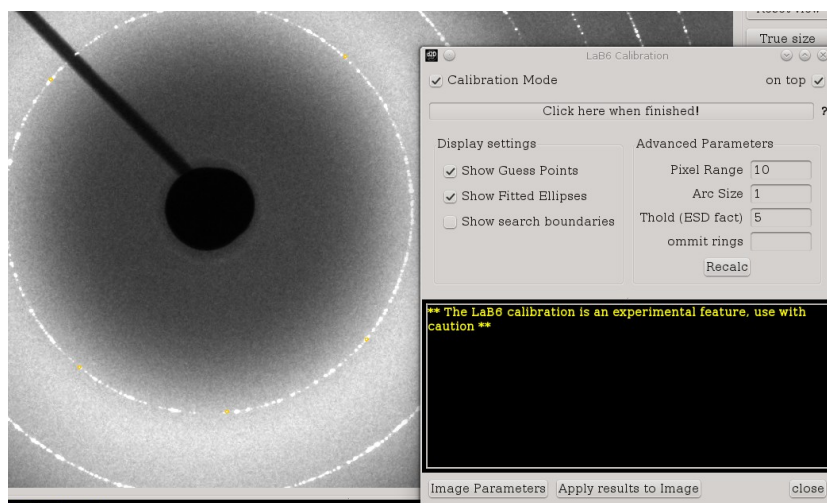
If *keep calibration info for the session* is selected, no calibration info will be read from the header of next opened images.

LaB6 calibration

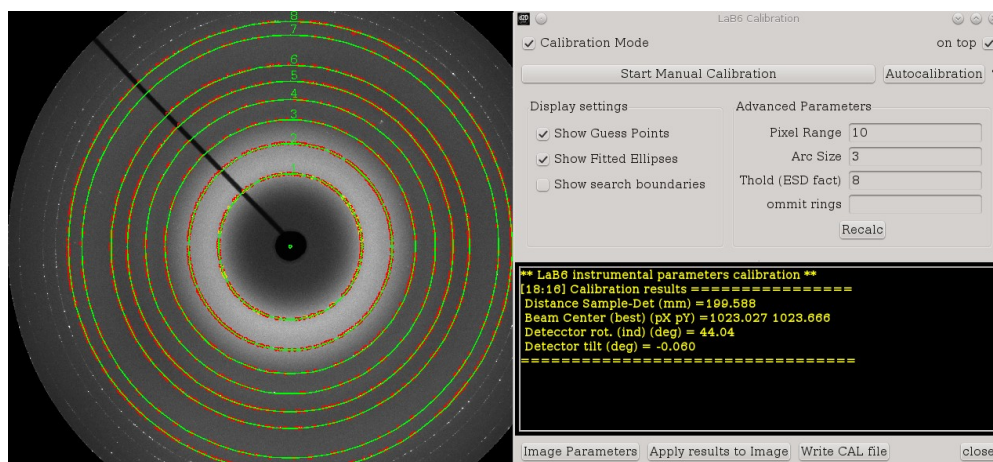


This module is for calibration of the sample-to-detector distance, the beam center and the detector tilt/rot angles from LaB₆ calibrant. This module has not been fully tested, use with caution and always check the obtained parameters. There are two options to do it:

- a) Click on Autocalibration. It will use the image header info (distance, wavelength, center, ...) as initial guess values to find the LaB₆ rings automatically. Try this method first.
- b) Select point on the first ring of LaB₆ manually:
 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

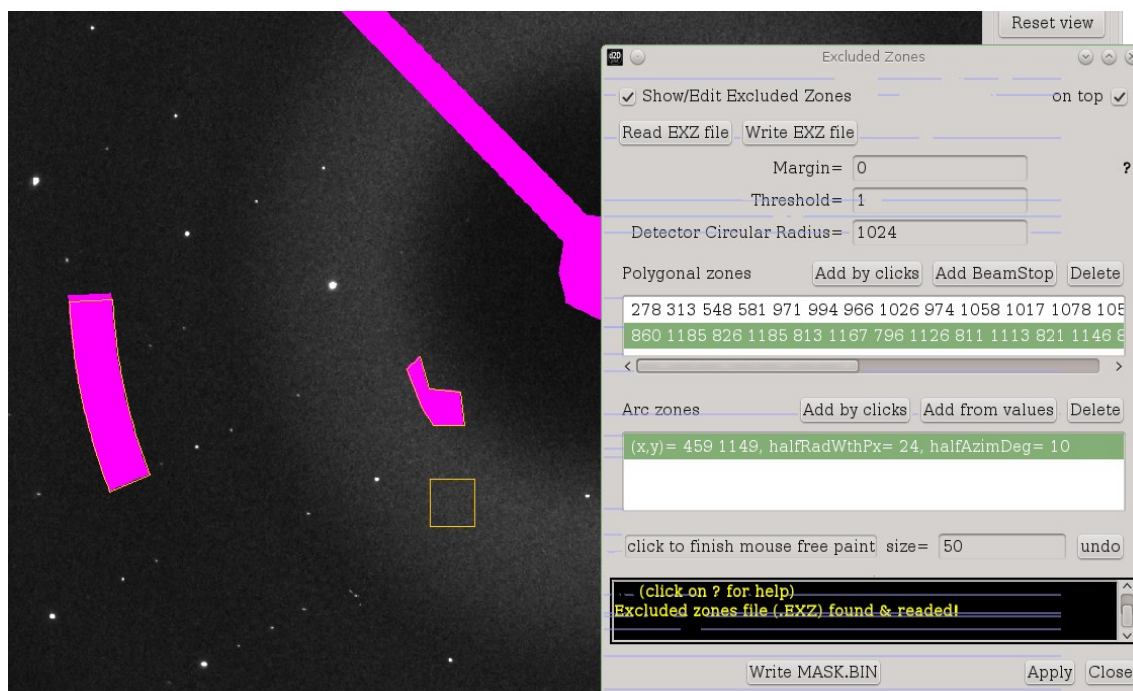


5. It can be repeated by clicking on the **Recalc** button (changing the parameters from the search rings if necessary).

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

Buttons below allow to apply the calibration results to the current image or write a CAL file to be used as calibration info for batch processing of images (and/or when the header info is not enough or correct).

Excluded zones



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

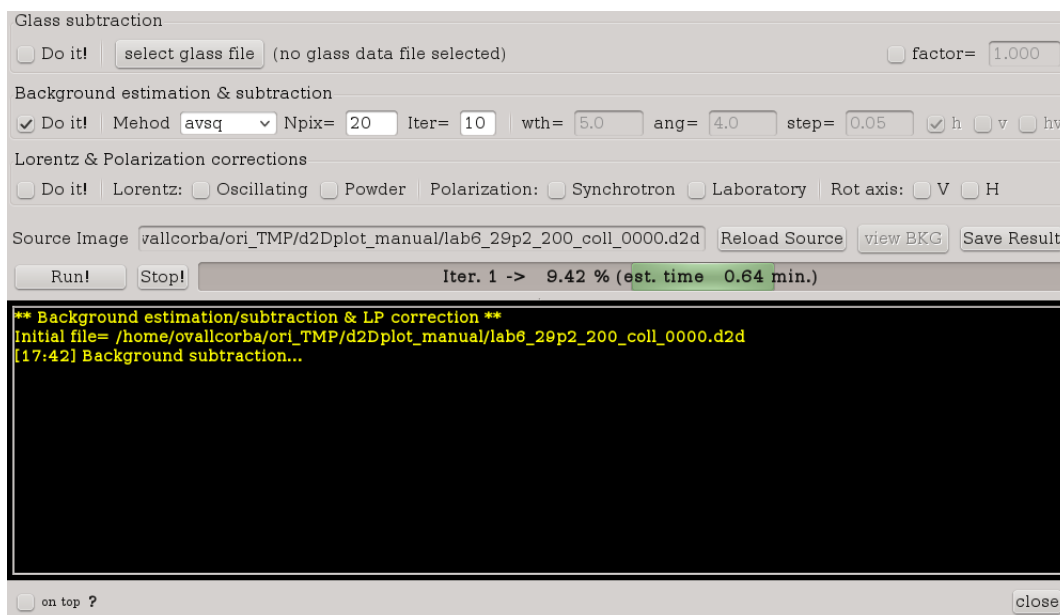
- Define a threshold such as if $Y < \text{Threshold}$ the pixel will be excluded
- Define a margin for the image (pixels on the borders to be excluded)
- Define a detector radius in case the detection area is circular.
- Add beamstop shaped excluded zone by giving a radius of the central part of the beamstop, a pixel inside the arm of the beamstop and the width of the arm.
- Add a polygonal excluded zone click ADD and click several points to define the zone.
- Add an arc-shaped excluded zone by clicking 3 points to define the zone in the following order: center, half radial width, half azimuth aperture. Adding this type of zones may be computationally slow.
- Paint with the mouse the zones you want to exclude by clicking **Mouse Free Paint** and left-click and drag with the mouse. You can select the size of the square-shaped “brush” and undo the last change with the button if desired.

After defining excluded zones, you may do one of the following:

- Save an Excluded Zones (ExZ) file to be loaded later and/or to apply the zones to other images.
- Save a MASK image, which is an image in BIN format with all the intensities at zero except for the mask pixels which have intensity -1.
- Save in a format (D2D, BIN) that contain the information.

On the main program window there is an option to show/hide the excluded zones, which are painted in magenta (paint ExZ) if activated.

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.

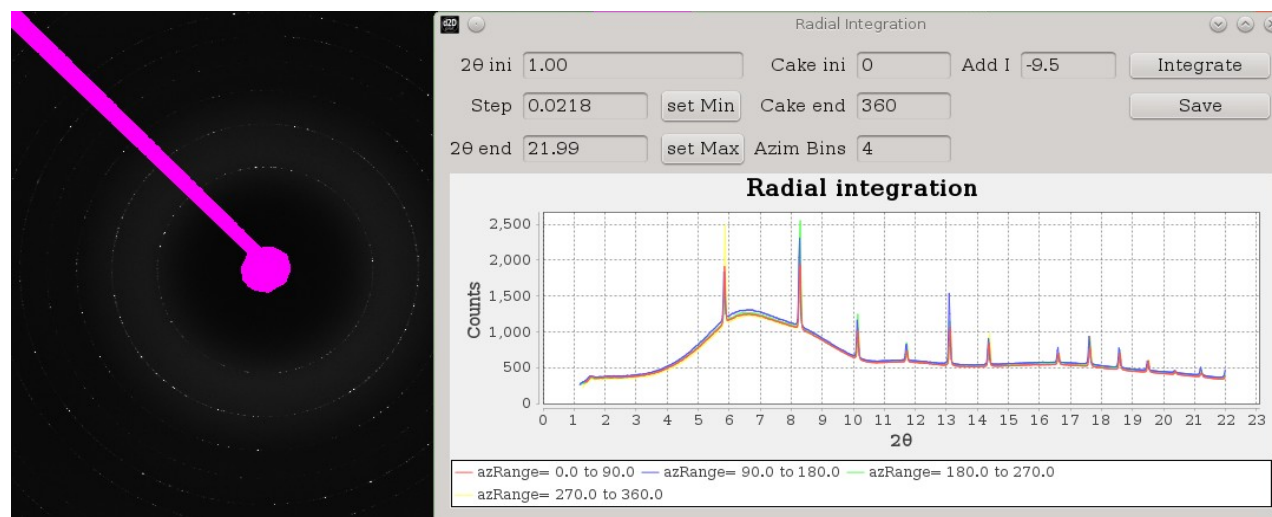
- minarc: The same as minsq but using an arc shaped zone for each pixel. Set the operations (v,h,vh) and the factors for width and angular aperture (wdt,ang).
3. The third one is to apply the corrections for Lorentz & polarization to the image pixels. Select the proper conditions (single grain oscillating/powder, 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

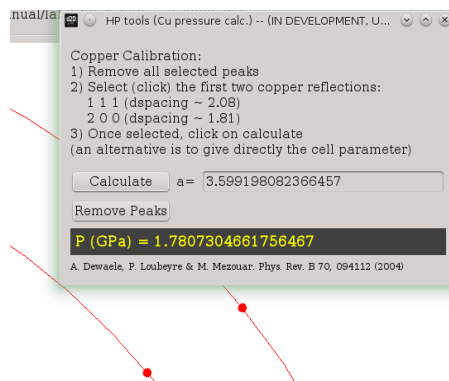


Give the range and conditions (fields are self-explanatory) to integrate the image. You can save it in a two columns file (2-theta intensity). Considerations:

- The cake ini/end units are degrees and starting from the vertical (12h. on a clock) going positive clockwise.
- Azim bins (usually will be 1) is to divide the cake in parts, so one pattern is generated for each part (check image above).
- Add I is to add intensity to the pixels of the image. It is useful in case the detector by default adds intensity to avoid zero. To subtract this extra intensity we need to

introduce a negative value here.

Copper pressure calculator (for High Pressure experiments)

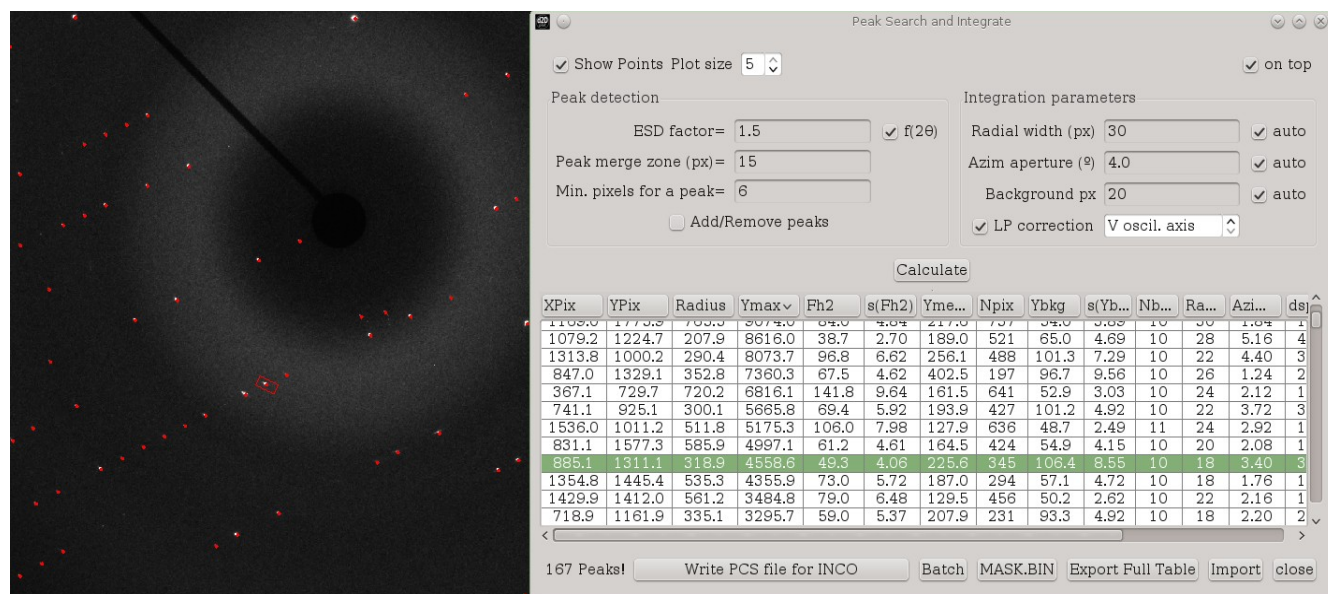


This module is still very preliminary and the only function it has implemented is the calculation of the pressure by the selection of two copper peaks (or alternatively directly from a given cell parameter).

4. Grain Analysis module

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

Find/Integrate Peaks



This one is probably one of the most important modules of d2Dplot. It finds and integrates spots on the image. The options for the peak detection are:

- ESD factor: It acts as a threshold related to the intensities standard deviation and optionally as a function of 2theta, useful when there are substrates producing circular backgrounds, e.g. glass
- Peak merge zone: to avoid very close peaks.
- Minimum number of pixels for a peak.

The integration options are:

- Radial width of the integration zone (in pixels). Can be set to auto.
- Azimuthal aperture of the integration zone (in degrees). Can be set to auto.
- Number of pixels to calculate the background. Can be set to auto.
- Lorentz correction according to the oscillation axis.

The results are shown on a table with a lot of information:

- XPix, YPix = Pixel coordinates.
- Radius = Center to pixel vector modulus.
- Ymax = Maximum intensity.

- $Fh2, s(FH2)$ = Integrated intensity and the associated standard deviation.
- $Ymean$ = Mean intensity.
- $Npix$ = Number of contributing pixels
- $Ybkg, sYbkg$ = Background intensity that has been subtracted and its standard deviation.
- $Nbkg$ = Number of background pixels used for the background estimation.
- $RadWth$ = Radial width in pixels of the integration area.
- $AzimDeg$ = Azimuthal aperture in degrees of the integration area.
- dsp = d-spacing of the spot.
- $p = \pi \cdot (ymax/yint)^{2/3}$
- $Swarm$ = If the peak has more than one maximum of intensity (may be overlap?)
- $Satur$ = If the peak contain saturated pixels (indicates the number).
- $nearMsk$ = True if the peak is close to a mask zone.

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

Checking add/remove peaks, additional peaks can be added or removed by clicking with the left or right mouse button respectively. They are automatically integrated.

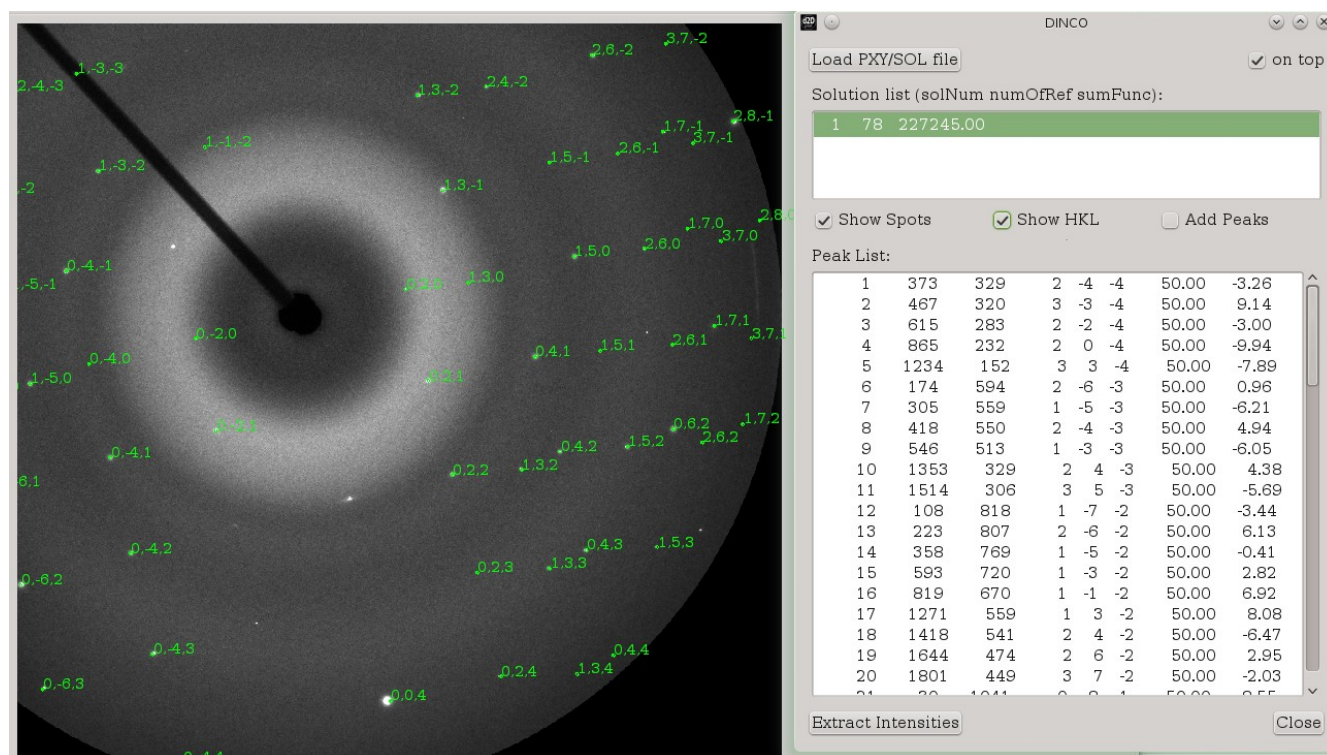
The peak list and intensity info can be exported as:

- PCS file to be used in tts-INCO program.
- A text file containing all the information of the table.

With the batch button several images can be processed using the same peak detection and integration parameters. Also, if the image on the main frame is changed (for example with the arrows on the top to navigate images), the peak search module is not closed and can be used to integrate directly the new image.

Load tts-INCO SOL/PCS files

Here the output files from 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/integrate peaks** will be opened.

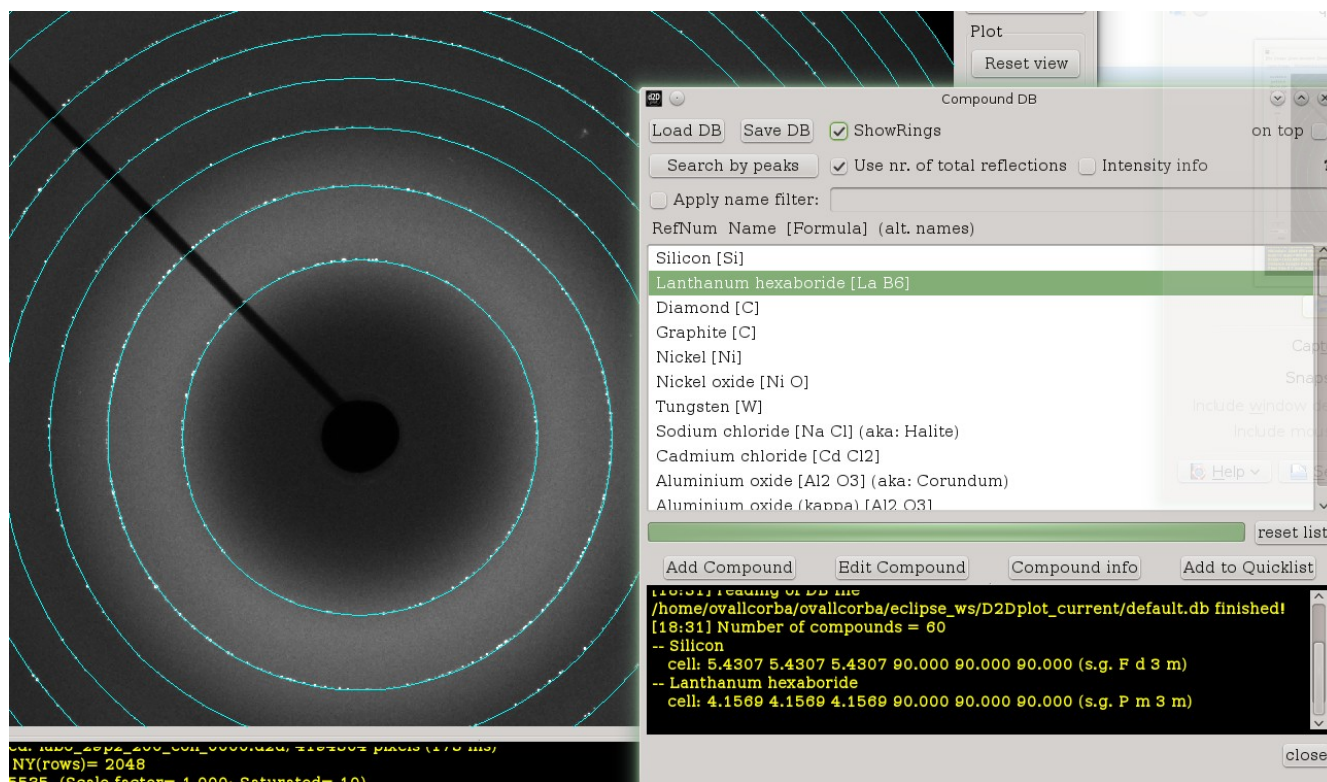
Load XDS file

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.

Name: Lanthanum hexaboride

Name (alt):

Formula: La B6

Cell parameters: 4.1569 4.1569 4.1569 90.000 90.000 90.000

Space group: P m 3 m

Reference: National Institute of Standards and Technology

Comment:

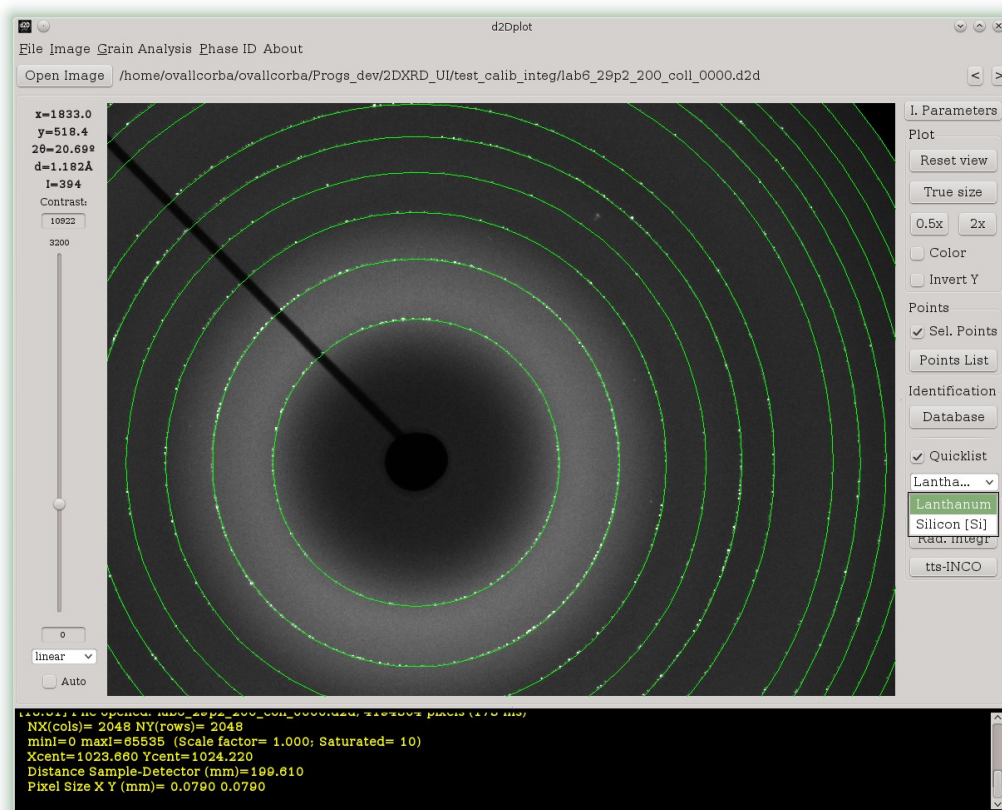
list of (one per line): h k l d-spacing intensity

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	4.19

import HKL

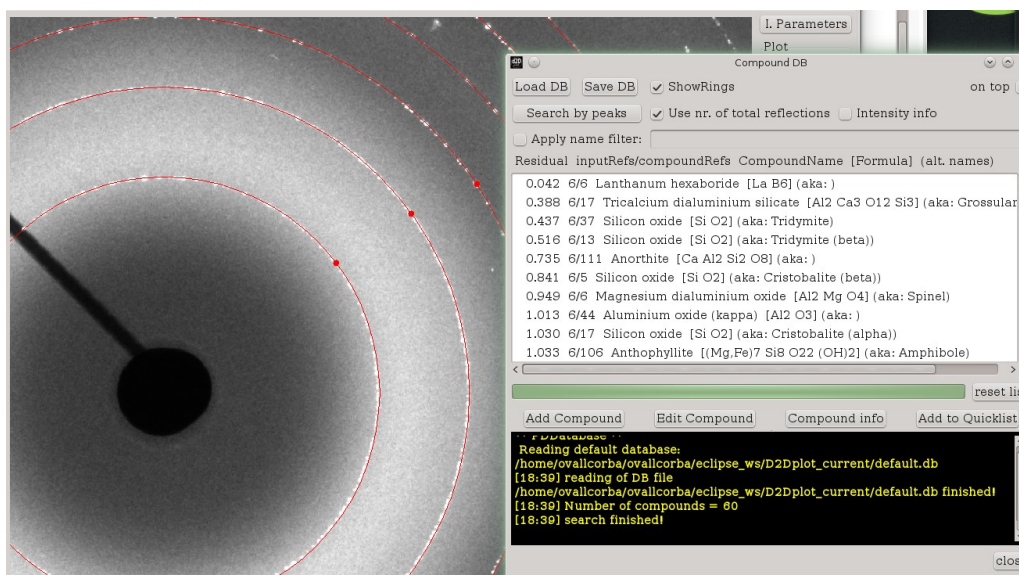
Remove Save Changes Cancel

- 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

6. **Macro mode**

This is a very recent feature of the program. It is the way to make the program do some operations to images and get directly the output, without opening any GUI if possible. The *macro* mode can be accessed via the command line. It is accessed by entering *-macro* as first argument when launching the program from the command line followed by the filename to the image to be processed. Then following arguments are available:

-sol

Displays directly a tts-inco SOL file (same filename as the input image).

-rint [CALfile] [-outdat DATfile]

Performs radial integration.

If no CALfile is specified, calibration parameters are taken from the image header.

If no DATfile is specified, same name as the input image (but .dat) is used.

-cal [dist] [wave] [-outcal [CALfile]]

LaB6 calibration.

If no dist or wave are specified they are taken from the image header.

Add *-outcal* option to generate a CAL filename with the same name as the input image as long as no CALfile is specified.

-show

To open graphical display and do not exit after processing.

(if the first argument is *-help* then the different options are listed)

(as it has been said before, if the only command line argument is a path to an image it will be opened directly)

Examples:

```
./d2Dplot -macro lab6_180_0003.edf -cal 180 0.3187 -outcal lab6_180.cal
```

```
Running on Unix or Linux
[19:25] 10 vava33.d2dplot.D2Dplot_global [CONFIG] ** LOGGING DISABLED **
Console logging DISABLED
[19:28] MACRO MODE ON
[19:28] Reading img file: lab6_180_capillary_0003.edf
[19:28] CAL option found, performing LaB6 calibration
[19:28] Using entered distance 180.000
[19:28] Using entered wavelength 0.3187
-----
[19:28] REFINEMENT RESULTS:
-----
CenterX=1023.43250
CenterY=1023.45001
S-D_distance=181.57628
ROT=35.75453
TILT=-1.25287
-----
[19:28] Writting output CAL file: lab6_180.cal
```

```
./d2Dplot -macro lab6_180_0003.edf -rint lab6_180.cal
```

```
Running on Unix or Linux
[19:25] 10 vava33.d2dplot.D2Dplot_global [CONFIG] ** LOGGING DISABLED **
Console logging DISABLED
[19:26] MACRO MODE ON
[19:26] Reading img file: lab6_180_0003.edf
[19:26] RINT option found, performing Radial Integration
[19:26] Using integration parameters from CAL file: lab6_180.inp
[19:26]
[19:26]   x-beam center: 1023.430
[19:26]   y-beam center: 1023.450
[19:26]   distance:      181.576
[19:26]   wavelength:   0.3187
[19:26]   tilt rotation: 35.8
[19:26]   angle of tilt: -1.25
[19:26]
[19:26]   t2ini:      0.000
[19:26]   t2fin:      23.866
[19:26]   stepsize:   0.0236
[19:26]   start azimuth: 0.0
[19:26]   end azimuth: 360.0
[19:26]   subadu:    -9.5
[19:26]
[19:26] Writting output DAT file: lab6_180_0003.dat
```

7. 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
EXZdetRadius=1024
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
EXZarc1=1325 1067 52 14
EXZarc2=507 1167 33 8
}
```

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 Y (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).
```


8. 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=0
EXZdetRadius=1024
EXZpol1=997 581 889 385 646 530 847 510 855 592
EXZarc1=1325 1067 52 14
!
! EXZmargin      Margin of the image in pixels (if any)
! EXZthreshold   Pixels with Y<threshold will be excluded
! EXZdetRadius   To exclude corners of the image in case detection area is circular(radius in px)
! EXZpol#        Sequence of pixels (X1 Y1 X2 Y2 X3 Y3...) defining a polygonal shape
! EXZarc#         Arc-shape defined as: ArcCenterX ArcCenterY ArcHalfRadialWthPx ArcHalfAzimWthDeg
```

9. Miscellaneous

Release notes

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 lot since then (although I could not dedicate as much time to it as I would like...) and while it remains basically a tool to visualize diffraction images I find it useful and interesting for a general usage.

Feedback to the author would be greatly appreciated. Also, if you find interesting to add a certain functionality it can also be considered.

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™

Acknowledgments

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

Copyright © Oriol Vallcorba 2016

(document last revision on Nov 17, 2016)