- User's Guide -

(for version 1805)

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d2Dplot is programmed with Java™

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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. 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).

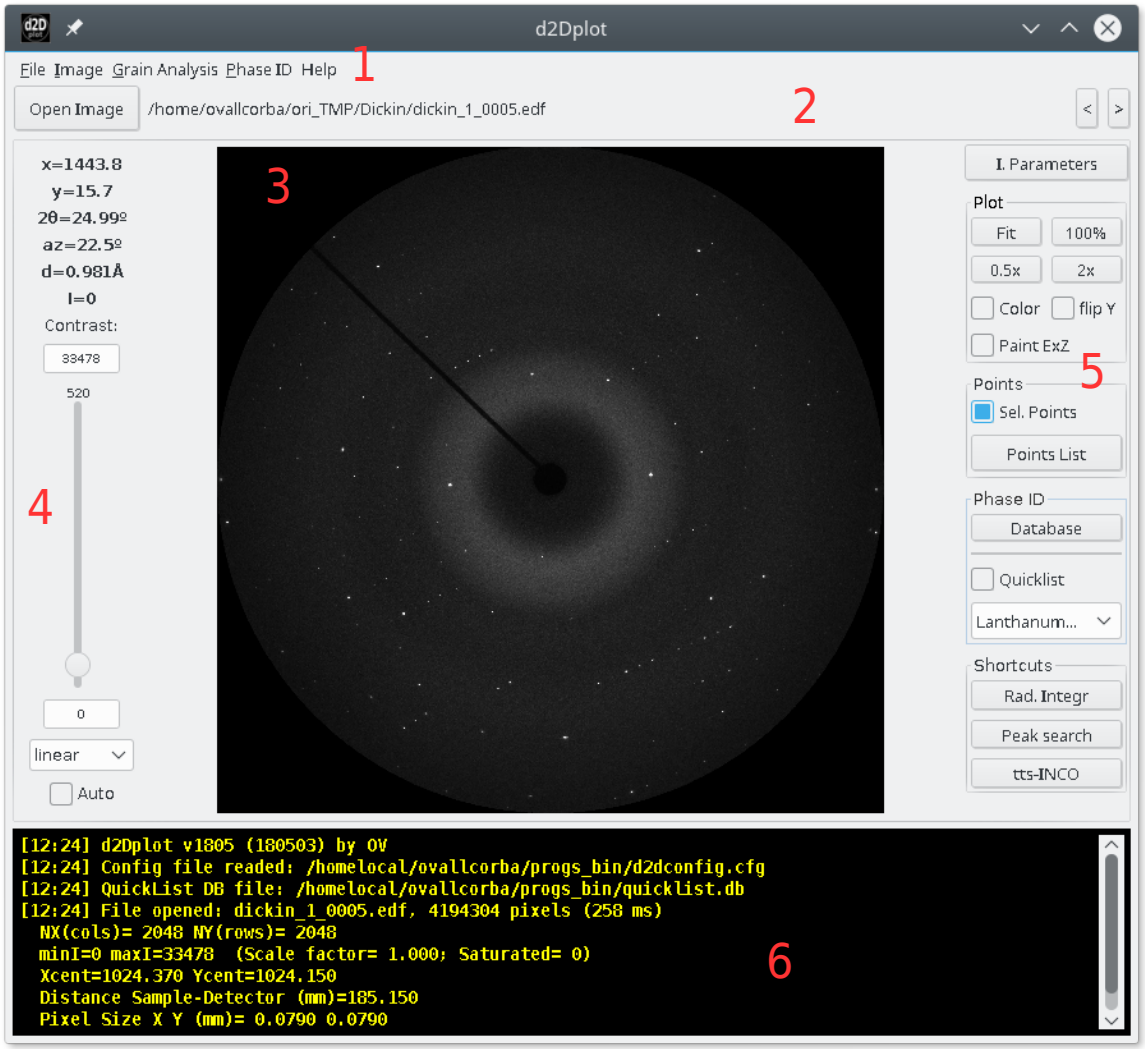
Configuration file

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 most important parameters are the default paths to the compound databases (`defQuickListDB` and `defCompoundDB`) which can be modified according to our preferences.

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.
- `Fast Viewer`. To open a series of images to be displayed sequentially.
- `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.
  - `Azhimuthal Integration.` To get the 1D pattern corresponding to a azhimuthal 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`**
  - `Find/Integrate Peaks`. Locate diffraction peaks on the image.
  - `Load tts-INCO SOL/PCS files.` Open the files generated by tts-INCO or tts-REDUC programs to check the correctness of single grain orientations (Rius *et. al.* 2015, 2016).
  - `Load XDS file.` Open a spot.xds file from XDS (**X**-ray **D**etector **S**oftware, CCP4; Kabsch, 1988) to show the position of the peaks.
  - `SC data to INCO.` Convert single-crystal dataset (small angular step) to a wider step angle format for INCO.
  - `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 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... (depend on the opened module)
- Middle mouse button: Press and drag to move the image. Click with no movement to fit the image to the display area.
- 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:

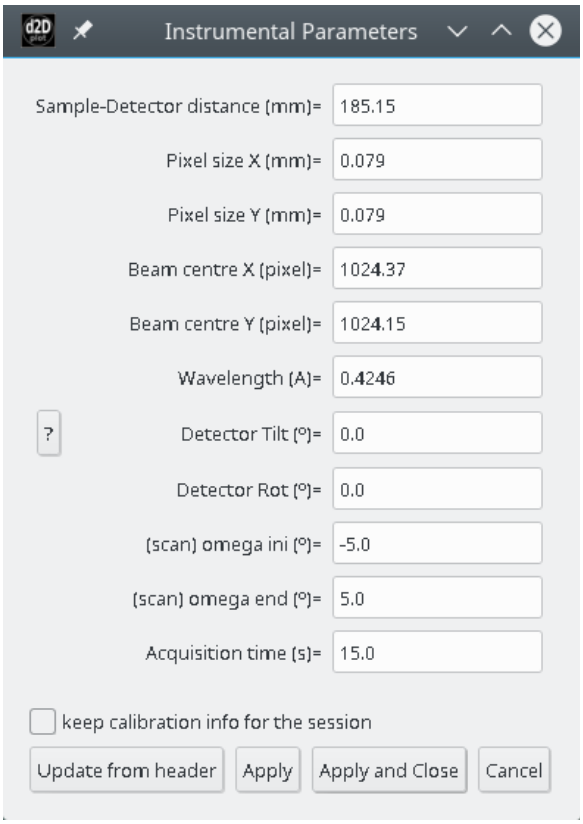
- Shortcuts for the instrumental parameters, radial integration, grain analysis, peak search/integrate and compound database.
- Plotting options regarding the image display (`100%` means that a pixel of the screen corresponds to a pixel of the image). ExZ = Excluded zones.

- 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

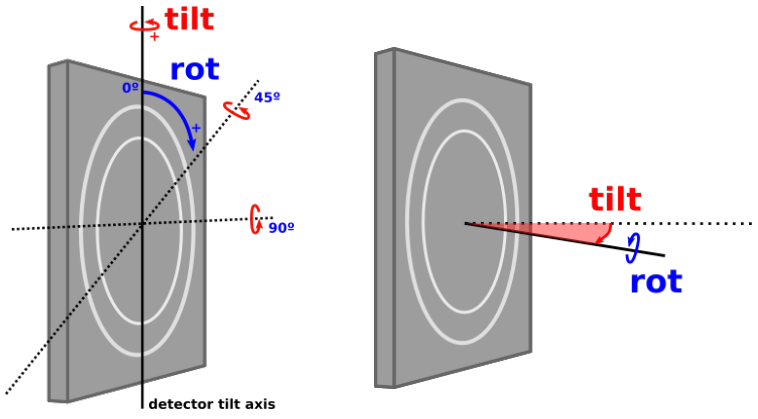
Instrumental parameters



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...)

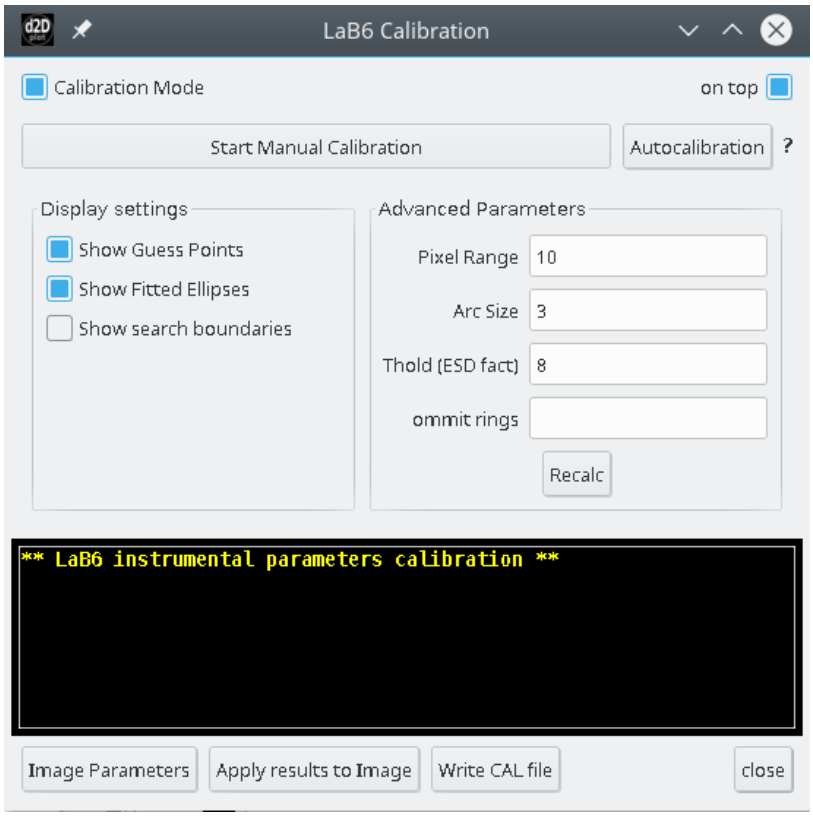


The convention used is compatible with calibrations with *Fit2D* program (Hammersley, Svensson & Thompson, 1994).

In the "?" dialog, a simulated LaB_6 diffraction image can be generated entering custom calibration values.

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

LaB6 calibration

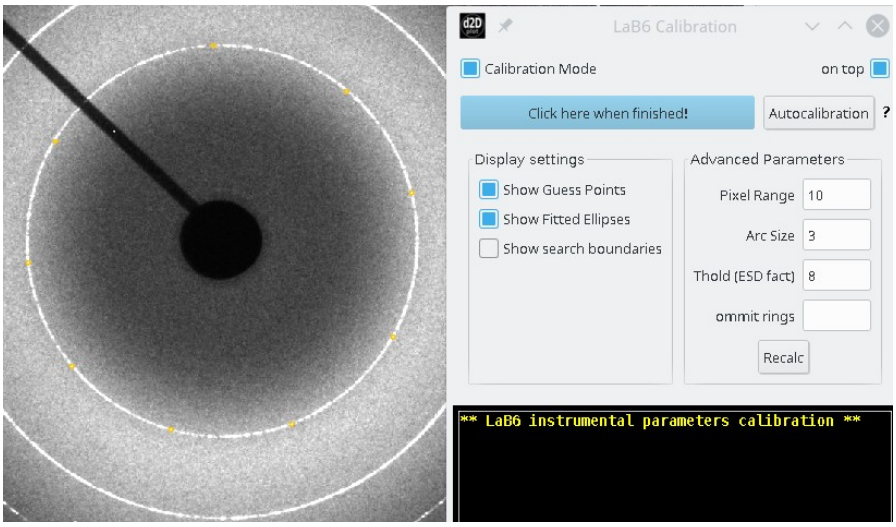


This module is for calibration of the sample-to-detector distance, the beam center and the detector tilt/rot angles from LaB_6 calibrant. There are two options to do it:

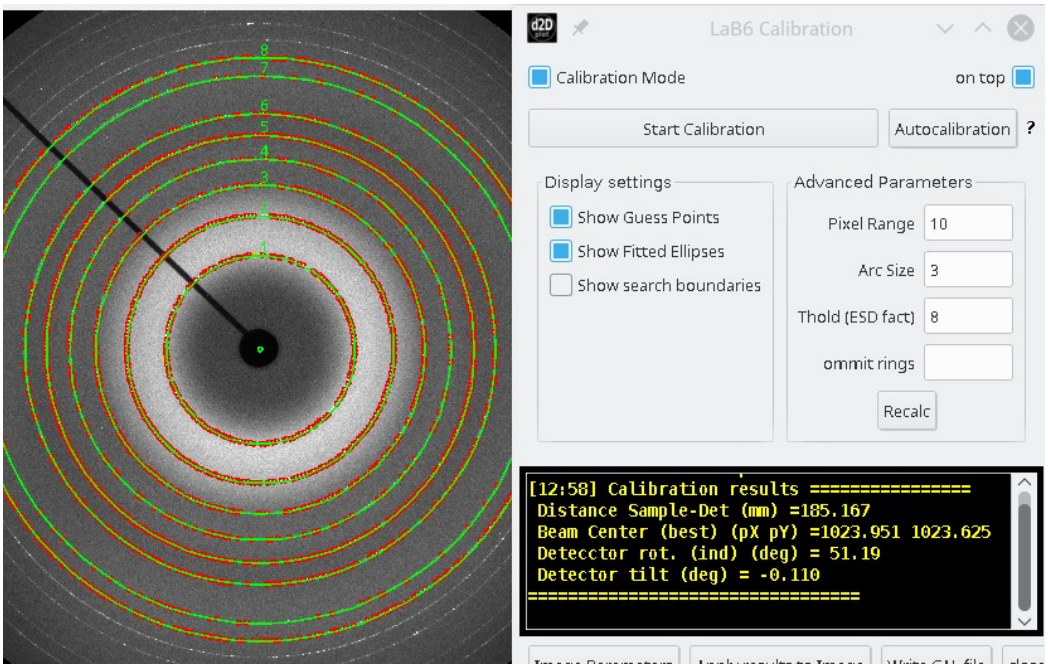
a) Click on `Autocalibration`. It will use the image header info (distance, wavelength, center, ...) as initial guess values to find the LaB_6 rings automatically. Try this method first.

b) Select point on the first ring of LaB_6 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

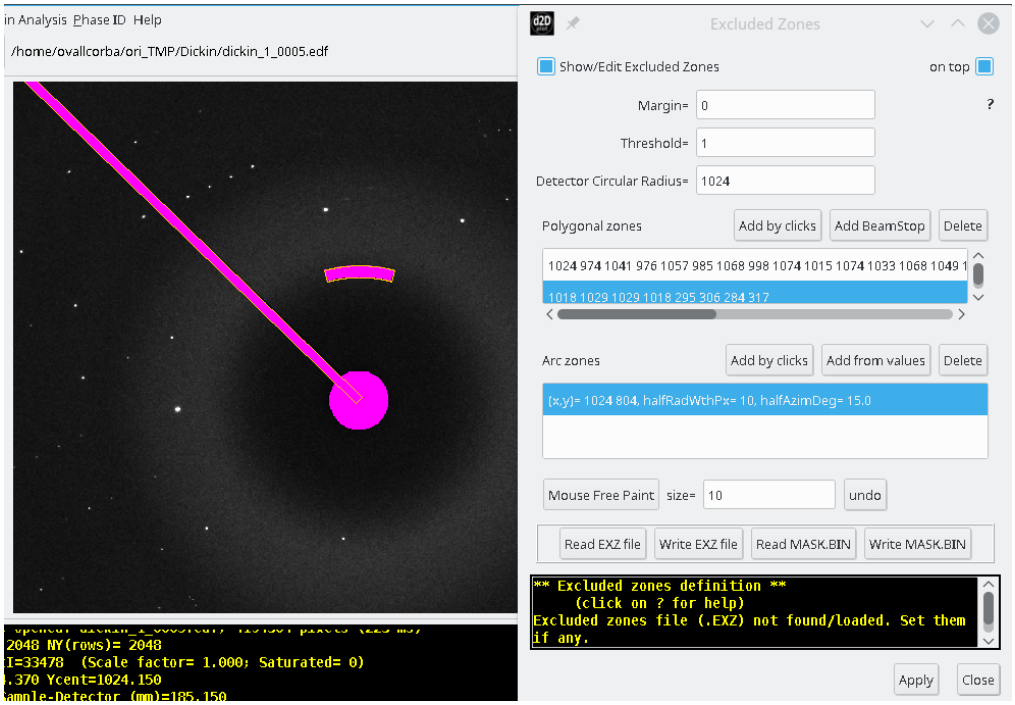


5. It can be repeated by clicking on the `Recalc` button (changing the parameters from the search rings if necessary).

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<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 azimuthal aperture.
- 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:

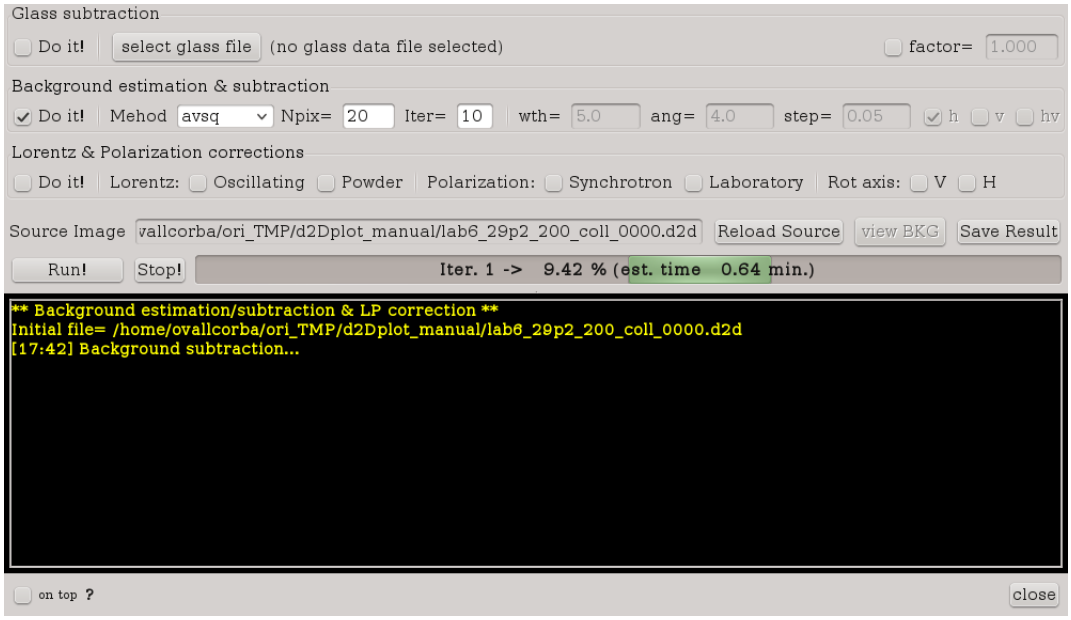
- Save an Excluded Zones (ExZ) file to be loaded later and/or to apply the zones to other images.
- Save a MASK image, which is an image in BIN format with all the intensities at zero

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.

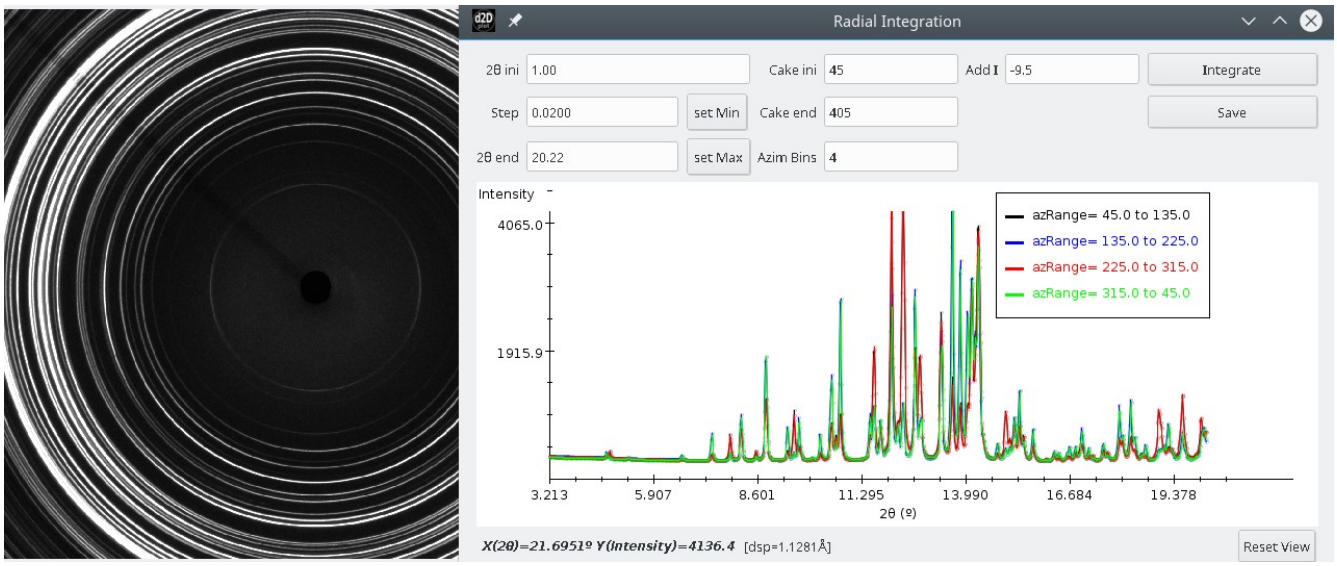
Visual inspection for residual peak intensity in the subtracted background can be done by clicking the [view BKG] button. Result images can be seen on the main window and source image can be reloaded if wanted. It is recommended to save the result to an image file before applying more corrections to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

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

Radial Integration

It performs the radial integration of the diffraction image given a 2-theta range and conditions (fields are self-explanatory). Result can be saved in a two columns file (2-theta intensity). Considerations:

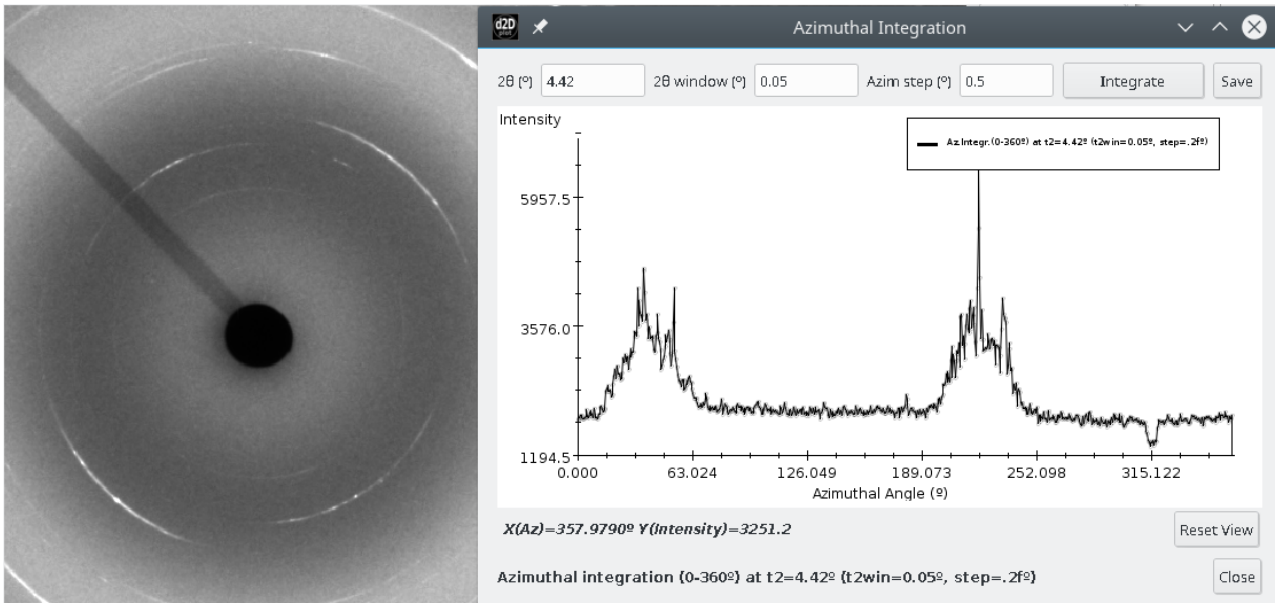
- The cake ini/end units are degrees and starting from the vertical (12h. on a clock) going positive clockwise.
- Azim bins (usually will be 1 for the full integration) is to divide the full integration (caki ini/end) in different cake fragments, so one pattern is generated for each part (check image above). It may be used to check for homogeneity or texture.
- 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.



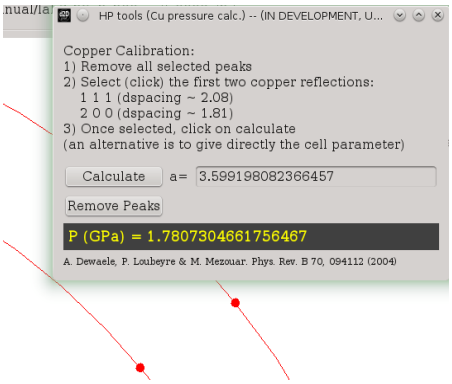
Information for the radial integration methodology and geometrical corrections can be found on Hinrichsen, Dinnebier & Jansen, 2008; as the methodology implemented in d2Dplot follows the definitions on the book.

Azimuthal Integration

It performs an integration along the circle (or ellipse if detector tilt is not zero) specified by a 2-theta value with a tolerance (2-theta window) and an angular step (azim step). It is useful to check for graininess and for texture in powder samples.



Copper pressure calculator (for High Pressure experiments)

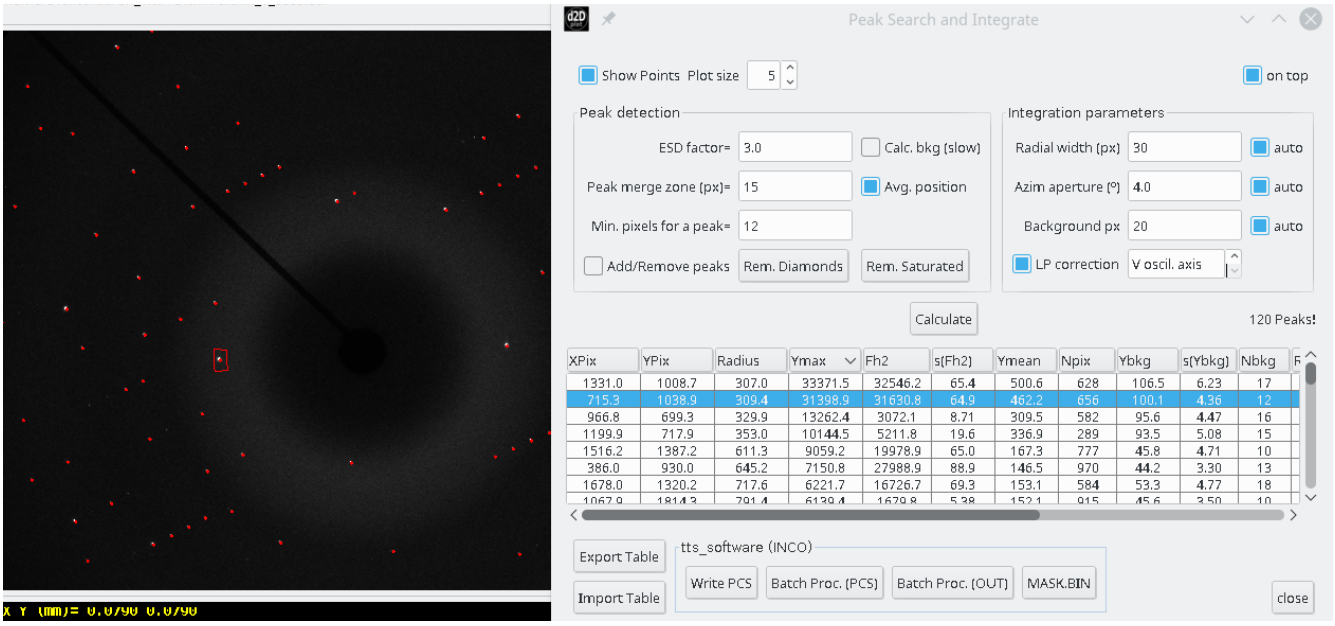


This module is still very preliminary and the only function it has implemented is the calculation of the pressure by the selection of two copper peaks (or alternatively directly from a given cell parameter).

4. Grain Analysis module

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

Find/Integrate Peaks



This is an important module of *d2Dplot* for the *TTS_software* interaction. 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 it can estimate the background for a better detection (it is slower).
- Peak merge zone: to avoid very close peaks. Avg. position means that when the merging is done it is taking the mass center of the peaks as the final peak position.
- Minimum number of pixels for a peak.
- By 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.
- Remove Diamonds tries to detect and remove the peaks coming from diamonds in case of Diamond Anvil Cells.
- Remove Saturated removes the saturated spots from the list.

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.

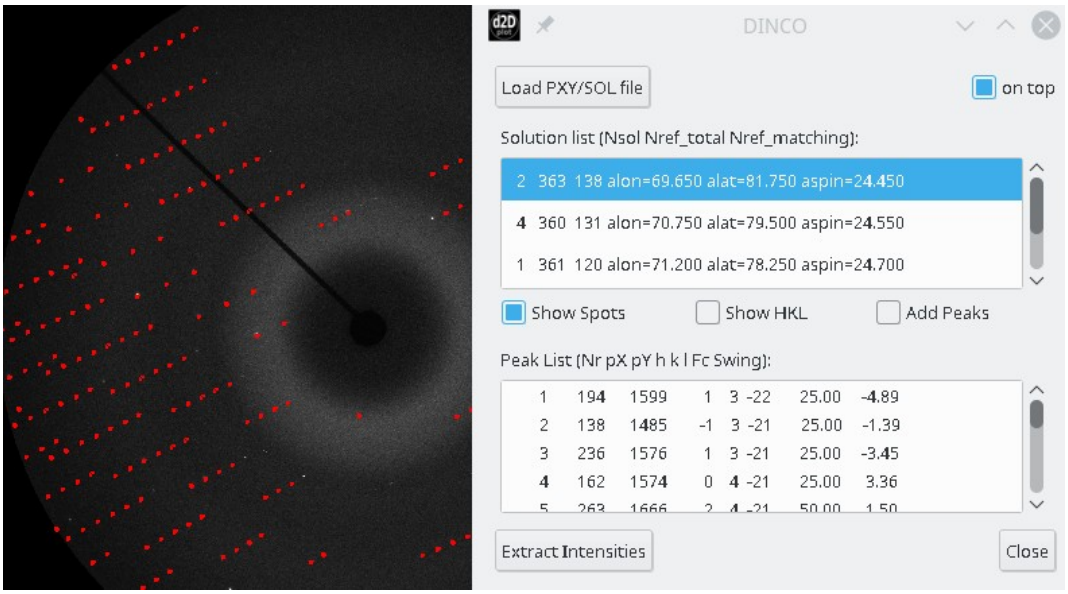
The peak list and intensity info can be exported as:

- A text file containing all the information of the table (it can be imported back).
- PCS file to be used in *tts-INCO* program (Rius *et. al.* 2015, 2016).

With the batch button several images can be processed using the same peak detection and integration parameters. The batch PCS generates an individual PCS file for each of the processed images. The batch OUT generates only one file containing the information of all the processed images. 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).



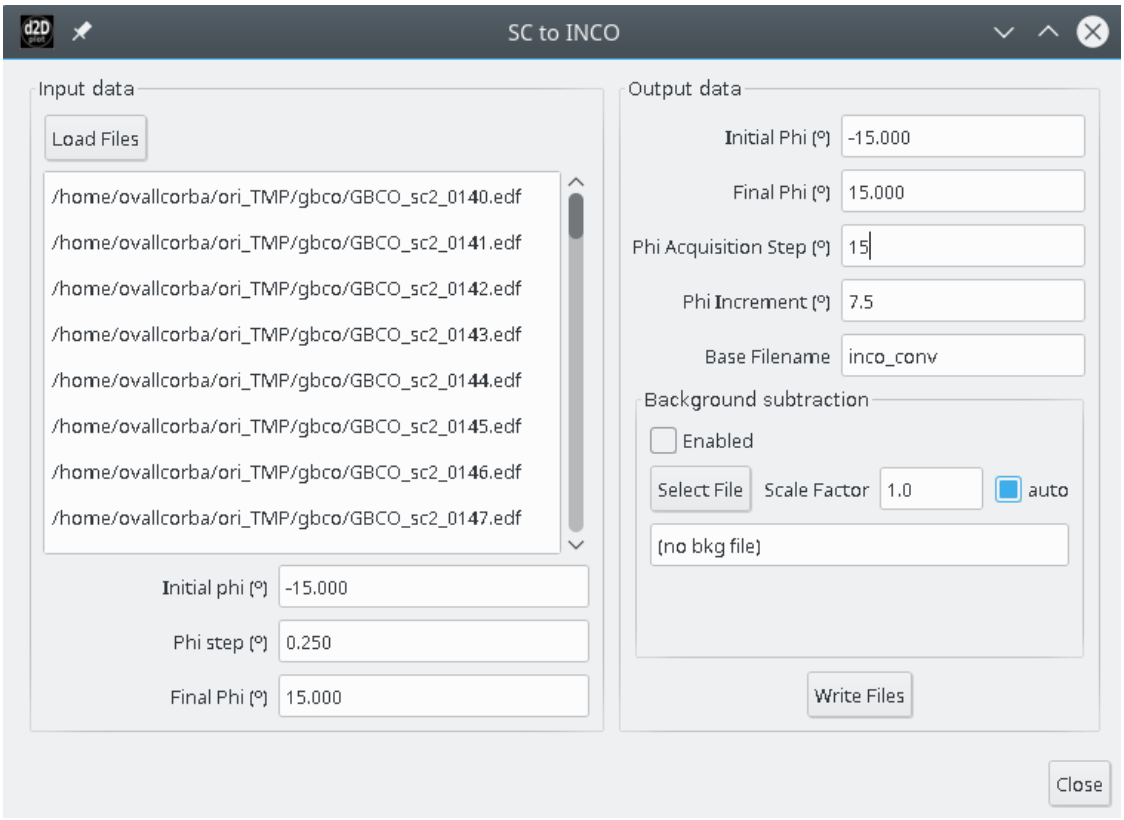
Also the peaks can be integrated by clicking `extract intensities` and a window equivalent as the one in find/integrate peaks will be opened.

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; Kabsch, 1988).

SC data to INCO

This option is used to sum image files specifying ranges of measurement.

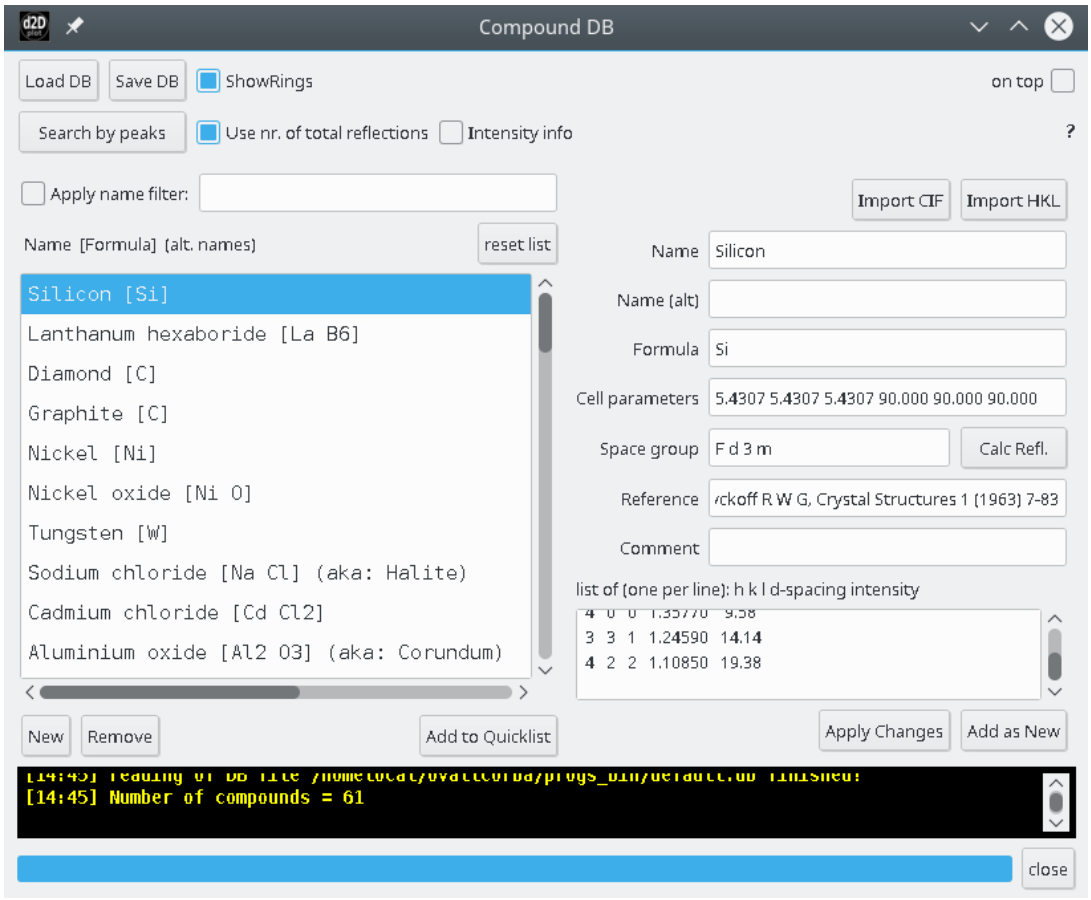


For example, taking single crystal data collected from -15º to 15º rotation with steps of 0.25º (120 images), it can be converted to 3 images of 15º rotation each with overlapping of 7.5º. In this case, 3 images will be generated: 1) data from -15 to 0º; 2) data from -7.5 to 7.5º; 3) data from 0 to 15º. Usually if you have single crystal data there is no need to perform any sum of the data, this is only intended in case tts_INCO wants to be used for any specific reason or to check data by performing other combinations of sums. Optionally, a background file can be subtracted to all the individual files before adding them up.

5. Phase ID

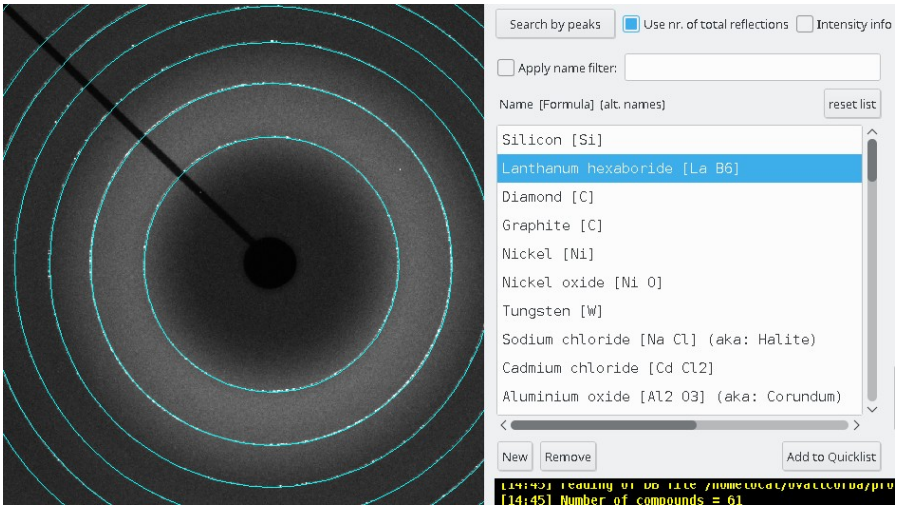
This is a strong part of *d2Dplot* which allows the fast identification of compounds from a custom database. There are two different "compound databases" considered in the program (actually lists will be the correct term to refer to them and not database). The full database, which is accessed via `Phase_ID - 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

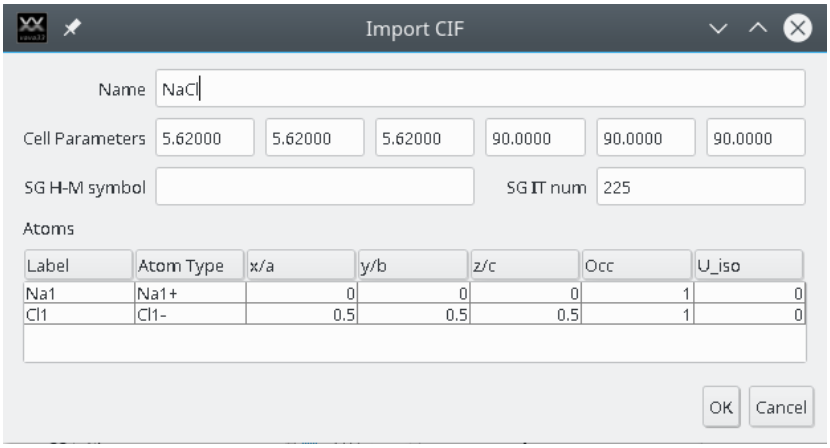


Here a plain-text DB file can be loaded. By default it opens the file `default.db` (which is in the program folder) as the example one coming with *d2Dplot*. Once loaded:

- Click on any compound to see the expected diffraction rings position on the image (if `ShowRings` is selected)

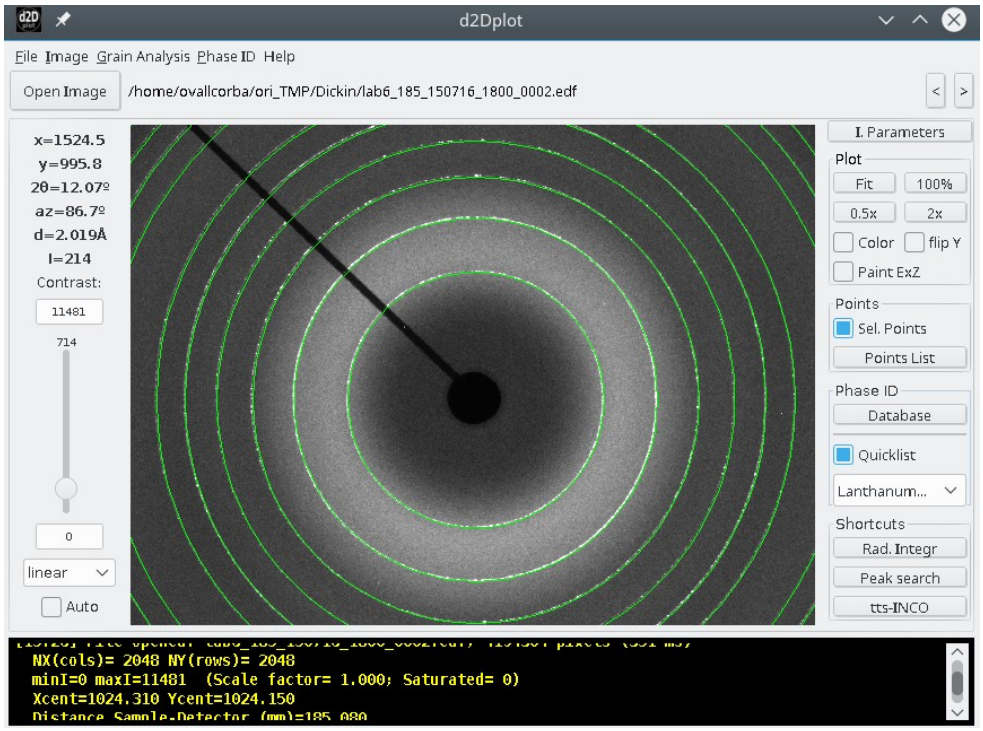


- Check `apply name filter` and type to easily find the desired compound
- Any selected compound may be edited from the fields on the right section of the window and clicking `apply changes` to update it or `add as new` to copy it as a new entry. Also new compounds may be added or removed by clicking `new` or `remove`. For new compound the information should be introduced. If the unit cell and space groups are known, the expected reflection positions can be calculated with `calc Refl` and the hkl list will be updated automatically. Alternatively, an HKL file or a CIF file can be imported. For CIF files, the hkl list (with calculated structure factors) will be automatically generated taking the cell parameters, symmetry and atom positions from the file. A confirmation window will show the information retrieved from the CIF to check for correctness.



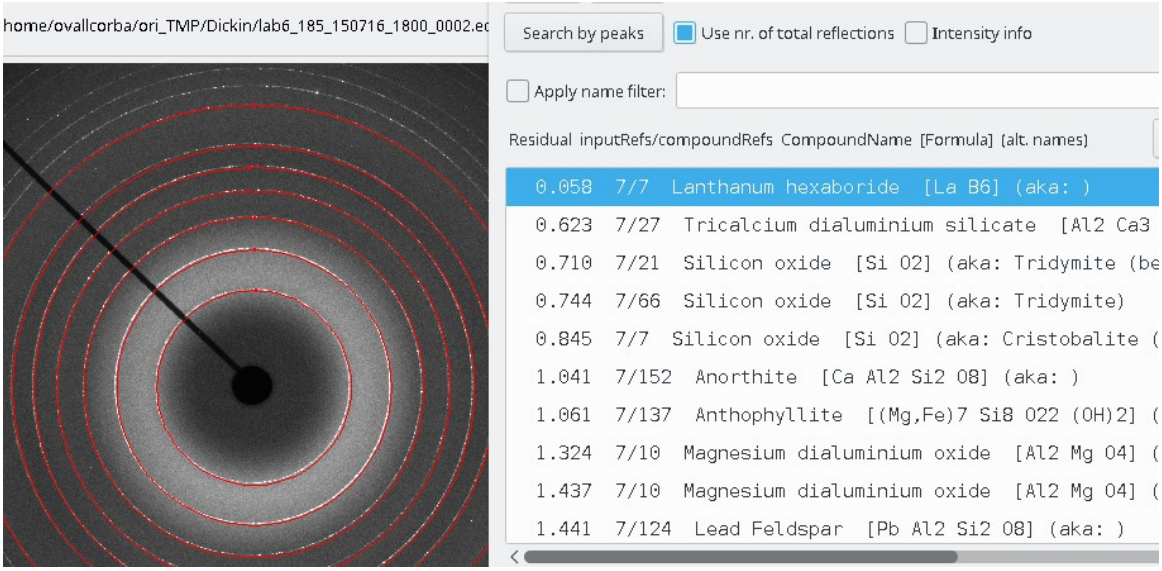
- Alternatively you can edit manually the DB file. It is a simple self-explanatory text file and its format is explained in another section of this guide.

- `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



There is the possibility to search in the database by image peak positions (selected on the main image window by the select points tool). 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 there is a good 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). 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 from the `reference` field on each entry of the database. If any of these entries should be removed (for whatever reason) please contact the author and they will be removed immediately.

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 azim: 0.0
[19:26]    end azim:   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 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 [Arvai, A. J., & Nielsen, C. (1983). ADSC Quantum-210 ADX]. 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, A. X. S. Area Detector Frame Format [e.g. GADDS detector, Bruker, A. X. S. "General Area Detector Diffraction System (GADDS) User Manual." *Madison, WI* 4 (1999)]

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).
```

TIFF format

TIF image format.

CBF format

DECTRIS Pilatus (Henrich *et al*. 2009) image format.

[https://www.dectris.com/technical_pilatus.html?.../pilatus/]

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. References

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B. Hinrichsen, R. E. Dinnebier & M. Jansen. Two-dimensional Diffraction Using Area Detectors. In: *Powder diffraction: theory and practice* (Royal Society of Chemistry, 2008).

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J. Rius, O. Vallcorba, C. Frontera. *TTS_software: A computer software for crystal structure analysis from tts microdiffraction data*. Institut de Ciència de Materials de Barcelona, CSIC, (Spain) **2016**. Available at http://departments.icmab.es/crystallography/software.

10. 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 develop the technique. The program has grown a lot since then, and while it remains basically a tool to visualize diffraction images it may be useful and interesting for a general usage. This is why after a little polishing it has been made available for use.

Feedback to the author would be greatly appreciated. Also, if you find interesting to add a certain functionality ask me and I will try my best.

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).

Major recent changes:

- 1805. Redesigned database module for easier editing. Added import CIF and the possibility to calculate the reflections from symmetry..
- 1805. Added Azimuthal integration, fast viewer and SC to INCO.
- 1805. Changed convention of tilt/rot.
- 1805. Improved peak integration (added background support).
- 1704. Reading of TIFF and CBF formats.
- 1704. Save PNG with scale factor and image “drawings”
- 1704. Read/write tilt and rot from/to EDF headers.

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
- ImageJ 1.50i. https://imagej.nih.gov/ij/index.html
  Public-domain: https://imagej.net/Licensing.
  CBF reader plugin for ImageJ (Jcbf) by J. Lewis Muir. (ISC-style licence: https://www.imca.aps.anl.gov/~jlmuir/repo/license.txt)

(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).

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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™

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