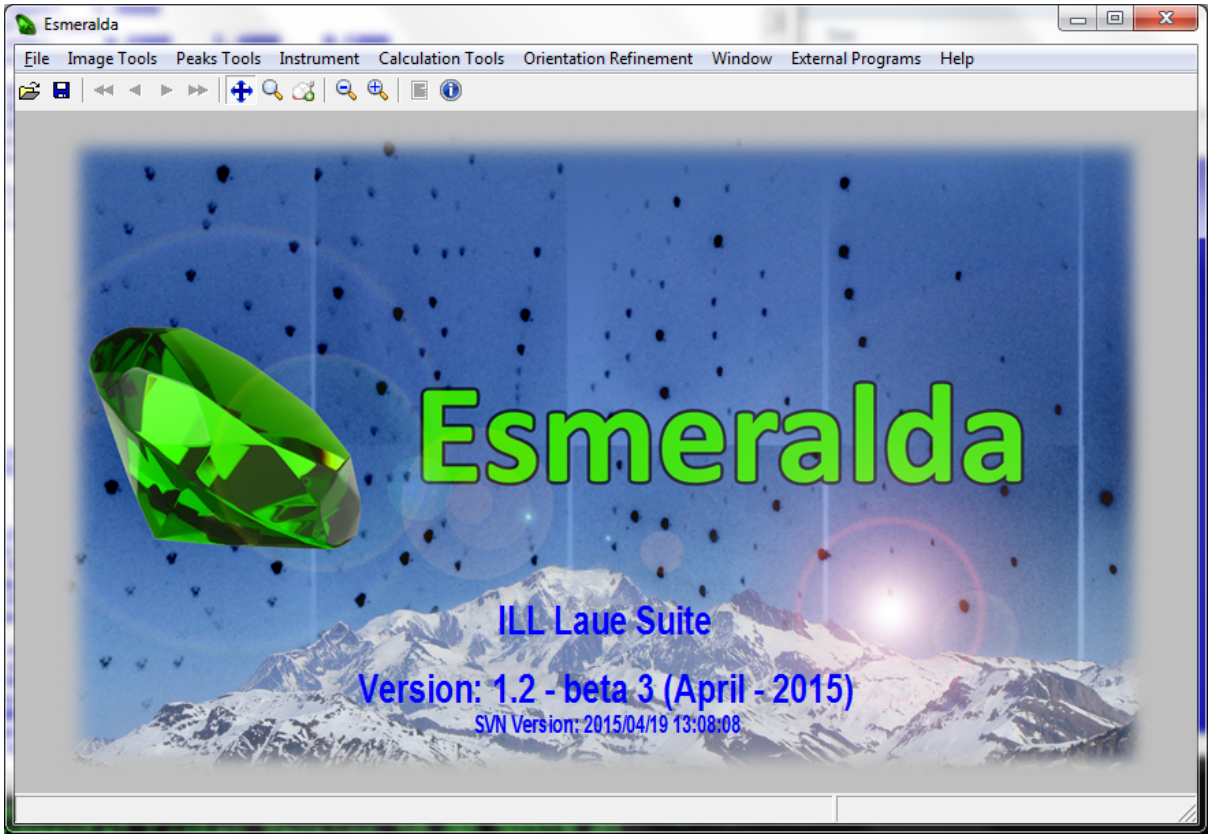

MANUAL OF THE PROGRAM:

Esmeralda

A program for Laue Diffraction data treatment

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The **Esmeralda** program is the main GUI for the Esmeralda Laue Suite. It is a program in strong current development and a series of bugs are still present. The program allows reading Laue image files (TIF, bin, raw or hbin formats) in order to perform a series of tasks.

Currently the most important tasks are the following:

1: Create (or read) an (existing) input file of extension ".cfl", called hereafter CFL file, in which the cell parameters and the space group of the crystal under study are explicitly written. Creation of CFL files for running the console program Laue_Orient.
2: Create (or read) an (existing) instrument file in which the geometrical characteristics of the instrument are described.
3: Read experimental images and visualise them in different conditions (zooming, 3D visualization). Display the different images and changes of the colour and contrast preferences. Save section of images.
4: Automatic search of Bragg peaks (two algorithms)
5: Manual selection of principal nodal spots
6: Display the calculated spot positions together with an experimental image. Rotate manually the crystal and calculation and display the spot positions on the fly.
7: Automatic orientation of the crystal by getting the UB matrix (or the rotation angles: Phi_x, Phi_y, Phi_z corresponding to the U-matrix) for the current image. If the spindle angle is known for each loaded image, the calculated spots are adjusted automatically when moving from one image to the other. There are three orienting algorithms currently implemented in Esmeralda.
8: Interactive refinement of the orientation corresponding to the current image.
9: Preparation of scripts for refining a series of images and prepare a file per image containing the visible Bragg spots with all the necessary information for the integration step.
10: Perform interactively the integration of Bragg peaks using a simple method that takes into account the overlap of close reflections.
11: Run external console program. In particular the following programs:
- **Cyclops2cyl:** Conversion of the raw Cyclops TIF images to hbin format transforming them to cylindrical geometry and performing the appropriate corrections.
- **Laue_Orient**: for roughly get the orientation of the crystal using a large set of images
- **Ref_UB_Laue**: Program to refine the orientation, cell parameters and instrumental offsets of a series of images.
- **Argonne_Boxes_ILL**: Program (written by Clive Wilkinson with contribution of Garry McIntyre, Ross Piltz and JRC) to perform integration of Bragg peaks of the Laue images.
- **CyrsCalc**, **Search_TwinLaws**, **Get_Conv_Cell** utility program (see the corresponding documentation).
- **Normalize_Laue**: Normalization of the integrated intensities in order to get lambda-free squared structure factors

12: Consult the documentation of the different programs constituting the Esmeralda Laue Suite.

Getting started with Esmeralda

Normally, **Esmeralda** is used with the aim of obtaining a list of integrated intensities of well identified Bragg spots collected in a series of images differing by the spindle angle associated with the rotation of the crystal.

The first thing to do is to prepare a CFL file in which there is, as minimal information, the cell parameters, the space group and the name of the instrument file. This can be done by using a text editor by copying pre-existing files and adapting them to the current problem. Another way of doing that is by using directly **Esmeralda** from the scratch: `File > Create Instrument and CFL files`. In the Esmeralda distribution there is an `Examples` directory in which one can find a series

of detailed examples for the ILL instruments: VIVALDI, CYCLOPS and ORIENT_EXPRESS. If the CFL file exists already, one can open it directly (`File > Open CFL file`).

The second step is to open a Laue image that should have the appropriate characteristics, in particular the same number of pixels as those described in the instrument file. One can add the name of the image files in the CFL file. In such a case the images are opened directly.

Meaning of Toolbar buttons

Icon 1: Open a `CFL` file
Icon 2: Create/Save a `CFL` file containing eventually information about orientation, conditions for searching peaks, list of images, conditions for orienting.
Icon 3: Go to the first loaded image and show it.
Icon 4: Go to the previous image and show it.
Icon 5: Go to the next image and show it.
Icon 6: Go to the last loaded image and show it.

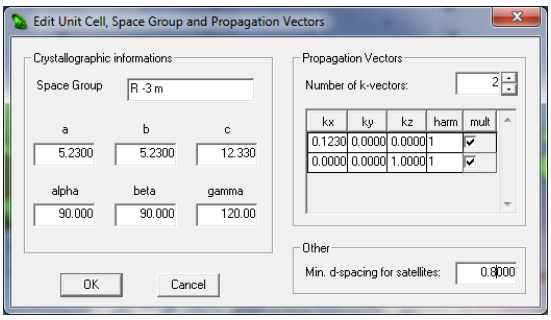
The icons 7, 8 and 9 are exclusive. You may select only one of them.

Icon 7: Default. Working in drag mode. When clicking on the left button we can drag the current image to put in the centre of the windows another part of the image.
Icon 8: Working in zoom mode. We can select a rectangular area and then zoom it on leaving the finger from the left button. Clicking on the right button it comes back to the standard view of the full image.
Icon 9: Mode for selecting points (peaks). When clicking with the left button a point is selected. Useful for promoting peaks to the first positions on the list of peaks (nodal peaks) or for removing existing peaks (double click).
Icon 10: Zoom out.
Icon 11: Zoom in.
Icon 12: Show the calculated peak positions with the current orientation.
Icon 12: Open a window with information about the current image.

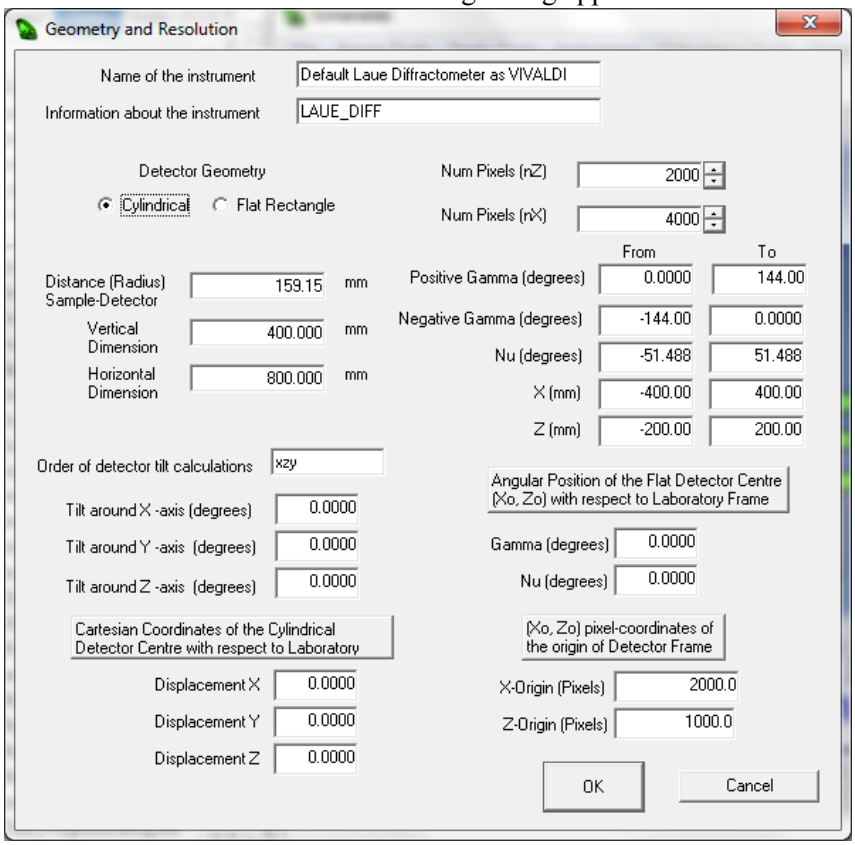
Menu item `File`

`New`: Selecting this option the program allows to create, from the scratch, an input `CFL` file and an instrument file. A series of dialogs appears sequentially and the user should provide the appropriate figures

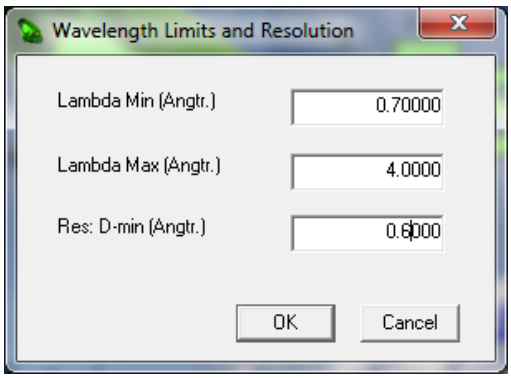
The first dialog is:



After clicking on `OK` or `Cancel` buttons the following dialog appears:



The values appearing in the above dialog correspond to those for VIVALDI. Only cylindrical and rectangular detectors are allowed. After filling carefully the appropriate values for the current instrument the user should click on `OK` or `Cancel` (if abandoning).
Finally the third dialog corresponding to `File > New` item is the following:



Once the values have been provided the program ask for saving the `CFL` and instrument files. The user should provide the appropriate names for those files.

`Open`: This option, as well as the corresponding toolbar icon, allows opening a previously existent `CFL` file.

`Save`: This option is not yet operational.

`Save as`: This option is not yet operational.

Modify Cell, Space Group or k-vectors: This option allows to change whatever of the named parameters by opening the first dialog appearing in `File > New` menu item (see above).

Edit a CFL file: This option allows opening a `CFL` file within the editor associated to **Esmeralda** (see below)

Edit results files: This option allows opening a file within the editor associated to **Esmeralda** (see below)

Reset All: This option closes all images and comes back to a state similar to that existing after opening **Esmeralda** for the first time.

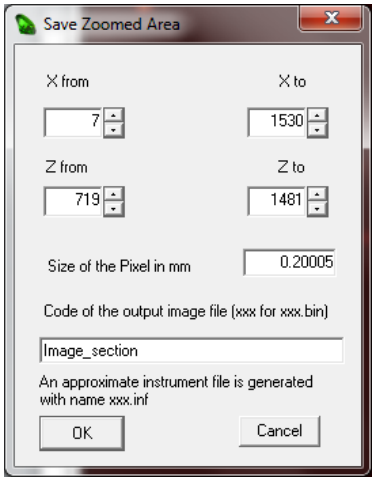
Load Instrument Parameters from File: This option loads the instrument parameters from an existing instrument file.

Save Instrument Parameters into File: This option writes an instrument file using the current instrument parameters.

Open Laue Images: This option allows opening Laue Images by selecting them from a directory. Only files with extensions: `tif`, `bmp`, `hbin`, `bin`, `img`, `raw` and `reo` are recognized. If the size of the image does not correspond to the number of pixels specified in the instrument file the image is not opened.

Open images buffer file: This option allows opening all the Laue Images written in the buffer file containing the full names of the corresponding files. All images should be given in the same format and correspond to the size specified in the instrument file.

Save Zoomed Area as Image: This option allows saving a portion of the current image, which has been previously zoomed, into an `hbin` file. The following dialog is opened when this option is selected:



The user should provide the name of the image file.

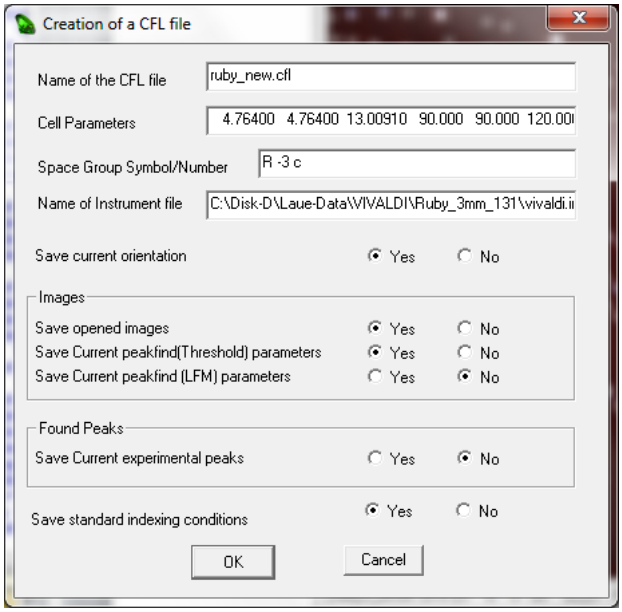
The program calculates an approximate set of parameters for creating an appropriate instrument file corresponding to the section of the image. The instrument type correspond to a *rectangular* detector, so if the image has been selected from a cylindrical detector the calculation of spots by re-reading the image and the instrument file are not properly done. This option is appropriate to select portions of a multi-detector formed by rectangular sections. This is the case of CYCLOPS images before transforming them to cylindrical.
This option should be used for fine studying the geometrical aberrations of the multi-detector in order to perform the most precise corrections if they are needed for some special purpose.

Generate a Dummy Image: This option allows creating a black image that may be used for simulation purposes. This is only needed if one wants to see the aspect of calculated Laue patterns from a theoretical unit cell and space group.

Close All Images: This option allows closing all loaded images maintaining the information from the `CFL` and instrument files.

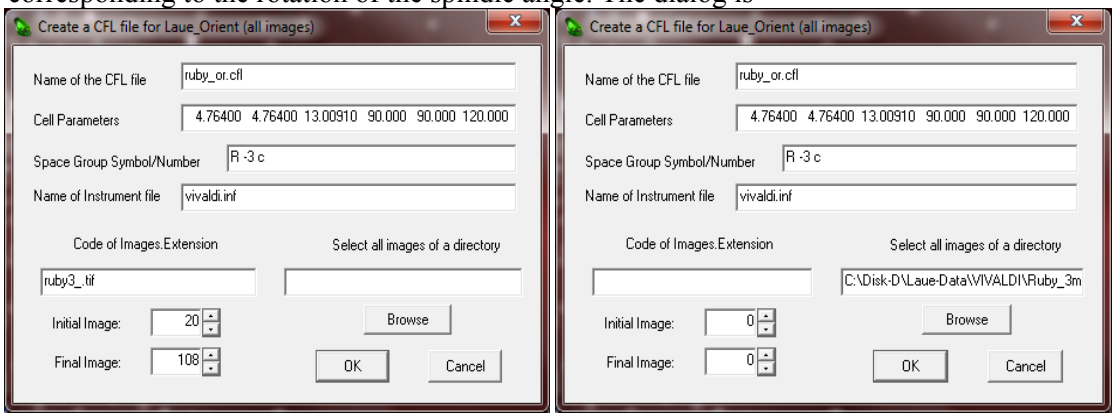
Export: This option gives access to saving different files.

Export> CFL file for Orienting: This option opens a dialog for creating a new CFL file containing the available information and for adding new one needed for running the program **Laue_Orient**. This program allows finding peaks and pre-orienting all the images provided by the user. It generates the appropriate files for refining all orienting parameters with **Ref_UB_Laue**.
The dialog is



This is typically for adding the images already opened or to save the already found experimental peaks and run **Laue_Orient**. Further edition is needed, in general, for running the program.

Export> CFL file for Laue_Orient (batch): This option opens a dialog for creating a new `CFL` file for running the program **Laue_Orient** using all the images corresponding to the rotation of the spindle angle. The dialog is

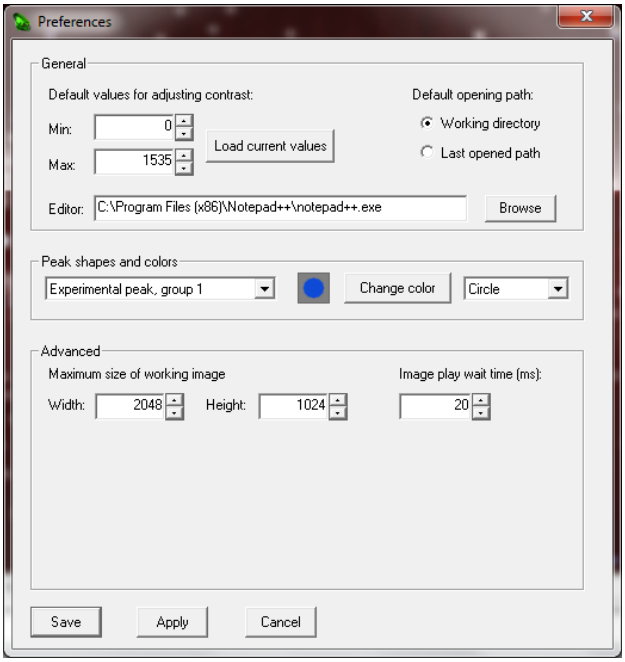


Much shorter than the previous one. It creates a `CFL` file for running **Laue_Orient** from the scratch using the initial orientation found by **Esmeralda**. In the example on the left, the code of the images is `ruby3_` which is the common part of the file name for all images, the extension is `.tif`. The names of the files written in the `CFL` file start with `ruby3_20.tif` and finish with `ruby3_108.tif`. In the example on the right all the images of a particular directory will be saved in the output `CFL` file.
After saving the file one can run **Laue_Orient** directly from the menu item `External Programs > Laue_Orient` in **Esmeralda**.

Export> All experimental peaks (method 1): This option creates a file (called `Peaks_All_Images.pks`) containing the list of all peaks found in the opened images for further inspection. This file contains the number of the peak, the number of the image, the number of the peak in the current image, the centre of mass of each peak (in mm) the position of the maximum in pixel units, the intensity, the angles gamma and nu, the parameters of the variance-covariance tensor (ellipse axes and angle) and the orienting angles: Omega, Chi, Phi of the image.

Export> All experimental peaks (method 2): This option creates a file per image (called `image_filename.peaks`) containing the list of all peaks found in the images for further inspection. A graphic dialog with a histogram is opened for each image so that the user can select the number of peaks to save. This file contains the position of the maximum and the peak intensity. It may be used by **Laue_Orient** as input peak-file for orienting.

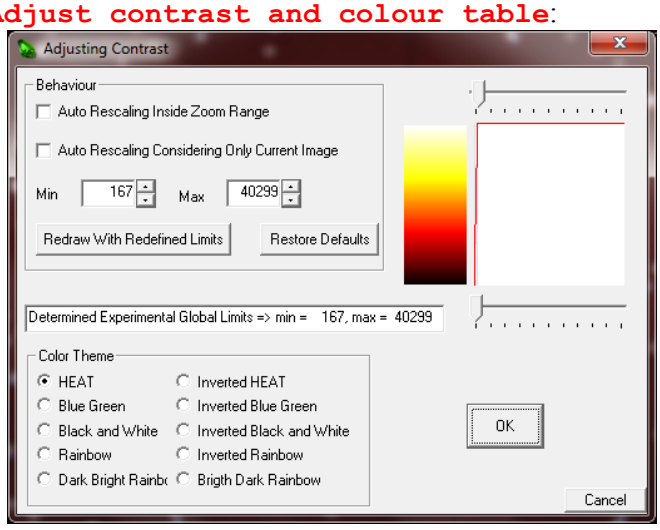
Preferences: This option gives access to saving preferences. It opens a dialog of the form:



The user may provide intensity values for adjusting the contrast, select his(her) favourite text editor, select colours and shapes for peaks of different types (experimental peaks, calculated peaks, satellites, etc.)

Menu item Image Tools

Adjust contrast and colour table:

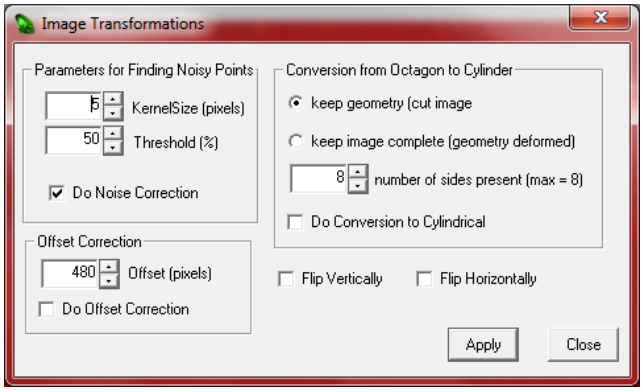


This option allows the user to select the colour of the images and the contrast. The dialog is shown on the left.

The use may play with the different options and select the colour theme.

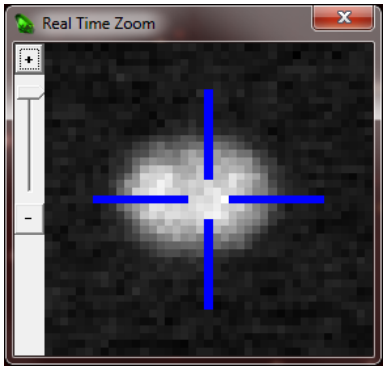
Invert Intensities:
This option changes the values of the intensities. This is needed for certain images in bitmap format; otherwise the search of the peaks cannot be done properly. For a normal image (positive intensities) with peak intensity values higher than the background, the image shown does not change, however the values are changed in memory. This can be seen selecting the option `Visualize Current Area in 3D` (see below).

Image Transformations:

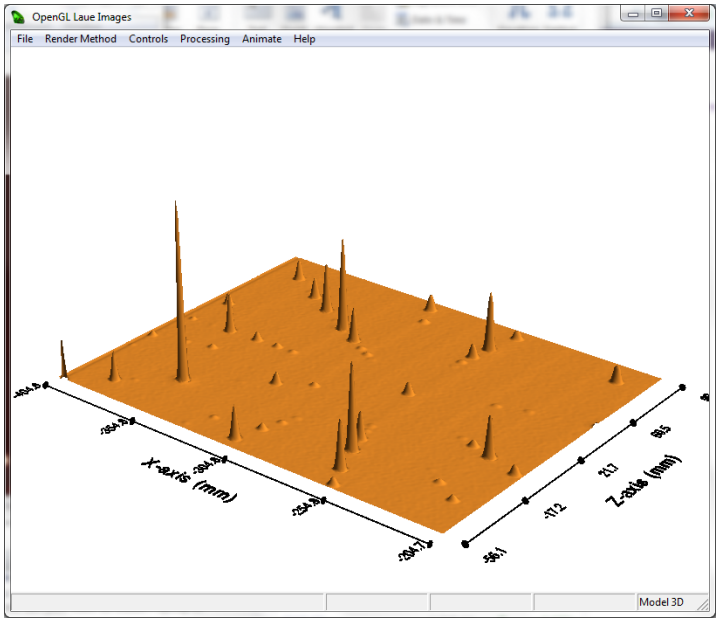


This option allows correcting noise in the images, flip the image or do an offset correction, and, finally, transform octagonal detector geometry to cylindrical geometry (CYCLOPS). This is done better using the program **Cyclops2cyl** that is able to correct and create cylindrical geometry for images coming from CYCLOPS.

Real Time Zoom:
This option opens (or close) a small window showing a zoom of the area of the image that is close to the mouse.
This option is useful when it is needed clicking on peaks for selecting them or for promoting them to *nodal peak* or to delete a single peak.



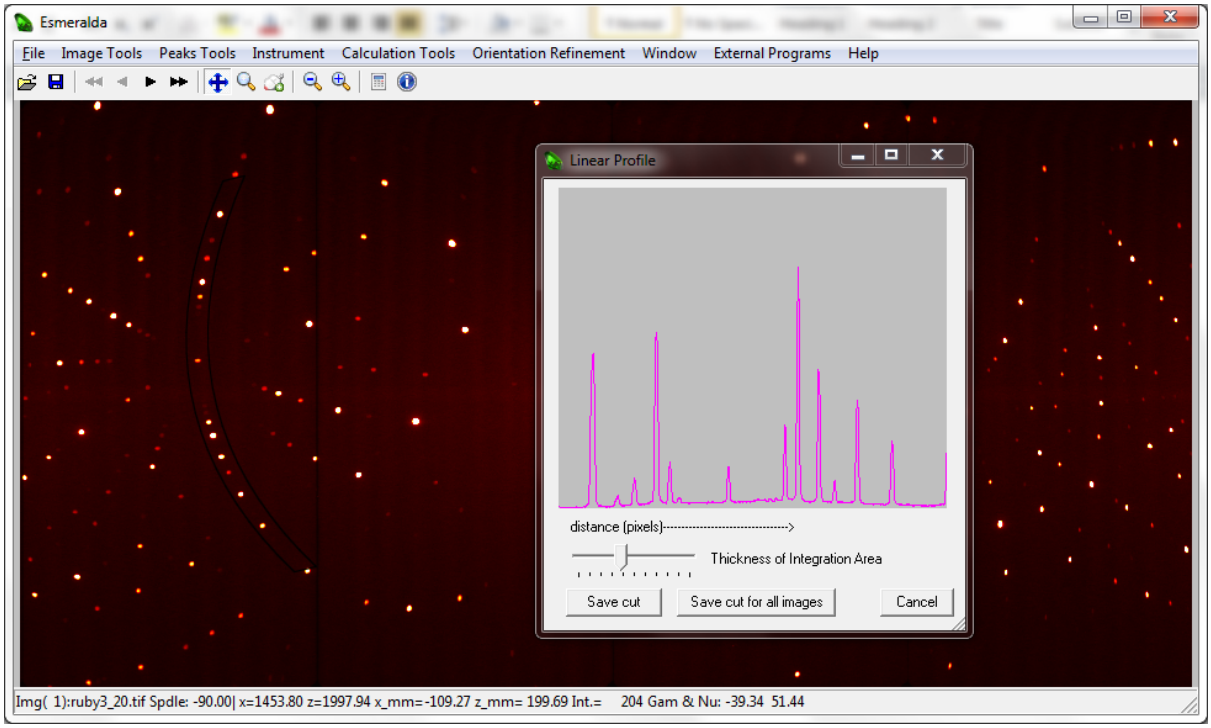
Visualize Current Area in 3D:



This option opens (or close) a window showing a 3D representation of the intensity of the Laue pattern of the area of the image currently visible in the main window. The aspect of the visualization is provided in the image on the left. The use can change different things (colours, illumination, apply filters, etc.) in the image as shown in the menu bar. Moving the mouse with the left button down the user can orient the image as wished.

Profile along a Curve:

This option allows selecting a Bezier curve, of a certain thickness, and representing the profile of the peak intensities in another window as shown in the image below.



The user can modify the thickness of the integration area using the cursor in the window containing the line profile. For selection the area to plot the user should start by clicking with the left button of the mouse in one extreme of the curve to construct, then, without leaving the finger, drag the mouse up to the end of the curve (a straight line is drawn) and finally select a point of the line and drag it up to reproduce the arc to be plotted.
If calculated peaks are present and the orientation of the crystal has been already performed the Miller indices of the reflections appear in the profile.
The user can save the profile in a file for the current image or for all the opened images.

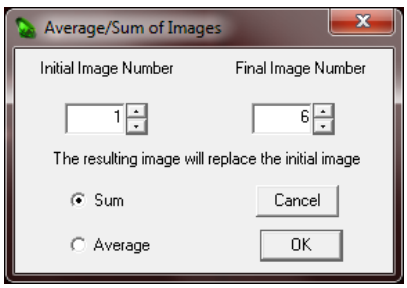
Previous Image: Shows the previous image in the list of opened images

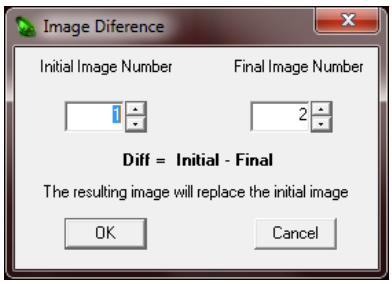
Next Image: Shows the next image in the list of opened images

Show all Images (Forward): Shows sequentially all the opened images, starting with the first image, during a small time (controlled by the `Image Play wait time` item in the Preferences dialog)

Show all Images (Backward): Shows sequentially all the opened images, starting with the last image, during a small time (controlled by the `Image Play wait time` item in the Preferences dialog)

Go to Image: Opens a dialog to introduce the number of the image to be shown in the main window



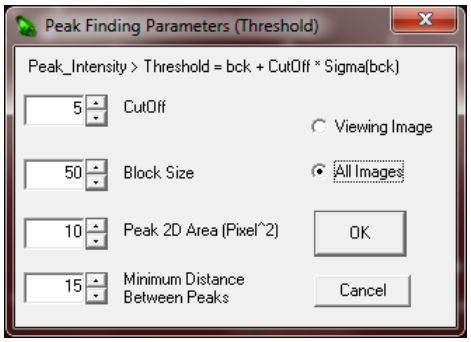


Add (Average) Images: Opens a dialog to select the images that have to be summed (or averaged).

Difference of two Images: Opens a dialog to select the images that have to be subtracted.

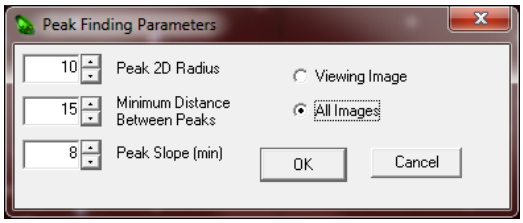
Menu item Peak Tools

Automatic Peak Finding (Threshold):



Search for peaks using a threshold algorithm from Clive Wilkinson (SNAIL). This algorithm is faster than the next one and has the advantage of getting information about the centroid and the width of the peaks through the variance-covariance matrix of the point distribution for each peak. The user can select the conditions of the algorithm by changing the appropriate values in the dialog on the left.

Automatic Peak Finding (LFM):



Search for peaks (maximum of intensities) using the LFM algorithm.

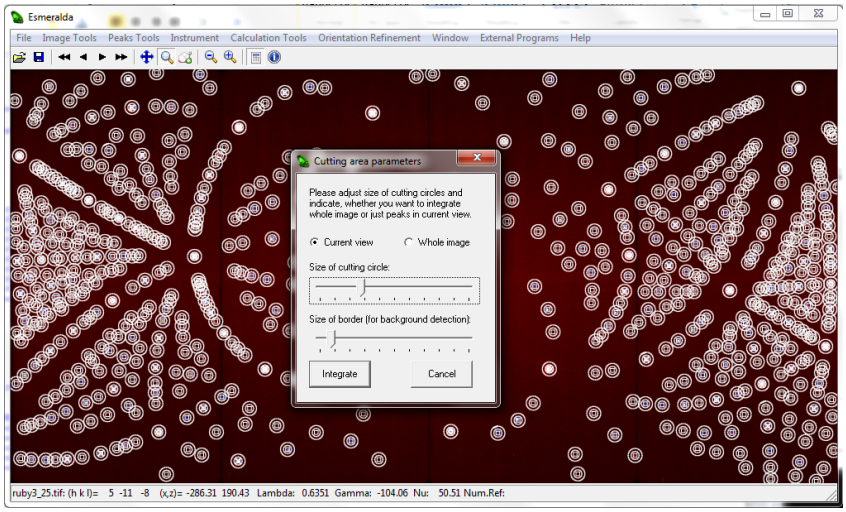
Clear Peaks of the current image area: Remove the (selected or found) peaks.

Clear All Peaks of All Images: Remove all peaks of all images.

Save Initial Indexed Peaks (All Images):
Save files of indexed and unindexed peaks of all opened images after finding interactively the orientation of the crystal. The names of the files are of the form `image_file_name_peaks.inf` and `image_file_name_unindexed_peaks.inf`. The files can be used by **Ref_UB_Laue** for refining the orientation for each image.

Integrate Peaks (experimental positions):
Integrate the experimentally found peaks using circles around the maximum for calculating the background.

Integrate Peaks (calculated positions):



Integrate the area around the calculated peak positions using circles around the maximum for calculating the background. This is illustrated in the image on the left. After clicking on "Integrate" the program calculates the approximate background corresponding to the current view of the whole image and shows, in

3D, the aspect of the calculated background. Closing the 3D view window the programs asks for continuing the process. If the user is satisfied clicking on OK initiates the process of integration.

Show Multiplicity (On/Off):
Change the aspect of calculated peaks as a function of the Laue multiplicity of the spot.

Select Closest Peak Tool (On/Off):
This switch allows selecting the position of the maximum of the closest peak to the mouse at the moment of clicking with the left button and if the mode of the mouse is "Clicking On" (see below).

Mouse Clicking (On/Off):
This switch allows changing the status of the mouse to "Clicking On" or to "Clicking Off". It is equivalent to the icon number 9 in the toolbar (see above). The `Real Time Zoom` window facilitates the use of the "Clicking On" status of the mouse for selecting peaks. If the `Select Closest Peak Tool` option is "On" it is clearly seen in the `Real Time Zoom` window that the peak to be selected appear with red dots.

Show Complete Mask:
This option allows visualizing the "mask" of the image after interactive integration of the peaks.

Adjust Pointer Size:
This option allows changing the size of the symbol representing the spots. The change can be done interactively by moving a slider and visualizing the radius (for a circle) in millimetres.

Menu item `Instrument`

Geometry and Resolution:
This option allows the user to visualize the current instrumental parameters. The dialog is the same as the second appearing after selecting in the `File` menu the item `New`. The use can change whatever parameter, but in general it is not needed unless the user is trying to set up a new instrument file.

Wavelength Limits:
This option allows the user to change the wavelength range and the resolution for the current session. The values supersede those provided in the instrument file. The dialog is the same as the third appearing after selecting in the `File` menu the item `New`.

Show excluded regions:
This option allows visualizing the excluded regions.

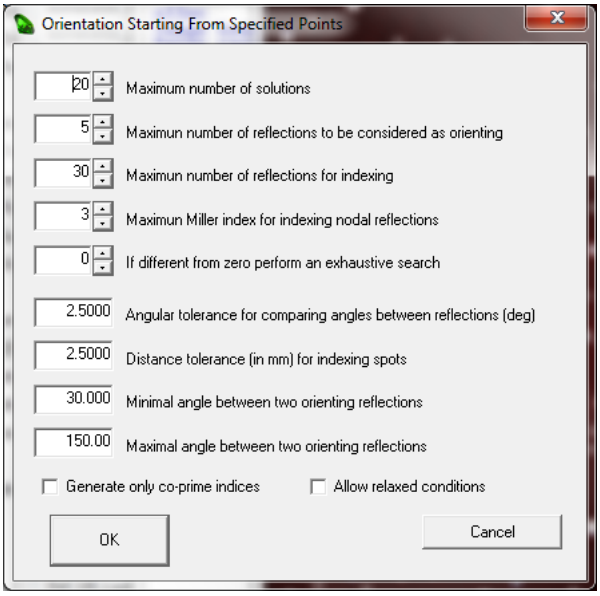
Manage Excluded Regions:
This option allows the user to select the areas of the image that should be considered as excluded regions for preparing a new instrument file. It is not currently operational.

Menu item `Calculation Tools`

Superposition of Calculated Peaks:
This option allows the user to visualize calculated spot positions for the current orientation. This is the same as the option corresponding to icon 12 in the toolbar, except that a dialog box is opened containing sliders for changing the rotation angles interactively. If no orientation has been calculated the spots appear in positions corresponding to the standard orientation of the crystal: Cartesian crystal axes coincide with the laboratory axes.

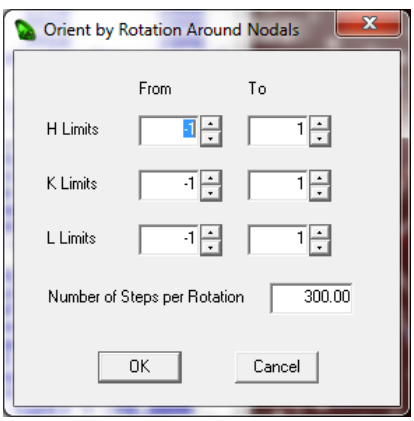
Automatic Orientation:
For using this options peak positions should exist in memory. This can be obtained by using one of the two procedures for finding peaks (see `Peaks Tools` menu item) together with manual selection of nodal peaks (if needed). Three procedures are provided that we describe below.

Automatic Orientation > Angle comparisons of Obs-Calc peaks:



This option opens a dialog (see it on the left) for selecting the parameters of the algorithm. This is based in the assumption that the first peaks in the list are nodal points (Bragg reflections of small Miller indices). The program uses systematically Miller indices for two reflections among the "Maximum number of reflections to be considered as orienting reflections". A pair of reflections is enough for calculating an orientation matrix. From the calculated orientation matrix the program tries to assign indices to the first "Maximum number of reflections for indexing", this is done by comparing the observed inter-reflection angles with those calculated from the indices, if a substantive fraction of these reflections are indexed the corresponding orientation matrix is retained as a solution.
Normally the default parameters (for neutron Laue patterns in instrument like VIVALDI or CYCLOPS) are enough for finding the orientation, however, if the instrument parameters are not very precise it may be useful to increase the angular and distance tolerance for indexing the spots.
This method is the fastest one if the nodal points are among the first peaks in the list. The peak finding procedures (menu item `Peaks Tools > Automatic Peak Finding`) order the peaks as decreasing intensities (the most intense peaks are on top of the list), but this method may fail if the most intense peak are not nodal. The best way is to select one of the images in which at least two nodal points are clearly visible (they are recognized because they are normally the intersection of few rows of peaks and they do not have other peaks close to them). For promoting observed peaks to the status of nodal one has to select manually those nodal points by clicking on the found peaks that may be nodals and repeat the procedure.

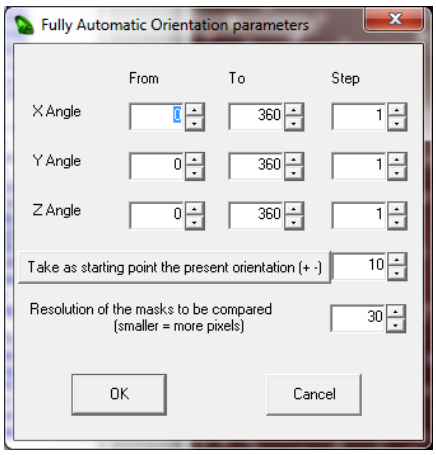
Automatic Orientation > Stepwise rotating around nodals: This option assign indices to the first peaks in the list supposing that they are nodal points (as in the method above) and the systematically apply a rotation to the calculated image until the maximum number of coincidences appear. This method is slower that the first one but it usually works in all cases. A change in the maximum value of the indices may be necessary as shown in the dialog on the left. The number of steps for a full rotation of 360º may be such that the order of a single step is between 1º and 2º. This



method should be used if the first one does not work for some reason.

T

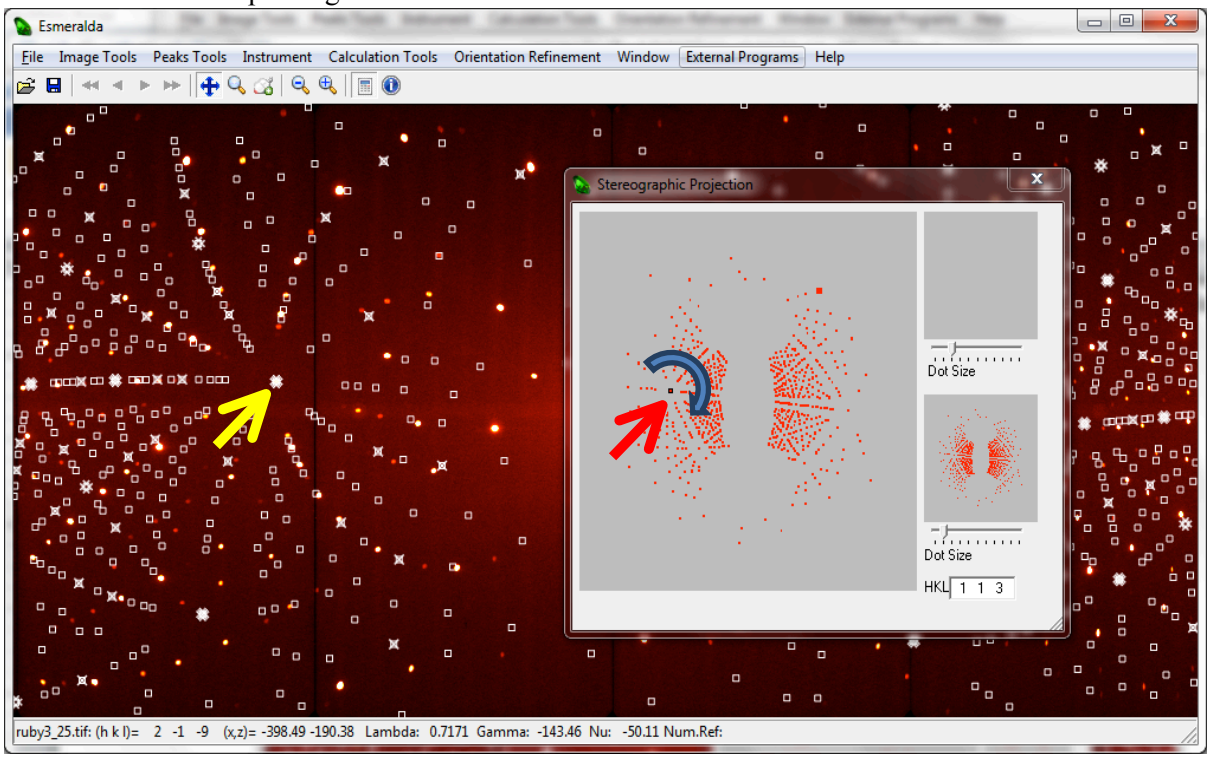
Automatic Orientation > All Possible Rotations (Slow): This option opens a dialog for controlling the parameters of the algorithm. The method works by successive rotations around the *x*, *y* and *z* axes of the image. The user can select the angular range for each rotation as well as the angular step (see dialog on the right). One can take the current orientation and select an angular range for the three rotations of the given amplitude in degrees (10 in the present example). The algorithm works using the principle of maximum number of matching spots as in the second algorithm, however a full exhaustive use of this method may be very time consuming.



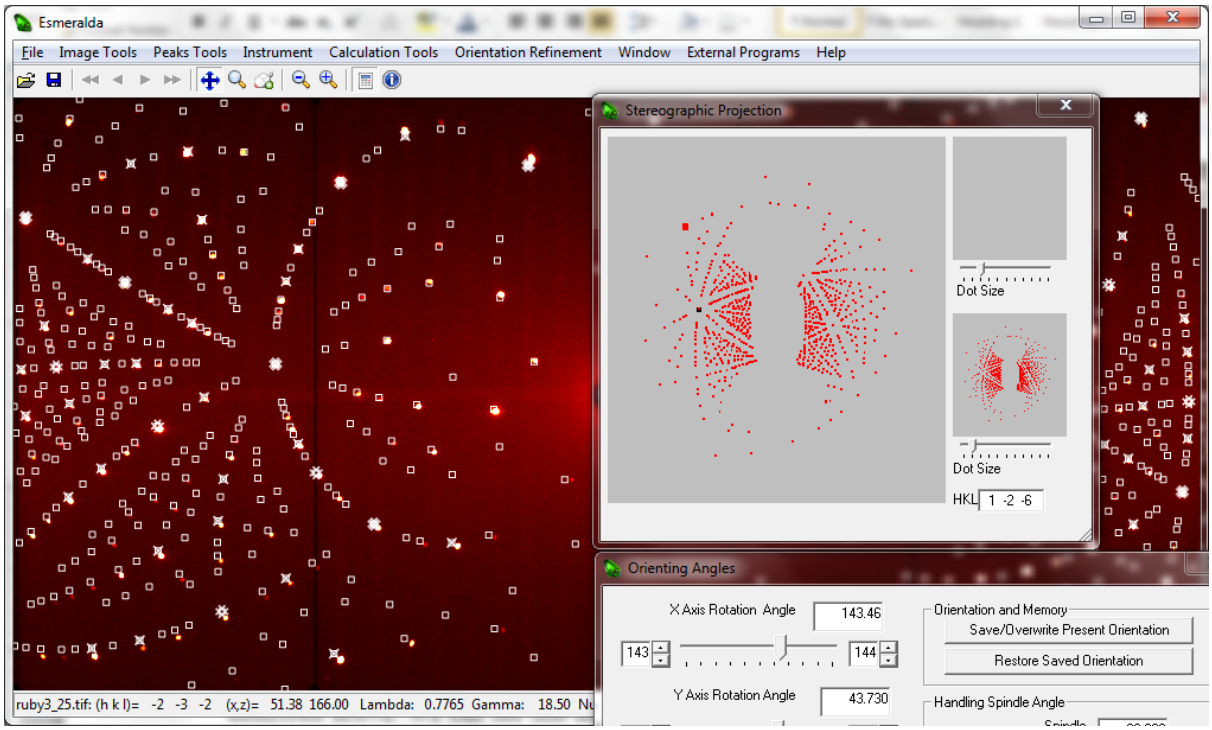
This method should not be used for routine orientation, however in cases of low quality of the Laue pattern on can find an approximate orientation that helps to find the reason(s) why the other methods fail.

Manually Orient Around a Fixed Spot:

This is a manual method of finding the orientation of the crystal based in visual recognition of the good orientation. For starting the orientation one has to visualize the calculated spots by selecting `Calculation Tools > Superposition of Calculated Peaks` and using the sliders of the orientation angles dialog move the calculated spots to make a coincidence of a calculated nodal point with one of the suspected nodal points in the experimental images. This can be done also from the menu item `Window > Stereographic Projection` that opens a dialog in which the stereographic projection of the calculated pattern is visible, the surface of the projection works as an orienting device: clicking on the left button and dragging the mouse in the surface makes changes in the orientation. This procedure is better than the use of the sliders because it is needed for doing the rotation for orienting. One can use both the stereographic projection for doing the rough coincidence and the sliders for improving the coincidence.



Once we have a calculated spot in coincidence with an experimental spot we select the menu option: `Calculation Tools > Manually Orient Around a Fixed Spot` and then move the



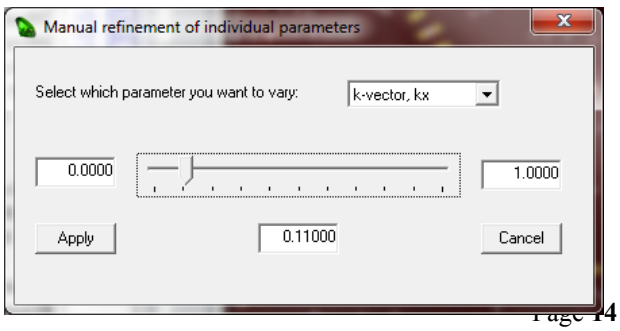
mouse to click on the desired spot. In the example of the image above we have emphasised the nodal spot and the corresponding point in the stereographic projection. Dragging the mouse on the surface of the stereographic projection (as indicated with the semi-circular arrow) one can see that the spots are all rotating keeping fixed the selected nodal point. If the selection is good we can determine the orientation manually by inspection. This is an interactive version of the second automatic method described above. We can see that after rotating around the fixed spot as indicated above we arrive to an approximate orientation that can be saved by clicking on the button `Save/Overwrite Present Orientation` of the `Orienting Angles` dialog.

`Output Reflection Files`:
This menu item allows outputting a list of reflections into a file.

`Output Reflection Files > Full List of Reflections`:
All excited reflections are output into a file called `Reflections_File.hkl`. A status is associated to each reflection. Only when status=0 the reflection is visible in the detector.

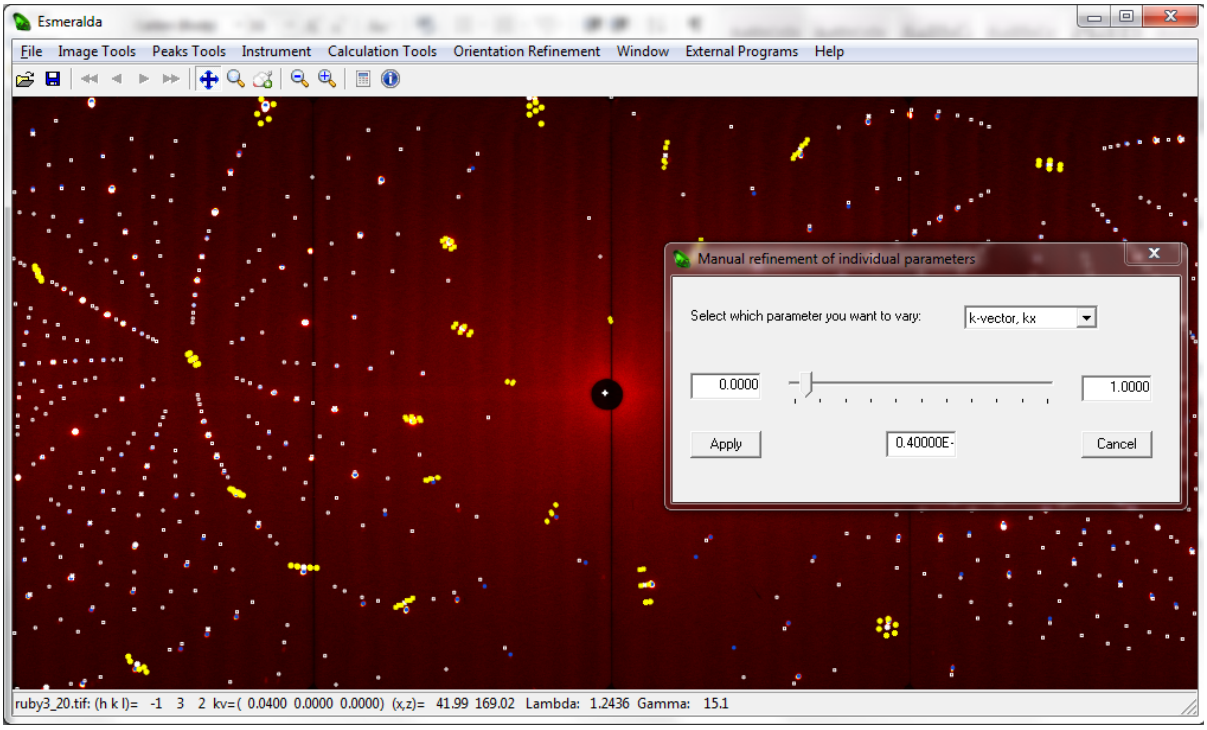
`Output Reflection Files > List of Reflections in Detector`:
All reflections actually visible in the detector (status=0, depend on the geometrical characteristics given in the instrument file) are output into a file called `Reflections_File.hkl`.

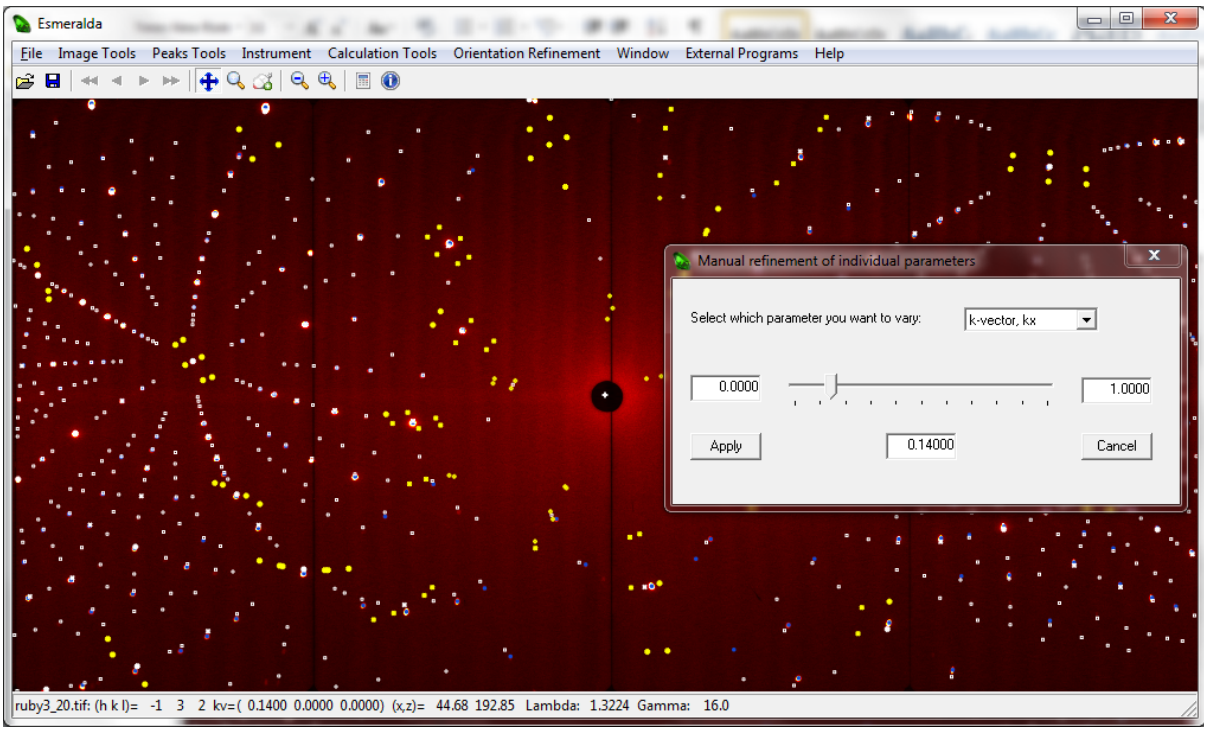
`Manual Change of Parameters`:



This menu item opens a dialog that allows the change of a series of individual parameters interactively. The effect on the diffraction pattern is seen automatically. For instance changing the resolution or the minimum wavelength one can see the appearance or disappearance of reflections. This dialog can also be used to find propagation vectors quite easily.

For the moment the list of parameters that can be changed interactively is the following: x-offset, z-offset, cell parameters, propagation vector components, number of harmonics, minimum d-spacing for propagation vector calculations (dk-min), resolution (d-min) and wavelength range.
In the following images one can see two different positions of the satellites calculated using the variation of k_x (k_x =0.04 and k_x =0.14).

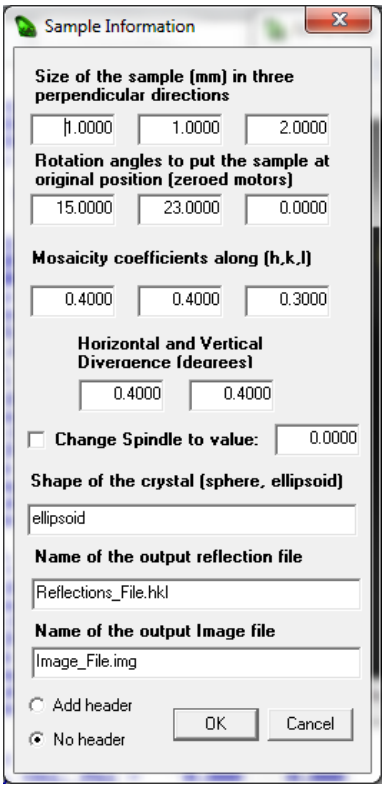




The manual change of parameters dialog is modeless, so other actions are permitted during its use. However it may remain unhandled situations, if something wrong happens it is safer to close the dialog and reopen it.

Apply Distortions (On/Off):
This menu item (switch) is automatically put *On* after an interactive refinement corresponding to a particular image. For the image that has been refined the coincidence of the calculated spot positions with those of the experimental peaks is assured by the application of the refined distortions, however the application of the distortions to other images may make worse the agreement between observed and calculated positions.

Calculate Theoretical Image:

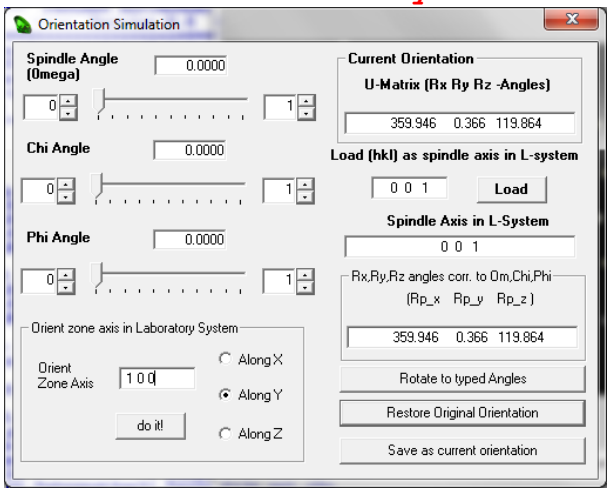


A full Laue image is calculated according to the information provided in the CFL file. This item is accessible only if atom positions have been provided in the CFL file. The calculation is currently performed for neutron diffraction assuming a Maxwellian thermal incident spectrum. The characteristics of the sample and the divergence of the incident beam have to be provided by filling the dialog box on the left.
The orientation of the crystal can be input by giving three rotation angles (Phix, Phiy, Phiz) in degrees. The mosaicity of the crystal along *h*, *k* and *l* directions in reciprocal space should also be provided, as well as the horizontal and vertical divergence of the incident beam. These parameters determine the size of the spot for the current instrument parameters. If the shape of the crystal is assumed to be a sphere the size of the sample is assumed to be the first size parameter (along "x" in mm) as diameter.

Adding a header, the output file is of the time *.hbin, otherwise it is a simple binary image also recognized by **Esmeralda**.

The calculated image can be used for testing the program (using it as an experimental image) or for comparison with an experimental image.

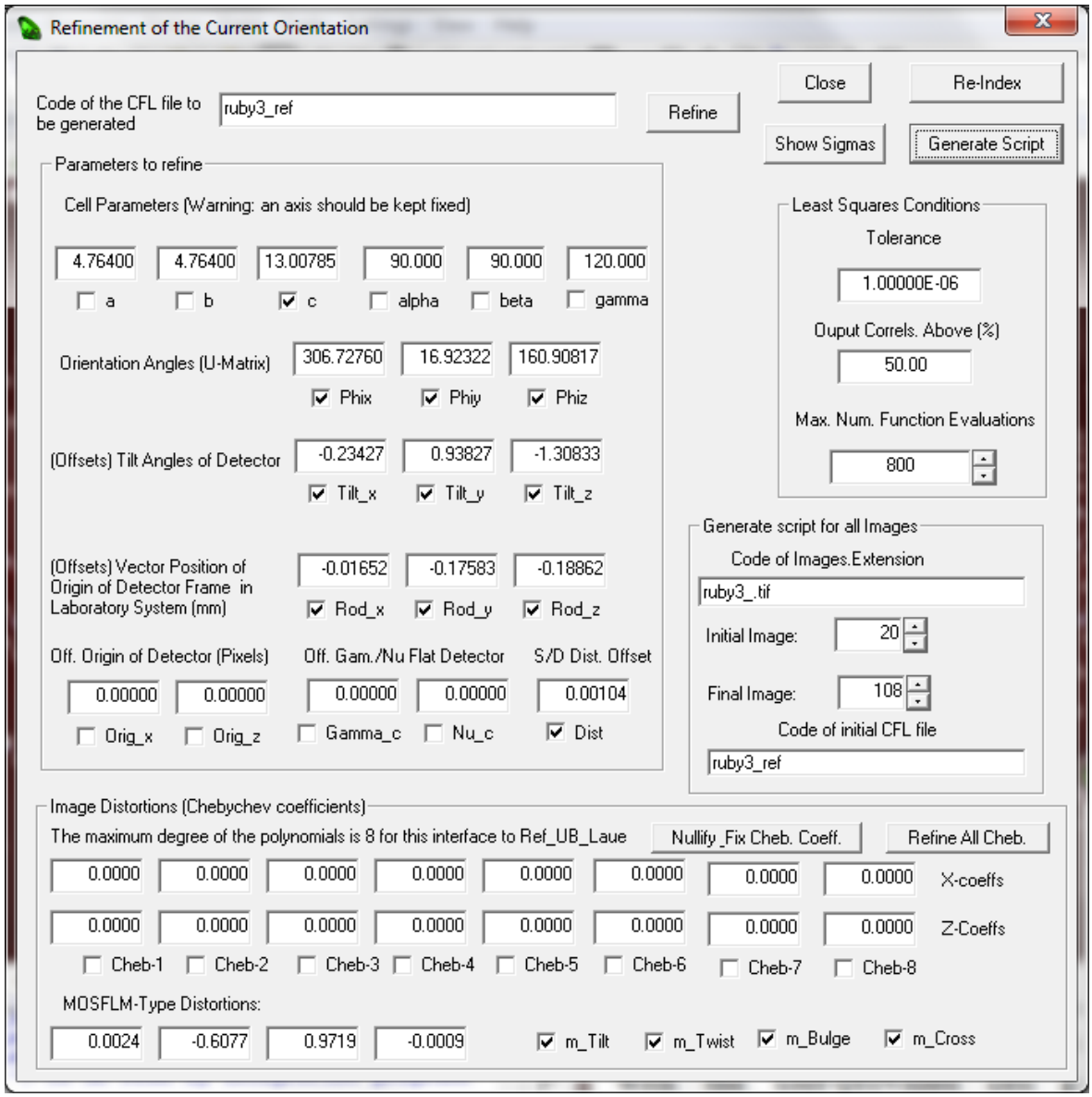
Simulation of Laboratory Rotations:



This item opens a dialog as shown in the left. On that dialog box there is the possibility to move the motor controlling the angles (Omega, Chi, Phi) of an orienting device and the spot positions motions can be seen directly in the image window. The current orientation of the crystal is loaded as three angles in the right-top of the dialog. This is not moved when the angles are changed.
The area titled: Orient zone axis in Laboratory system, allows the calculation of the angular motions to be applied to the crystal in order to orient a particular zone-axis along one of the principal directions of the Laboratory reference system. The output of the angles is done in the console after pushing the button "do it!"
This part of the program is not yet finished and some buttons are not behaving as expected

Menu item `Orientation Refinement`

`Refinement of the Current Orientation`:
This option allows the user to refine interactively the orientation corresponding to the current image. This option does not aim to refine the whole set of images corresponding to a full experiment. One can do that but it may be tedious. For treating the whole set of images (corresponding to different positions of the spindle angle) it is better to use a batch mode by running **Laue_Orient** and then **Ref_UB_Laue**. After selecting an image in which the user has found an orientation using one of the

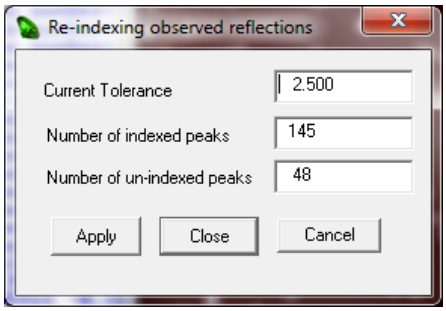


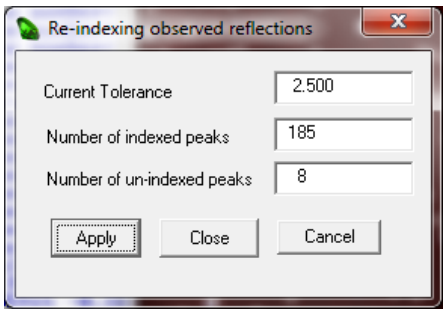
methods available in the menu item `Calculation Tools`, the following dialog is opened:

The default refinement parameters are good for an image taken in a well aligned instrument and with a good instrument file. The meaning of the parameters is clear from their given names. For details the user can consult the documentation accompanying **Esmeralda** (in particular the documents Laue_Basic_Equations.pdf and Ref_UB_Laue.pdf).

On the console opened by Esmeralda one can see something like:

In which we can see how the refinement proceeds. The average distance is the sum of all the distances between the calculated and the observed peaks divided by the number of peaks.

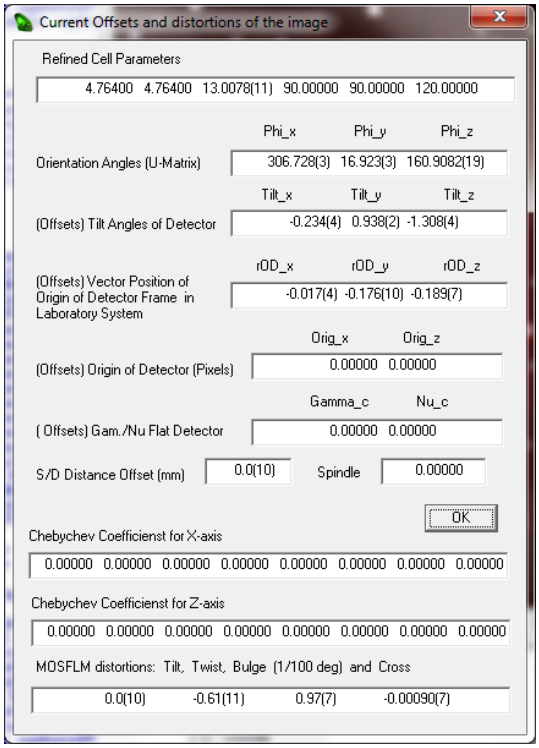




The button `Re-index` allows the inclusion of more experimental points for refinement because the first time the user clicks on the `Refine` button only the rough orientation with the user-provided cell parameters and instrument parameters are used, and this is normally a fraction of the found experimental peaks. In the example on the left there were 145 peaks indexed and 48 unindexed. When the user clicks on the `Apply` button, new peaks are promoted to the list to be refined within the given tolerance. In the example 40 new peaks have been indexed within the tolerance of 2.5 mm. There are always experimental peaks that may be too close to excluded regions that the orientation method does not consider or there are some spurious peaks that are not real spots. This is not important to get a proper refinement of the orientation angles, cell and instrumental parameters.

At whatever moment the user can see the value of the refined parameters and the corresponding standard deviations by clicking on the button `Show Sigmas`, then a dialog with all values appear with the standard deviations in parentheses as is common in crystallographic conventions.

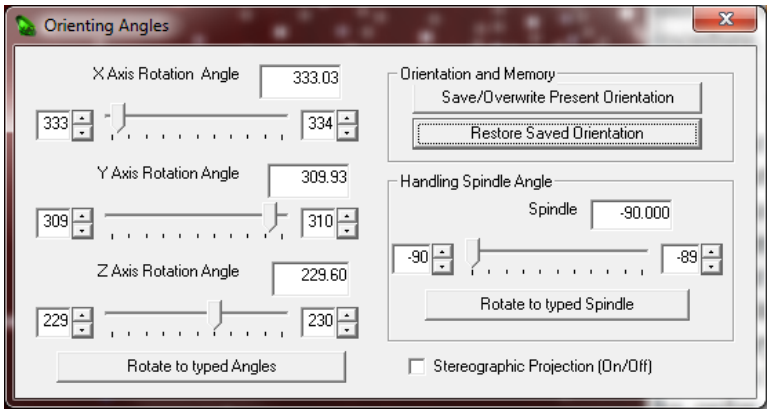
Finally one can use the button `Generate Script` for preparing a script that will be used by **Ref_UB_Laue** for refining all the images as input in the `Generate script for all Images` area of the `Refinement of the Current Orientation` dialog. The program generates then a file `called code_of_images.reflaue` (in the example above `ruby3_.reflaue`) that contains the name of the initial `CFL` file that will be used for each image (in the example above `ruby3_ref.cfl`) and the name of all the images constructed from the code and the numbers given in the dialog. This kind of file allows a refinement of individual images without connections between them. Each image has its own cell parameters, etc. If the user prefers to refine the parameters having a more physically sound content the best is to use **Laue_Orient** to generate a file for **Ref_UB_Laue** (see the menu item `File > Export> CFL file for Laue_Orient (batch)`) that allows the treatment of all images simultaneously in which one can refine the offsets of the spindle angles and individual $\mathbf{r}_{OD}$ (vector position of the origin of the detector frame with respect to the laboratory system, always in the centre of the crystal) because a small precession of the crystal is unavoidable when changing the spindle angle.



`Show Current Offsets`:
This menu item opens a dialog that is exactly the same as that obtained when clicking on the `Show Sigmas` button of the `Refinement of the Current Orientation` dialog. It is shown on the left as an example.
One can see that the origin of the detector is not refined because there is a strong correlation between those parameters and the components of the vector $\mathbf{r}_{OD}$. For closing this dialog it is necessary to click on the `OK` button.

`Re-index Observed Reflections`:
This menu item opens exactly the same dialog as that obtained when clicking on the `Re-Index` button of the `Refinement of the Current Orientation` dialog.

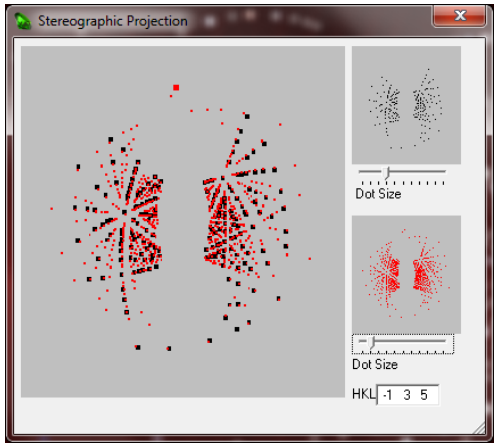
Menu item `Window`



`Zoom Window`:
This option is currently the same as `Image Tools > Real Time Zoom`.

`Orienting Angles`:
This option is a switch for opening or closing the `Orienting Angles` dialog shown on the left. This dialog is also opened with the option `Calculation Tools >`

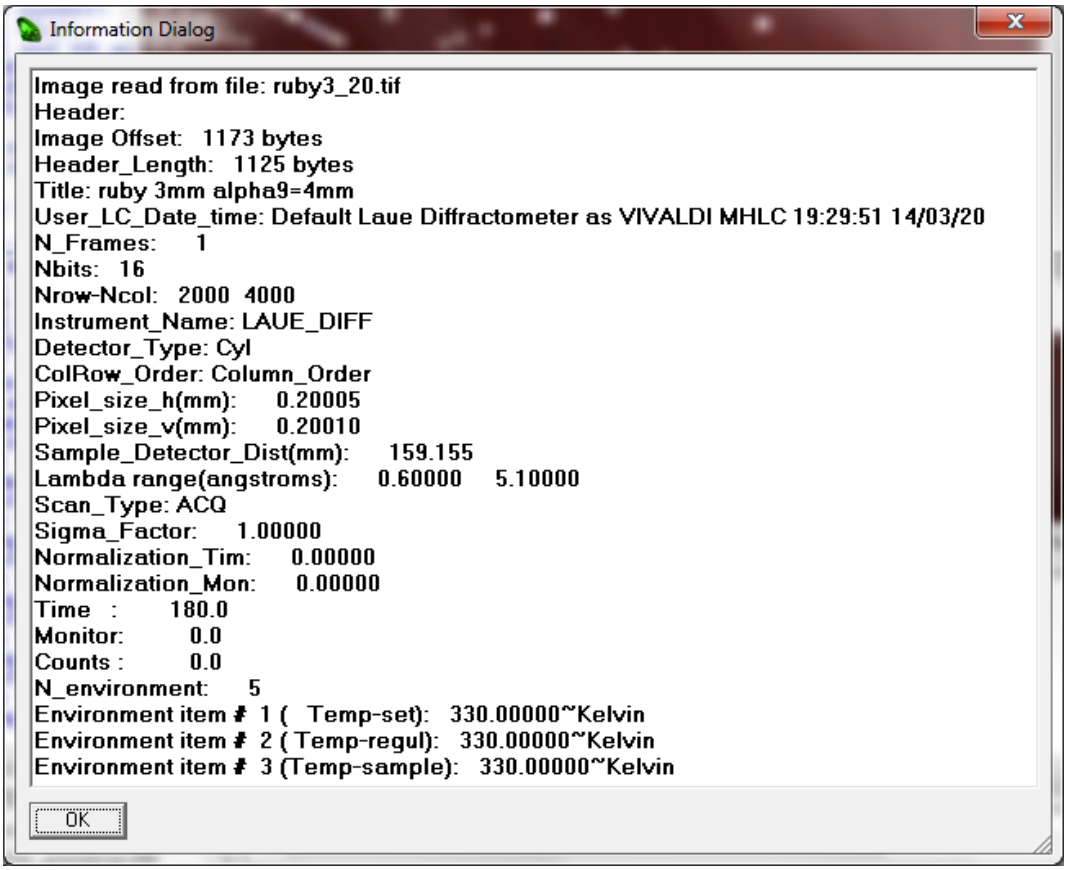
`Superposition of Calculated Peaks`. It may be used for changing the orientation angles to make coincidences of calculated peaks with observed peaks. See the section discussing the menu item `Calculation Tools > Manually Orient Around a Fixed Spot`.



`Stereographic Projection`:
This option is a switch for opening or closing the `Stereographic Projection` dialog shown on the left. This is another kind of view of the Laue Pattern; it may be used to move the calculated pattern with respect to the observed pattern for making coincidences between them.

`List of Peaks`:
This option is not yet operational.

`Information Dialog`:
This option opens a window in which all the available information concerning the current image is written. Below we give an example:



Menu item `External Programs`

`Cyclops2cyl`:
This option allows running the program **Cyclops2cyl**. For running this program the user should create an input buffer file as explained in the document Cyclops2cyl.pdf, accessible in the `Help` menu.

`Laue_Orient`:

This option allows running the program **Laue_Orient**. For running this program the user should create an input `CFL` file as explained in the document Laue_Orient.pdf, accessible in the `Help` menu.

`Ref_UB_Laue`:
This option allows running the program **Ref_UB_Laue**. For running this program the user should create an input `CFL` file as explained in the document Ref_UB_Laue.pdf, accessible in the `Help` menu.

`Argonne_Boxes (ILL) - Laue_Integration`:
This option allows running an integration program. Currently for both menu items the program is **Laue_Integration** (a modified version of the program Argonne_Boxes from Clive Wilkinson and Garry McIntyre). For running this program the user should create an input `ABX` file as explained in the document Argonne_Boxes_ILL.pdf, accessible in the `Help` menu.

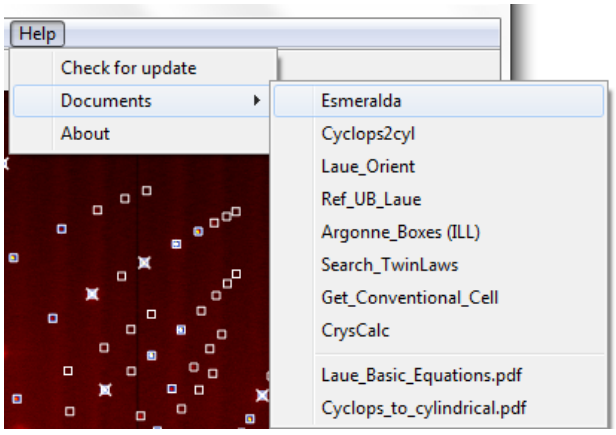
`Normalize_Laue`:
This item runs the program **Normalize_Laue** for obtaining normalized squares of structure factors from the total list of integrated reflections. The documentation of this program is not yet available.

`Utilities`:
This option allows accessing the following console utilities:

> **`Utilities > CrysCalc`**:
> This option runs the **CrysCalc** program (Crystallographic Calculations). A console terminal is opened and the menu appears. The different options are available in the document CrysCalc.pdf, accessible in the `Help` menu.
>
> **`Utilities > Search_TwinLaws`**:
> This option runs the **Search_TwinLaws** program. The explanations are available in the document Search_TwinLaws.pdf, accessible in the `Help` menu.
>
> **`Utilities > Get_Conventional_Cell`**:
> This option runs the **Get_Conventional_Cell** program. The explanations are available in the document Get_Conventional_Cell.pdf, accessible in the `Help` menu.

Menu item `Help`

`Check for Updates`:
This option allows accessing the most recent version of Esmeralda.



Documents:
This option allows accessing the documentation of Esmeralda.

In the figure on the left one can see the currently available documents.

About:
Open the last information about Esmeralda. Currently the following dialog is opened: