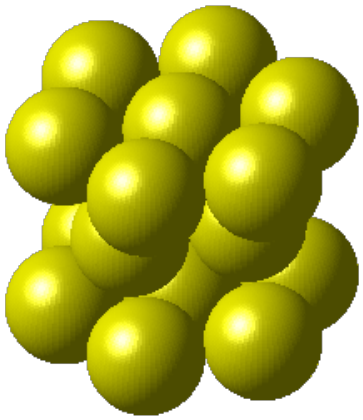

CrysTBox – Crystallographic Toolbox

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Contents

Introduction

This publication should provide the CrysTBox users with a reference manual and user guide. CrysTBox is set of tools for crystallographers, electron microscopists or generally for anyone interested in physics. The first chapter of this manual covers the installation procedure, troubleshooting, CrysTBox Server and specification of files describing user-defined materials. Each of following chapters describe one tool: cellViewer – a visualization tool and crystallographic calculator; diffractGUI – a tool for automated analysis of spot and disk diffraction patterns and ringGUI – a tool for automated analysis of ring diffraction patterns.

Further details and updated information can be found at `www.fzu.cz/crystbox`. In case of any questions, offers or comments please feel free to contact the author.

If you find this software helpful for your research, please cite it. The details can be found in the last chapter.

If you have any questions, offers or comments, please feel free to contact me: `klinger@post.cz`

Chapter 1

General information

This chapter covers some basic information about CrysTBox such as installation, material specification or CrysTBox Server. It does not focus on the tools, those are described in following chapters.

1.1 Installation and troubleshooting

Following lines should guide you through the installation of CrysTBox, DigitalMicrograph plugin and they should also offer some troubleshooting.

1.1.1 CrysTBox Installation

The installation procedure may slightly vary depending on your system, whether you choose MCR or WEB installer (see bellow) etc., but the main steps of the installation procedure remain the same as described below.

Step 1 – Get installation file

CrysTBox is available on demand. Please contact the author to obtain the installation files.

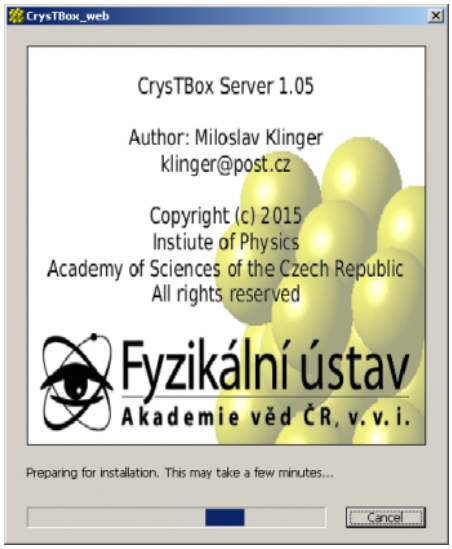
Installers are available **for Windows in 32-bit and 64-bit** version. CrysTBox is built using MATLAB Compiler and therefore it requires a package of supporting functions called MALTAB Compiler Runtime (MCR). The installer may or may not include MCR. There are two installer versions available:

- **MCR installer** – contains MCR, can be used on **offline** computers (about 700 MB)
- **WEB installer** – does not contain MCR, **requires the Internet** connection (about 30 MB)

As for the tools (diffractGUI, ringGUI...), both installers provide the same tools and features.

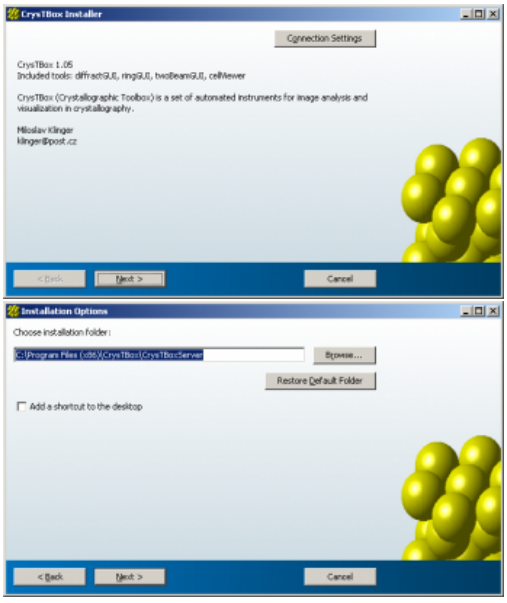
Step 2 – Launch installer

Once you have the installer, launch it. You should see this image (on the right) for a while. The length of "the while" may vary from seconds to tens of minutes. Only MathWorks knows why. Nevertheless, please, be patient.
Note: Before launching the installation of a new version, make sure, that old version of CrysTBox is not running.
Note: It may take the installer some time to appear (tens of seconds, especially for MCR installers). Again, only MathWorks knows why. Please, do not re-launch the installer.
Note: It may happen, that the installer window disappears at the end of this step. Again, only MathWorks knows why. Although there is no sign of the ongoing installation procedure, please do not re-launch the installer, it should reappear in several seconds... or tens of seconds.
Note: If the installer can not be launched, please check whether the installer version (32-bit or 64-bit) fits the version of your operation system.



Step 3 – Enter your preferences

You can specify where CrysTBox should be installed, whether to create a shortcut and so on.
Note: It may happen that the Next button does not work. If you face this problem, please try to use MCR installer (at least until MathWorks comes up with a solution). According to my experience, this is a problem of WEB installers only.

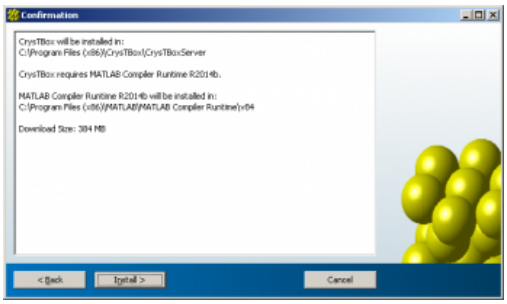


Step 4 – MCR installation (if not installed yet)

CrysTBox needs package of supporting functions – MATLAB Compiler Runtime (MCR). If it has not been installed yet, you can specify the destination folder and you have to agree with the license conditions.

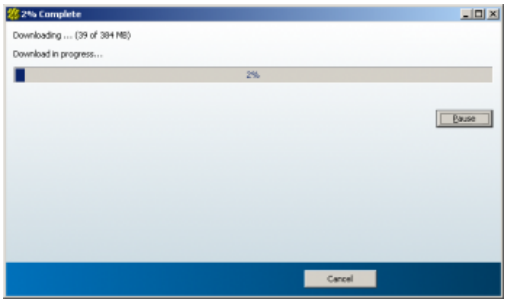
Step 5 – Confirmation

Here you can see the installation summary.



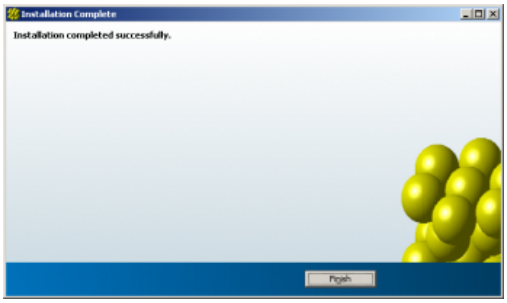
Step 6 – Wait a minute...

Now, CrysTBox and all other software (if needed) is being installed. It may take few seconds to several tens of minutes depending on the amount of data being installed, on your computer and on your Internet connection (in case of the WEB installer).
Note: The installation fails during this step, if an old version of CrysTBox is already running. Once it happens, please terminate the installation, close CrysTBox and launch the installation again.



Step 7 – Finished

CrysTBox has been successfully installed.



1.1.2 Installation of DigitalMicrograph plug-in

This guide should help you to install a DigitalMicrograph (DM) plug-in, which allows you to launch the CrysTBox directly from DM.

Step 1 – Locate plug-in file

The plug-in file is distributed with the CrysTBox. The file is named CrysTBox.gt1 and you should find it in the folder, where the CrysTBox is installed to. If you have not changed the destination folder during CrysTBox installation, the path should be
C:/Program Files/CrysTBox/CrysTBoxServer/application for 64-bit installation and
C:/Program Files (x86)/CrysTBox/CrysTBoxServer/application for 32-bit version.

Step 2 – Copy plug-in file to DM plug-in folder

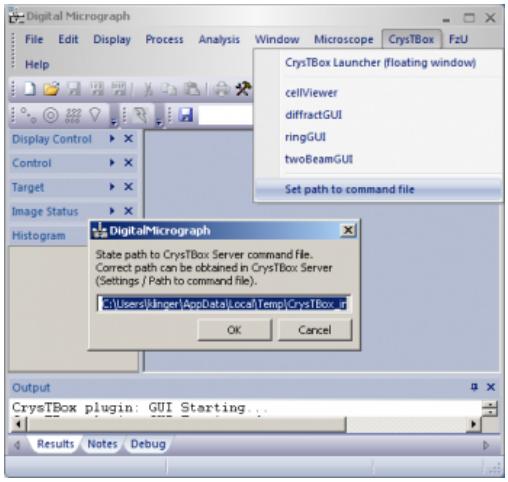
The file CrysTBox.gt1 needs to be copied to DM plug-in folder. This folder is located in the same folder, where the DM is installed. Typically the path to the plug-in folder looks like
C:/Program Files/Gatan/Plugins

Step 3 – Launch DM

Start DM (or restart if already running). There should be a new entry in DM main menu – CrysTBox.

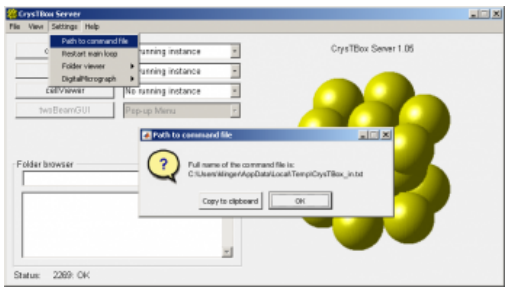
Step 4 – Open CrysTBox command file settings in DM

In DM main menu, select CrysTBox / Set path to command file. A dialog box with an edit field should appear.



Step 5 – Set path to CrysTBox command file

Specify path to the command file in the DM dialog box and press OK. The path can be found in CrysTBox Server main menu at Settings / Path to command file (see the image).



1.1.3 Troubleshooting

This section addresses problems which you may face during the installation procedure and after successful installation. In case of installation troubles, you may also refer to the previous sections which provide step-by-step guides covering the installation of CrysTBox and DigitalMicrograph plug-in.

Installer does not even start

Check whether the installer version matches the version of your operating system (32-bit vs. 64-bit).

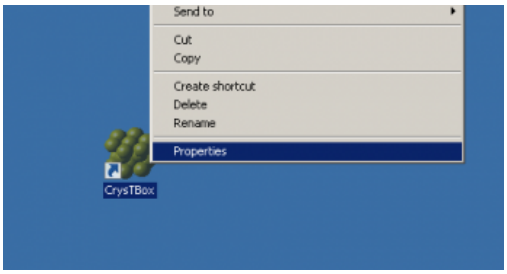
Installer button "Next" does not work

However sad it may be, it happens... I'm waiting for MathWorks answer for this bug. According to my experience, it happens for the WEB installers only, so using the MCR installer may help.

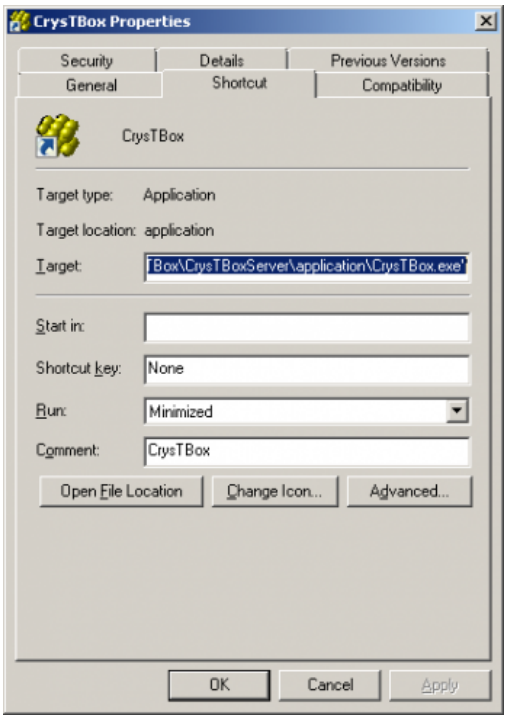
CrysTBox is installed, but crashes (software OpenGL)

According to MathWorks, these crashes may be caused by drivers of a graphic card. One way how to prevent those crashes is to use software rendering. CrysTBox offers this feature.

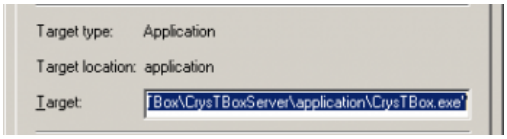
Right click on the CrysTBox shortcut and select Properties.



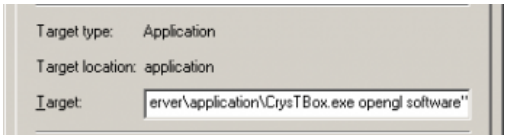
This window should appear.



We are interested in field Target.



Add text opengl software right behind CrysTBox.exe and before the ending quotes. Press OK and try to launch CrysTBox again.



Note, that the settings applies only on this particular shortcut (icon). If the problems preserve, please, contact the software author.

1.2 CrysTBox Server

The CrysTBox server allows the user to launch individual tools, handle the running instances of the tools and browse the directory structure for the input images. Individual tools can be launched directly using the buttons, or via external application (such as DigitalMicrograph).

Unfortunately, MATLAB does not allow the compiled application to utilize more CPU cores, so all the instances launched from one CrysTBox server need to share one single core. This may cause one tool to respond slowly (or even not to respond at all) if another is busy with ongoing analysis.

1.2.1 Window description

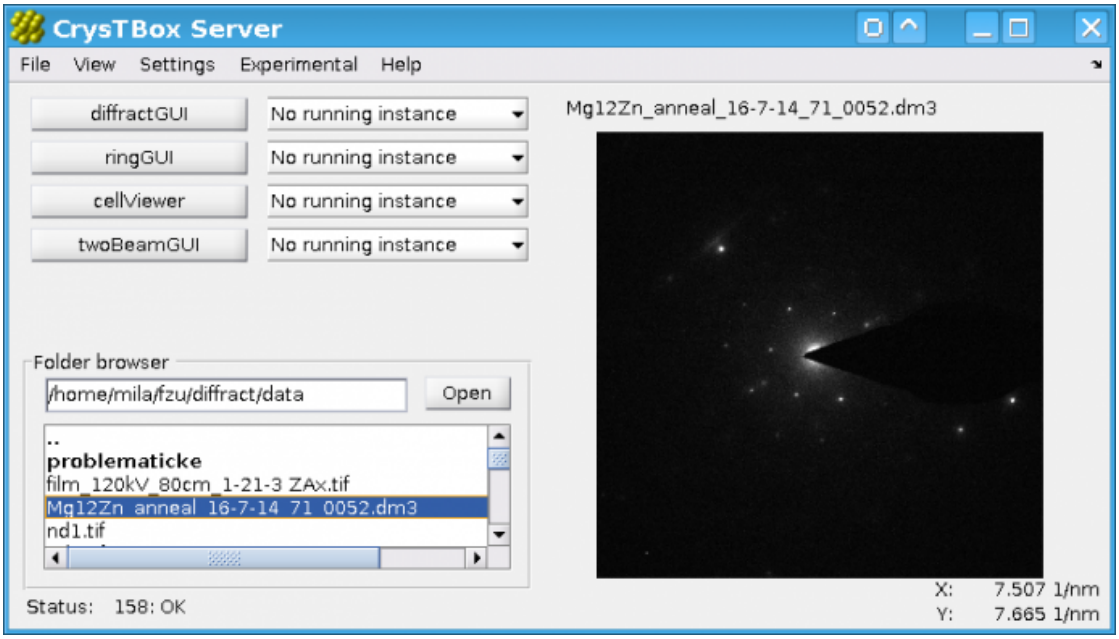


Figure 1.1: CrysTBox Server window.

The application window of the CrysTBox Server consists of one figure, buttons launching individual tools and a simplified file browser. A detailed description of the graphical user interface follows.

Image

This part of the interface shows screenshot-hints or provides preview of the images browsed in the **Folder browser**. The screenshot-hint is a screenshot of a particular tool (diffractGUI, ringGUI, cellViewer, etc.) displayed when the mouse pointer is hovered over the button launching the appropriate tool (see **Launching buttons**). The file preview is displayed if some supported image file is selected in the **Folder browser**. The preview can be zoomed in and out using a mouse wheel if the mouse pointer is located over the image. Coordinates of the mouse pointer within the image are shown below.

Figure 1.2: Image preview.

Launching buttons

Those buttons can be used to launch individual CrysTBox tools. To pass the launched tool an input image, please select the image in the **Folder browser** and then press the launch button. The pop-up menus next to the buttons list the instances launched by the CrysTBox Server. The user can raise an individual tool instance to the focus by selecting it in the pop-up menu. Names of individual instances can be changed allowing the user to easily handle many CrysTBox windows performing different analyses.

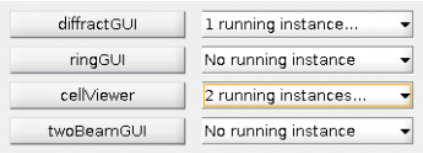


Figure 1.3: Launching buttons.

Folder browser

This panel allows for a simplified browsing and navigation in the directory structure of your PC. Enlisted folders (in bold) can be opened by a double-click, while the supported files can be highlighted and previewed in a single click. The highlighted file is automatically passed to the launched tool as the image to be analyzed (provided the launched tool accepts the images as an input).

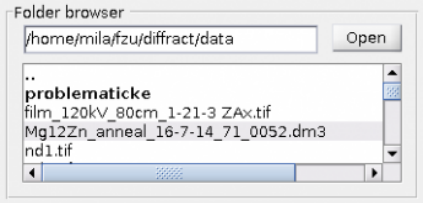


Figure 1.4: Folder browser.

1.3 Material specification

Users does not need to rely on the materials predefined in CrysTBox. They can specify their own material using a text file containing information about the unit cell. The file is expected to have an extension `.cell`. By default such files are located in subdirectory `fzuCommon/cellData/unitCells` in the directory, where CrysTBox is installed to.

A support of CIF format is currently under development.

File structure

The name of the file should reflect its content. Characters '#' and '%' denote comments – the part of the line behind them is not looked at. Multiple white characters are recognized as one, so they can be arbitrarily used by the user for the formating or alignment purposes.

The unit cell properties must be stated in following order:

1. lattice parameter a [nm]
2. lattice parameter b [nm]
3. lattice parameter c [nm]
4. lattice angle alpha [deg]
5. lattice angle beta [deg]
6. lattice angle gamma [deg]
7. material structure ('HCP', 'FCC', 'BCC', Diamond') or by fractional Miller indices of individual atoms in the unit cell written as decimal numbers or fractions
   - in case of Miller indices, one atom must have coordinates [0 0 0]
   - if there is no atom in [0 0 0] coordinates, all atoms are automatically shifted to fulfill this condition
8. atomic numbers – either one number if they are all the same for unit cell atoms, or space-separated values – one per each previously stated atom

Examples

File `Mg HCP.cell` describing Mg HCP unit cell:

```
# Mg HCP
# Lattice parameters - a, b, c [nm]
0.321
0.321
0.521

# Lattice angles - alpha, beta, gamma [deg]
90
90
120

# Structure
HCP
```

```
# Element
12
```

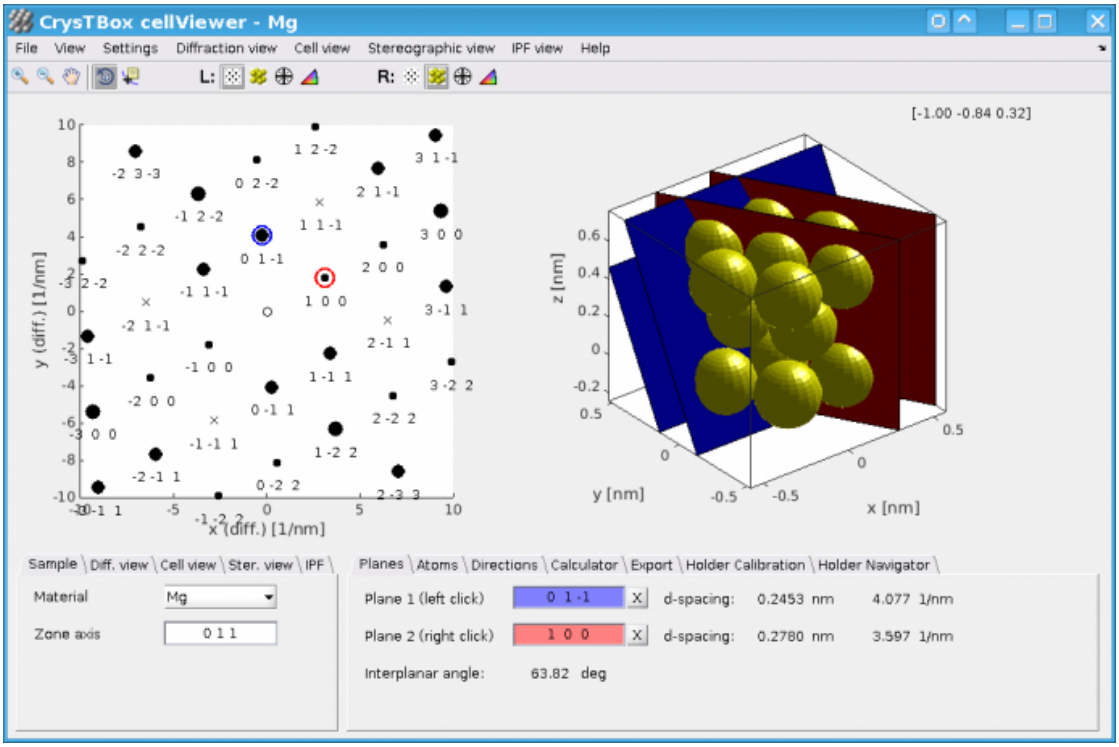
File `GaAs.cell` describing unit cell of GaAs compound:

```
# Lattice parameters - a, b, c [nm]
0.565
0.565
0.565

# Lattice angles - alpha, beta, gamma [deg]
90
90
90

# Positions of atoms in unit cell
[0 0 0]
[0 1/2 1/2]
[1/2 0 1/2]
[1/2 1/2 0]
[1/4 1/4 1/4]
[3/4 3/4 1/4]
[1/4 3/4 3/4]
[3/4 1/4 3/4]

# Element
31 31 31 31 33 33 33 33
```

Chapter 2

cellViewer

Crystallographic visualization tool and calculator.



2.1 About cellViewer

This tool offers a user-friendly interactive interface showing the material from four different perspectives: direct atomic lattice (**cell view**), reciprocal lattice (**diffraction view**), stereographic projection (**stereographic view**) and inverse pole figure (**IPF view**). CellViewer provides two separate slots or views (left and right), each of which can be occupied by one of the four mentioned views. The user can therefore select such combination of two perspectives, which fits his needs. The tool can be used to visualize crystallographic planes, directions, their mutual position and orientation, it provides crystallographic calculator or a tool which helps to calculate the TEM holder tilts leading to the desired sample orientation.

Both, left and right views are interactive and interconnected: if you click at the diffraction spot in the **Diffraction view** for instance, a corresponding crystallographic plane is rendered into the 3D unit cell the **Cell view** or a mark is drawn at appropriate position in **Stereographic view** or **IPF view**. The amount of influence of one view on another can be adjusted by user. For example, the 3D unit cell in the **Cell view** can be freely rotated without affecting other views. If it is needed, however, the diffraction pattern in the **diffraction view** can be instantly updated or the pole in the **stereographic view** can be adjusted so it matches the actual unit cell orientation.

2.2 Input

The only required input of this tool is the sample material. It should be defined as specified in section 1.3. Support of CIF format is under development.

An optional cellViewer input is results from diffractGUI. DiffractGUI can pass the zone axis and pattern orientation to the cellViewer, which can consequently provide a simulated diffractogram and the unit cell orientation directly corresponding to the diffractogram analyzed by diffractGUI.

2.3 Window description

As mentioned above, the window has two views or slots (left and right), each of which can be occupied by **cell view**, **diffraction view**, **stereographic view** or **IPF view**. Content of both views can be selected via context menu (appears after a right click on the view) or using toolbar buttons  ,  ,  and right below the main menu. Various properties and settings of individual views can be adjusted via main menu or more quickly via context menu and tabs in the bottom left part of the window. The tabs in the bottom right part of the windows show details about the selected crystallographic planes, directions, atoms, etc.

A detailed description of the graphical user interface follows.

2.3.1 Diffraction view

This view shows a theoretical spot diffraction pattern. It can be activated by pressing the toolbar button  . Individual diffraction spots are represented by disks. The disk size is derived from a structure factor. Crosses represent extremely weak or forbidden reflections. The sample does not need to be oriented in the exact zone axis and therefore, the diffraction condition is not perfectly met for certain diffraction spots. Those reflection then does not appear black, but they are shaded in gray scale – the darker the spot appears, the better satisfied diffraction condition is.

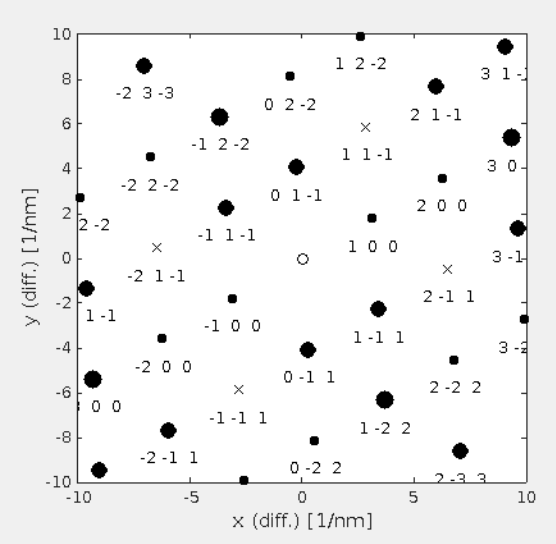


Figure 2.1: Diffraction view

The diffraction view is interactive. User can click on the spots to see the details about corresponding plane in the **Planes** tab and to get the plane itself drawn into the **Cell view**. Basic settings can be adjusted in the context menu or in tab **Diffraction view**, all settings is available in the main menu.

The mouse actions available for this view are following:

Left click
Selects Plane 1 (blue).

Shift + Left click
Selects Plane 2 (red).

Right click
Shows the context menu.

2.3.2 Cell view

This is an interactive view on the unit cell (or a broader atomic lattice) which can be activated via toolbar button . The atoms are represented as spheres coloured according to their element. User can zoom in, zoom out and rotate the unit cell using the toolbar buttons , and . As the cell is rotated, the actual crystallographic orientation can be seen in the top right corner. The actual orientation of the rotated lattice may or may not be instantly reflected in the **Diffraction view** or **Stereographic view**.

Similarly to the **Diffraction view**, user can select individual atoms using a mouse click. Selected atoms are highlighted and detailed information is shown in the **Atoms** tab. If only one atom is selected, its coordinates and element is stated there. In case of two atoms, information about vector between the atoms is printed. Three atoms generate a plane, which is described by normal vector and Miller plane indices. The plane is also rendered in the view. In case of four atoms, information about d-spacing is added.

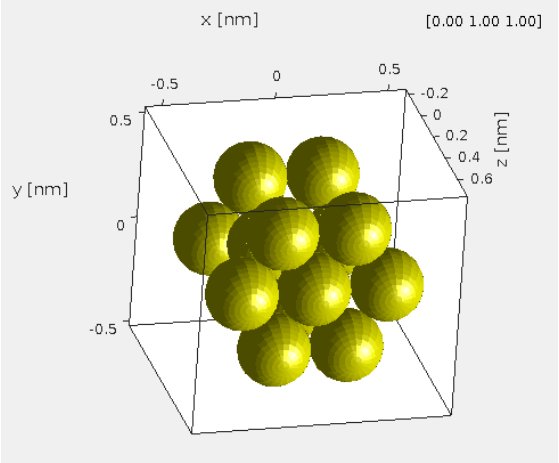


Figure 2.2: Cell view

The mouse actions available for this view are following:

Left click
Selects atom (green).

Shift + Left click / Ctrl+ Left click / Double Left click
Selects atom even if the rotation mode is turned on (toolbar button is highlighted).

Right click
Shows the context menu.

2.3.3 Stereographic view

This view can be activated by the toolbar button . The view is quite intuitive. It offers a stereographic projection of selected planes and direction. The projection pole can be fixed or updated instantly to match the unit cell orientation in the **Cell view**. The grid can reflect either the plane or direction indices.

Clicking the plot, you can select planes or directions which are consequently shown in other views.

The mouse actions available for this view are following:

Left click
Selects Plane 1 (blue).

Shift + Left click
Selects Plane 2 (red).

Ctrl + Left click
Selects Direction 1 (blue).

Ctrl + Shift + Left click
Selects Direction 2 (red).

Right click
Shows the context menu.

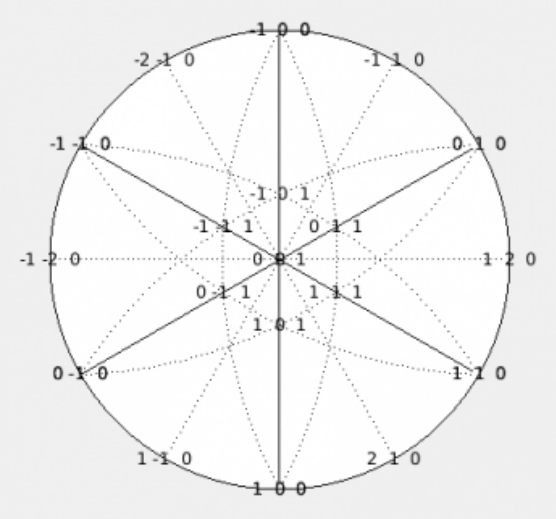


Figure 2.3: Stereographic view

2.3.4 IPF view

This view is quite similar to the **Stereographic view**. It can be activated by the toolbar button  . Compared to the **Stereographic view**, this view only covers a portion of the whole stereographic projection. The border of the shown area is given by three points, which can be set by user. The IPF triangle can be couloured. It can also be drawn into the **Stereographic view** or into the **Cell view** showing directly what the IPF stands for in the context of the unit cell.

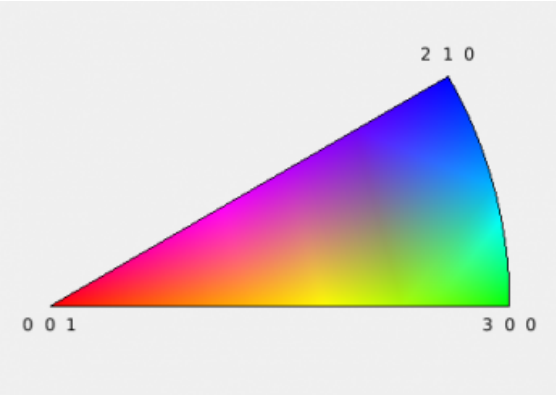


Figure 2.4: IPF view

Clicking the plot, you can select planes or directions which are consequently shown in other views.

The mouse actions available for this view are following:

Left click
Selects Plane 1 (blue).

Shift + Left click
Selects Plane 2 (red).

Ctrl + Left click
Selects Direction 1 (blue).

Ctrl + Shift + Left click
Selects Direction 2 (red).

Right click
Shows the context menu.

2.3.5 Sample tab

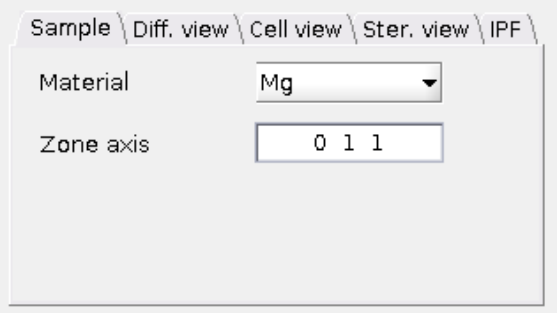


Figure 2.5: Sample tab

Material
Sample material can be specified using this field.

Zone axis
User can set desired zone axis here. Change of this field is always instantly reflected in both, left and right views.

2.3.6 Diffraction view tab

This tab allows for a basic settings of **Diffraction view**. Advanced settings is available in the main menu.

Max. spot index
Here, you can set maximum spot (plane) index of diffraction spots plotted in the **Diffraction view**.

Max. plane dev
This field specifies how tolerant the **Diffraction view** is to declination of actual orientation from the perfect zone axis. The higher is the value, the higher declination from the ideal zone axis is allowed to draw the spot in the diffractogram. Note, that the declination is reflected in the darkness of respective diffraction spot – the higher is the declination, the brighter is the spot.

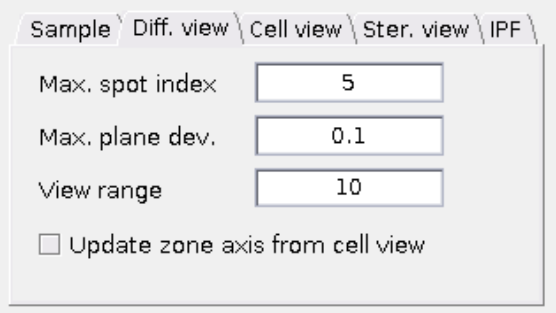


Figure 2.6: Diffraction view tab

View range
Specifies X and Y axes limits of the diffractogram.

Update zone axis from Cell view
If checked, the diffractogram is redrawn instantly as the unit cell is rotated in the **Cell view**.

2.3.7 Cell view tab

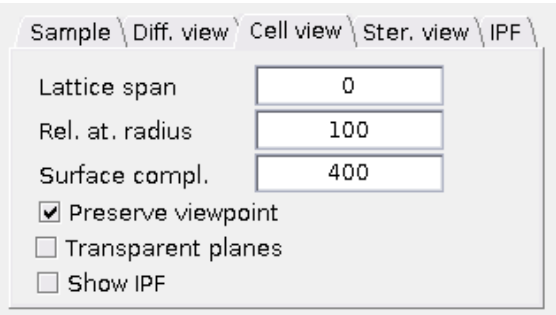


Figure 2.7: Cell view tab

Basic settings of the **Cell view** can be done in this tab. Advanced settings is available in the main menu.

Lattice span
Controls how many atoms are shown in the **Cell view**. Zero denotes "human friendly" unit cell (e.g. whole hexagon in case of HCP structure). Numbers higher or equal to one stand for a block of NxNxN "true" unit cells. Higher number of atoms may result in increased hardware requirements.

Rel. at. radius
Using the Relative atomic radius, you can set size of spheres representing the atoms as percent of distance between the two nearest atoms in the structure. In other words, value of 100 means, that two nearest atoms in the unit cell will touch each other. Numbers higher than 100 make some of the atoms intersect with each other, while Numbers lower than 100 make the **Cell view** sparser and easier to see through.

Surface complexity
Each atom visualization (sphere) consists of many flat faces. Number of the faces can be set here. Higher numbers make the atoms smoother. Higher number of faces may result in an increased hardware requirements.

Preserve viewpoint
The **Cell view** viewpoint is reset (to given zone axis orientation) after applying some **Cell view** changes (such as **Surface complexity**, **Rel. at. radius** and so on). This checkbox allows to preserve the unit cell orientation set by the user (e.g. by rotation, TEM holder tilting etc.).

Transparent planes
This checkbox makes the planes in the **Cell view** transparent, so that the atoms behind them can still be seen.

2.3.8 Stereographic view tab

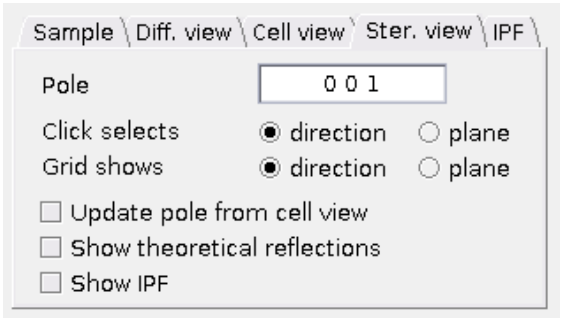


Figure 2.8: Stereographic view tab

Here you can control the **Stereographic view**. Advanced settings is available in the main menu.

Pole
Miller indices of the direction corresponding to the projection pole can be set here.

Click selects
This radio button determines whether the left mouse click selects a direction or plane. The other one can be selected with Ctrl.

Grid shows
Here it can be specified, whether the grid reflects directions or plane normals.

Update pole from cell view
This checkbox allows the projection pole and upper direction to be automatically updated if the unit cell is rotated.

Show theoretical reflections
If checked, the theoretical planes (corresponding to the reflections in the diffractogram) are shown in the stereographic projection. **Max. spot index** from **Diffraction tab** applies here.

Show IPF
Appearance of the IPF in the **Stereographic view** can be controlled here.

2.3.9 IPF view tab

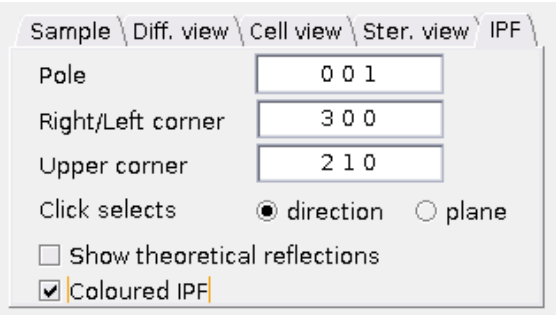


Figure 2.9: IPF view tab

The IPF can be adjusted here. Advanced settings is available in the main menu.

Pole
The IPF pole (corresponds to the bottom left/right corner) is specified here as a direction vector in Miller indices.

Right/Left corner
The side corner of the IPF triangle is set here as a direction vector in Miller indices.

Upper corner
The upper corner of the IPF triangle is defined in this field as a direction vector in Miller indices.

Click selects
This radio button determines whether the left mouse click selects a direction or plane. The other one can be selected with Ctrl.

Show theoretical reflections
If checked, the theoretical planes (corresponding to the reflections in the diffractogram) are shown in the stereographic projection. **Max. spot index** from **Diffraction tab** applies here.

Coloured IPF
This checkbox switches between white and coloured IPF.

2.3.10 Planes tab

This tab states details about the planes either given by a mouse click to the views or entered manually using fields **Plane 1** and **Plane 2** in this panel.

Plane 1
This field states the Miller indices of Plane 1 (the blue one). It can be filled manually or automatically after clicking to the **Diffraction view**, **Stereo view** and **IPF view**.

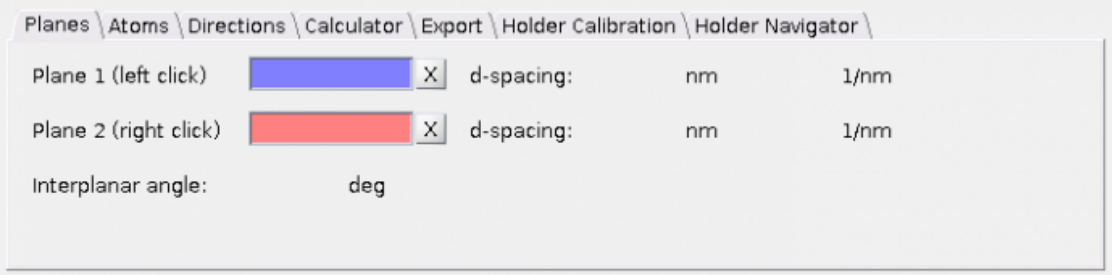


Figure 2.10: Planes tab

Plane 2
This field states the Miller indices of Plane 2 (the red one). It can be filled manually or automatically after clicking to the **Diffraction view**, **Stereo view** and **IPF view**.

d-spacing
D-spacings of both planes **Plane 1** and **Plane 2** are stated here.

Interplanar angle
If both planes, **Plane 1** and **Plane 2**, are specified, an angle between them is printed in here.

2.3.11 Atoms tab

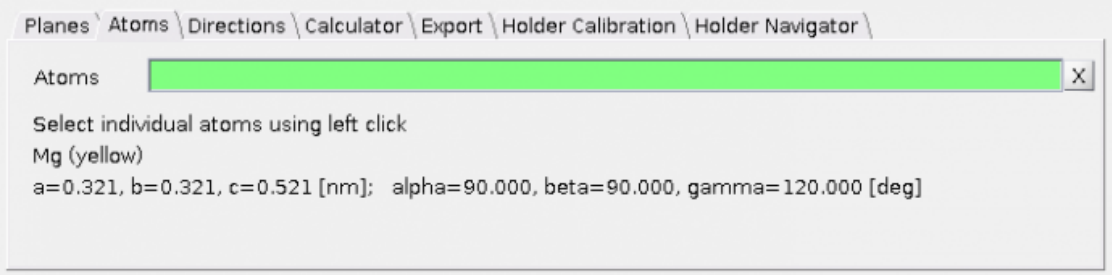


Figure 2.11: Atoms tab

Details about atoms selected by the mouse-click in the **Cell view** are mentioned here. As you click on particular atom, its coordinates (in Miller indices) are added to the field **Atoms**. Atomic coordinates can also be entered manually, separating individual atoms with semicolon. The details about the selection depend on how many atoms are selected:

- one atom – element, atom coordinates (Miller and Cartesian)
- two atoms – elements, direction of vector between the two atoms (Miller and Cartesian) and their distance (Miller and Cartesian)
- three atoms – elements, plane normal vector (in Miller and Cartesian coordinates)
- four atoms – elements, plane normal vector (in Miller and Cartesian coordinates) and d-spacing

2.3.12 Directions tab

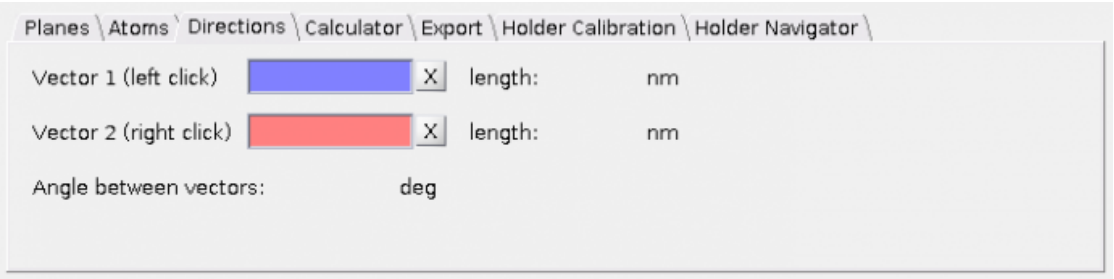


Figure 2.12: Directions tab

This tab states details about the crystallographic directions either given by a mouse click to the views or entered manually using fields **Direction 1** and **Direction 2** in this panel.

Vector 1
: This field states the Miller indices of Direction 1 (the blue one). It can be filled manually or automatically after clicking to the **Stereo view** and **IPF view**.

Vector 2
: This field states the Miller indices of Direction 2 (the red one). It can be filled manually or automatically after clicking to the **Stereo view** and **IPF view**.

Length
: Lengths of **Direction 1** and **Direction 2** are stated here.

Angle between vectors
: If both directions, **Direction 1** and **Direction 2**, are specified, an angle between them is printed in here.

2.3.13 Calculator tab

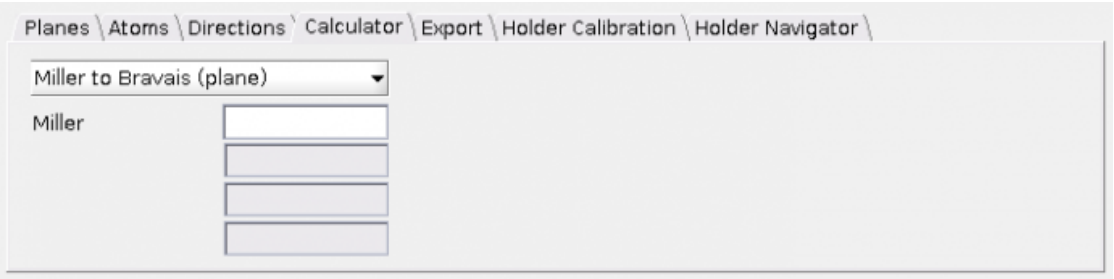


Figure 2.13: Calculator tab

This tab offers a crystallographic calculator. After selecting the quantity to be calculated in the pop-up menu, the descriptions of required parameters appear next to the text fields. When all the inputs are set correctly, the results are printed at the right hand side of the tab.

Supported calculations involve:

- conversion between Miller and Bravais notation for planes and directions
- conversion between Miller and Cartesian coordinate system for planes and directions
- enumeration of interplanar and interdirectional angles
- d-spacing enumeration and assignment
- calculation of structure factor, atomic scattering amplitude or extinction distance

2.3.14 Export tab

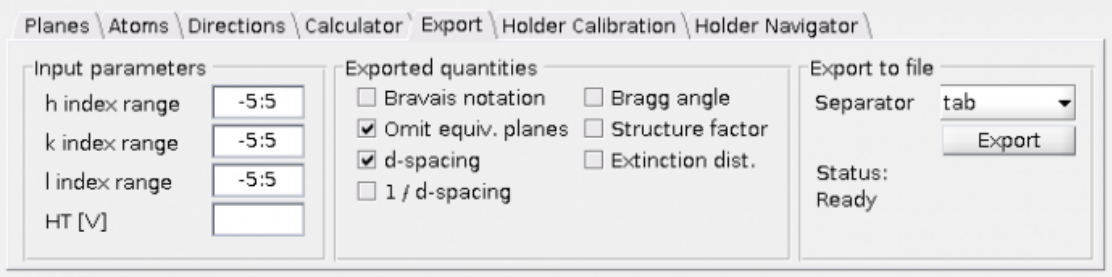


Figure 2.14: Export tab

Some of the crystallographic quantities can be exported to a text file using this tab.

Input parameters
This panel is used to set the calculation inputs – mainly the range of Miller indices of enumerated planes. Some calculations also require the acceleration voltage.

Exported quantities
Quantities exported to the table are specified here using the checkboxes.

Export file
In this tab, you can specify character separating individual values in the table using **Separator** pop-up menu. Then, you can launch the exporting procedure pressing the button **Export**. Status of the procedure is stated bellow.

2.3.15 Holder calibration tab

This tool allows you to simulate the TEM sample holder. Some basic calibration is required for this purpose. Holder visualization on the right hand side of the tab should help the user to check, whether all the values have been set correctly.

Holder azimuth
This field specifies orientation of the holder with respect to the sample orientation currently shown in the **Cell view**. This value is an angle between alpha tilt axis and Y (vertical) axis in degrees.

Direction of positive rotation angles
These pop-up menus allow you to specify whether the positive angles tilt the holder to the right or left for alpha tilt and upwards or downwards for beta tilt (watching from the holder handle towards the holder tip).

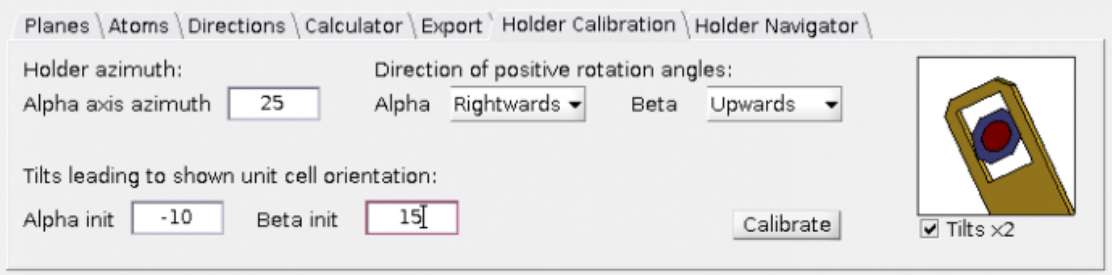


Figure 2.15: Holder calibration tab

Tilts leading to shown unit cell orientation
These fields are used to set alpha and beta tilt (in degrees) corresponding to the sample orientation as currently shown in the **Cell viewer**.

Calibrate
If all previously mentioned values are set and the holder visualization agrees with the reality, calibration can be confirmed pressing this button.

2.3.16 Holder navigator tab

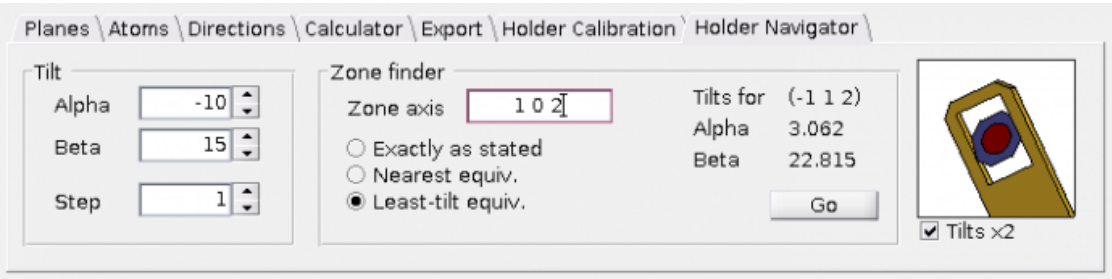


Figure 2.16: Holder navigator tab

This panel allows you to simulate TEM holder tilts. It can also calculate holder tilts required to get the sample to desired orientation.
Note: If the fields in this tab are not enabled, please perform the calibration using the **Holder calibration tab**

Tilt
Text fields **Alpha** and **Beta** (in degrees) can be used to tilt the sample in the **Cell view** and to see corresponding diffraction pattern in the **Diffraction view** (if the checkbox **Update zone axis from cell view** in panel **Diffraction view** is check-marked).

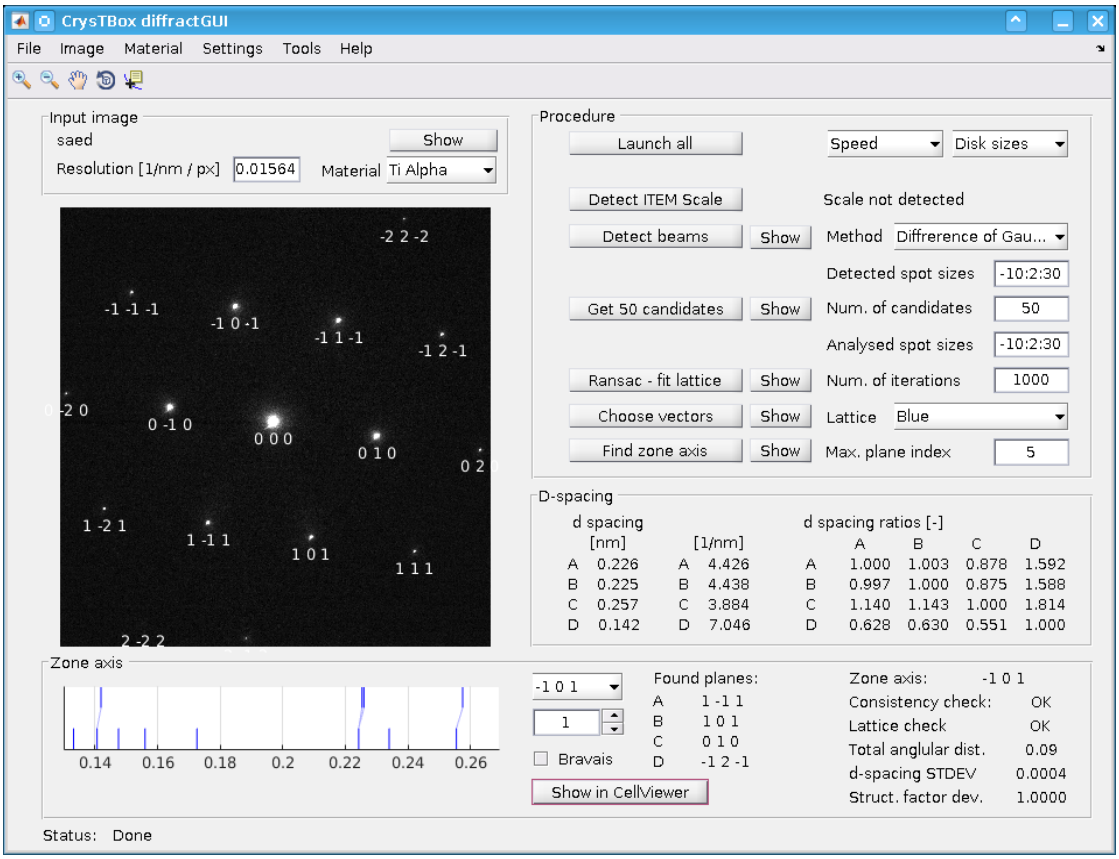
Zone finder
This panel allows you to find the alpha and beta tilts leading to the desired zone axis. Usually, the TEM holder tilts are limited to a certain range. Therefore, you can select whether you want to be navigated exactly to the zone axis which is stated in the text field (radio button **Exactly as stated**) or rather to such crystallographically equivalent zone axis, which is nearest to the actual sample orientation (radio button **Nearest equiv.**) or to the

crystallographically equivalent zone axis with the least holder tilts (radio button **Least-tilt equiv.**).

Chapter 3

diffractGUI

Automated analysis of spot and disk diffraction patterns.



3.1 About diffractGUI

The main purpose of this tool is to automatically determine the zone axis from a diffraction pattern, assign crystallographic indices to the diffraction spots and to measure the interplanar distances. The input image can be a spot pattern (SAED), disk pattern (CBED, nanodiffraction) or HRTEM image. Except of the automatic zone axis determination, diffractGUI can be helpful for manual analyses (it measures d-spacings and interplanar angles) or during camera length calibration.

3.2 Input

The tool requires two basic inputs: an image and sample material. The image should depict a spot or disk diffraction pattern or HRTEM image. The tool can process a wide range of diffractograms – from SAED (well defined diffraction spots), through nanodiffraction (blurry spots) to CBED (textured disks). The tool can even process patterns depicting more patterns at time (twins, intercrystalline boundaries). Preferred image format is DM3, as it contains scaling information. Nevertheless, all common image formats (JPG, PNG, TIFF, etc.) are supported.

The sample material should be defined as specified in section 1.3. Support of CIF format is under development.

3.3 Window description

The application window consists of one figure and several panels. The figure allows the user to see the input image and graphical visualization of the results. Surrounding panels provide control of the analysis, allow settings of the most important parameters and list the results.

A detailed description of the graphical user interface follows.

3.3.1 Input image panel

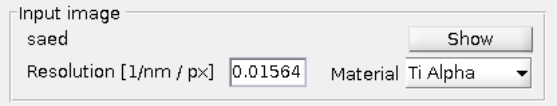


Figure 3.1: Input image panel

This panel contains basic information about the input image such as the image name, resolution and sample material corresponding to the depicted pattern.

Resolution
The image resolution can be set manually here.

Material
Material can be chosen from this pop-up menu. You can pick one from listed materials or you can select a file describing your own material (file specification). Material does not need to be chosen prior to the analysis, it can be changed during the procedure.

Show
Shows the input image.

3.3.2 Procedure panel

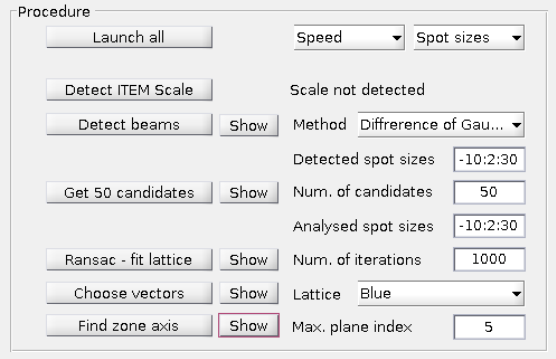


Figure 3.2: Procedure panel

This panel allows you to launch the analysis procedure and to control its individual steps if needed. The analysis can be launched by single click on the button **Launch all** or it can be performed step by step by clicking on buttons bellow corresponding to individual analysis steps. Partial results of the individual steps can be displayed using corresponding **Show** buttons.

Launch all
: This button launches all the steps of the analysis at once. Prior to launching the analysis, some basic settings can be done using **Speed** and **Spot size** pop-up menus

Speed
: This pop-up menu allows you to speed-up the beam detection and lattice fitting, which are normally the most time consuming steps. Fast mode, however, is recommended for the less tricky images. This settings applies on the blob detection only. It does not apply on disk detection using the Hough transform.

Spot size
: Here you can give the tool a hint whether to focus on smaller spots, larger spots or disks. In case of diffraction pattern consisting of textured disks (such as CBED) value **Disks (CBED)** shall be set.

Detect ITEM scale
: Detection of a scale bar burnt into the image by ITEM acquisition software is launched by this button. The result can be found next to the button. If the detection is successful, bar length should be stated together with the length stated in the scale bar – for example "Label: "10 1/nm", Length: 158 px".

Detect beams
: This button starts the detection of diffraction spots or disks in the image.

Method
: Method used for the detection of diffraction spots or disks can be set here. The spots can be detected using blob detection methods (all entries containing "Gaussian" or "Hessian"), while the disks should be detected using Hough transform.

Detected disk sizes
: Sizes of the spots to detect can be specified here for the blob detection methods.

Get N candidates
Picks N strongest detections for further processing. Number of the selected candidates can be changed using **Num. of candidates**.

Num. of candidates
This filed states number of the strongest detected spots/disks, which should serve for fitting a regular reciprocal lattice using RANSAC algorithm. Number of finally accepted candidates does not need to be equal to the number specified by the user. It can be lower (if there is insufficient number of detections) or higher (if there is more than one candidate with detection score equal to the score of the N-th candidate).

Analyzed spot size
The algorithm can analyze only a specific subset of the detected disks (**Detected disk sizes**). Here you can specify sizes of the spots from which the N strongest candidates are chosen.

Ransac – fit lattice
RANSAC algorithm fits a regular reciprocal lattice to the set of strongest detected spots or disks.

Num. of iterations
Number of RANSAC iterations.

Choose vectors
Several "basic" vectors are localized in the regular lattice found by RANSAC algorithm. The details about the vectors can be seen in **D-spacing** panel. If the vectors are not centered correctly on the transmitted beam, you can center them manually using menu **Image / Set primary beam**. If there is more than one lattice found by RANSAC, the vectors are localized in the lattice specified using **Lattice** pop-up menu.

Lattice
If there are multiple lattices in the image and RANSAC is set to detect them (**Settings / RANSAC / RANSAC Multimodel settings**), you can select the lattice to be processed.

Find zone axis
After this button is pressed, the algorithm tries to map the theoretical d-spacings and interplanar angles to the experimental ones measured in the image. If it succeeds, the results are shown in the **Zone axis** panel.

Max. plane index
This field sets a maximal plane index (in Miller indices) of the theoretical planes, whose d-spacings and interplanar angles are compared to the experimental values in order to identify the "basic" vectors (see **Choose vectors)** and determine the zone axis.

3.3.3 D-spacing panel

This panel shows the details about the lattice vectors measured in the image using **Choose vectors** button. Exact vector lengths, length ratios and d-spacings are stated. A diagram identifying the vectors in the image and showing the interplanar angles (see bottom left image) can be shown by the **Show** button next to the button **Choose vectors**.

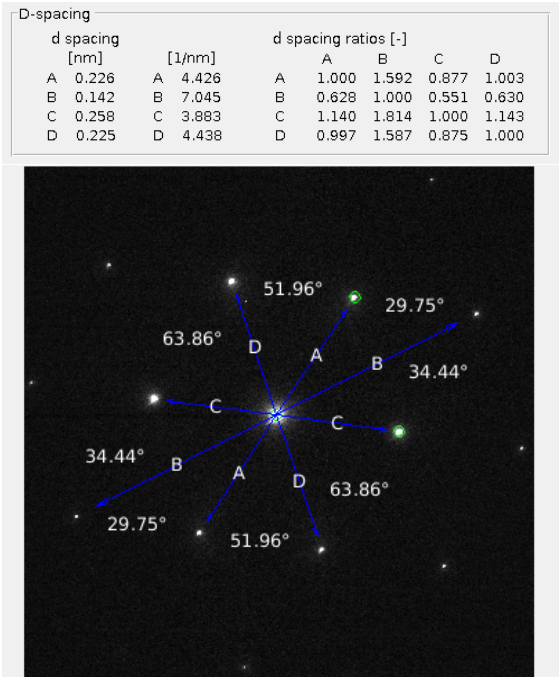


Figure 3.3: D-spacing panel (top) Chosen 'basic' vectors (bottom)

3.3.4 Zone-axis panel

The final results of the analysis are shown here. If there exist some valid assignment of the measured d-spacings to the theoretical ones, the details of such assignment are stated here. On the left hand side, there is a visualization of the assignment. The blue vertical lines on the bottom of the plot represent the theoretical d-spacings specific of the material chosen using **Material** pop-up menu. The vertical blue lines on the top of the plot stand for the d-spacings measured in the experimental image and listed in the **D-spacing** panel. Light-blue lines between the theoretical and experimental d-spacings represent the assignment – each measured d-spacing is paired with the theoretical one. Only those assignments which fulfill certain physical and crystallographical constraints (see **Lattice check** and **Consistency check**) are taken into account. Each assignment is scored. The score is based on a comparison of the experimental and theoretical d-spacing, interplanar angles and it optionally reflects the structure factor. Only certain number of the best-scored assignments (and corresponding zone axes) is listed in the **Zone ax.** pop-up menu. There are also some quality measures reflecting how chosen assignment comply with the theory (see **Total angular dist.** and **d-spacing STDEV**).

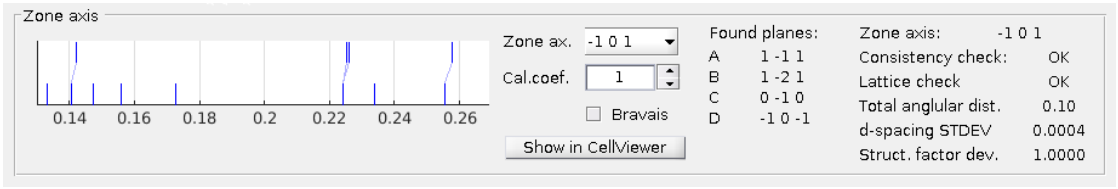


Figure 3.4: Zone-axis panel

Zone ax.
Typically, there are many possible assignments and therefore many possible zone axes, because the measured d-spacing may correspond to many crystallographically equivalent planes. Sometimes, it may also happen, that the experimental d-spacing can be paired with more than one theoretical d-spacing. Possible assignments (and corresponding zone axes) are listed in this pop-up menu. Only several best-scored zone axes are available here. Maximum number of enlisted zone axes can be set using **Settings / Max. number of resulting solutions**.

Cal. coef.
This value allows for an adjustment of camera calibration inaccuracies. Measured d-spacing values are multiplied by this coefficient prior to the comparison with the theoretical d-spacings.

Found planes
This table states the details of the chosen assignment – the plane indices corresponding to the experimentally measured vectors found using **Choose vectors** button.

Zone axis
Chosen zone axis.

Consistency check
Checks, whether all pairs of four "basic" vectors agree on resulting zone axis. If the chosen assignment fulfills this constraint, "OK" appears.

Lattice check
Checks, whether vector additions of all pairs of four "basic" vectors agree with Miller indices of corresponding spots. If the chosen assignment fulfills this constraint, "OK" appears.

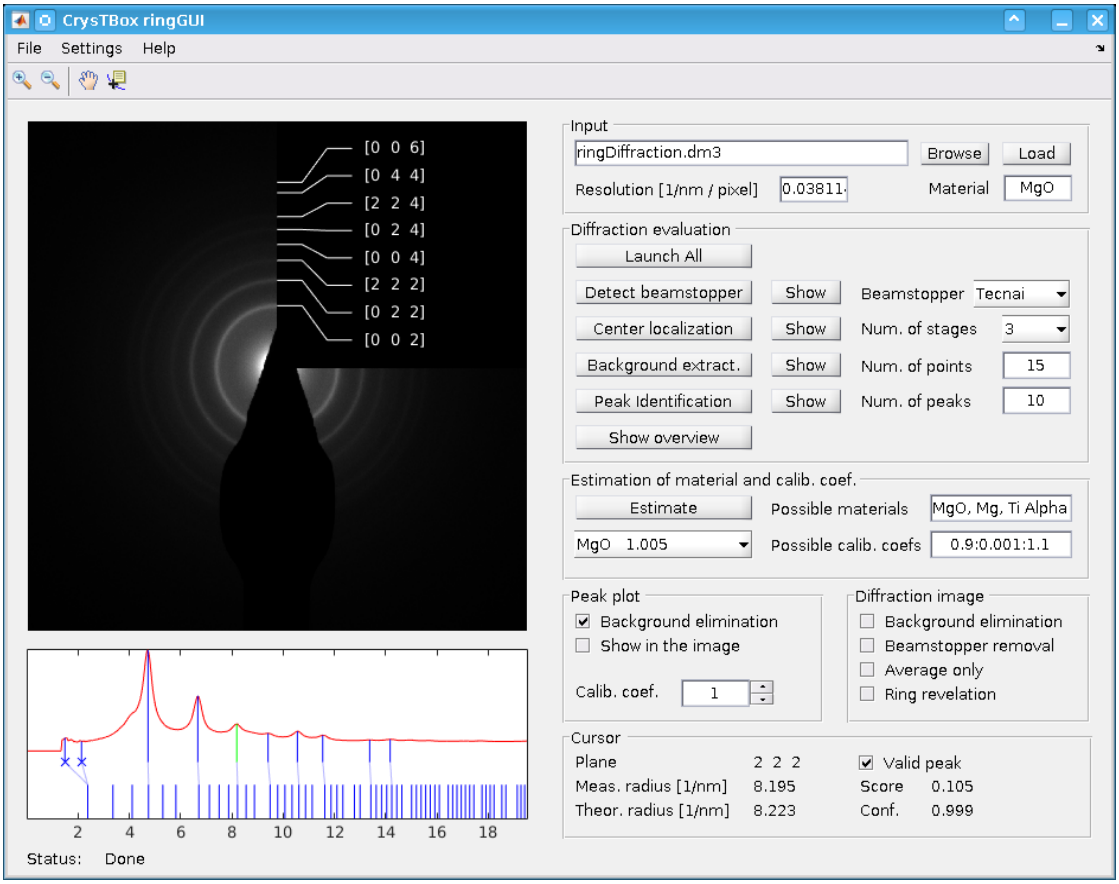
Total angular dist.
Sum of squares of angular distances between the four measured "basic" vectors and their theoretical counterparts. The lower number, the better. Values may differ from image to image, from material to material, however numbers higher than ten usually indicate a problem.

d-spacing STDEV
This number equals to the standard deviation of differences between the measured and theoretical d-spacing values. The lower numbers the better. Values may differ from material to material, from zone axis to zone axis, however reasonable values are thousandths or hundredths.

Chapter 4

ringGUI

Automated analysis of ring diffraction patterns.



4.1 About ringGUI

The main purpose of this tool is to automatically identify crystallographic planes corresponding to the rings depicted in the ring diffractogram. If the sample material is not exactly known, ringGUI can select the sample material from a list of candidate materials given by the user. The tool can also automatically enumerate the camera length inaccuracy, so it can be very helpful during the camera length calibration.

4.2 Input

The tool requires two basic inputs: a diffraction image and sample material. The image should depict a ring diffraction. The rings does not need to be complete. Even very spotty images can be successfully processed. The image, however, should not be significantly distorted – the rings should not be apparently elliptical for instance. Preferred image format is DM3, as it contains scaling information. Nevertheless, all common image formats (JPG, PNG, TIFF, etc.) are supported.

The sample material should be defined as specified in section 1.3. Support of CIF format is under development.

4.3 Window description

The application window consists of two figures and several panels. The figures allow the user to see the input image and a graphical interpretation of some results. The surrounding panels allow to control the analysis procedure and list some results.

A detailed description of the graphical user interface follows.

4.3.1 Diffraction image

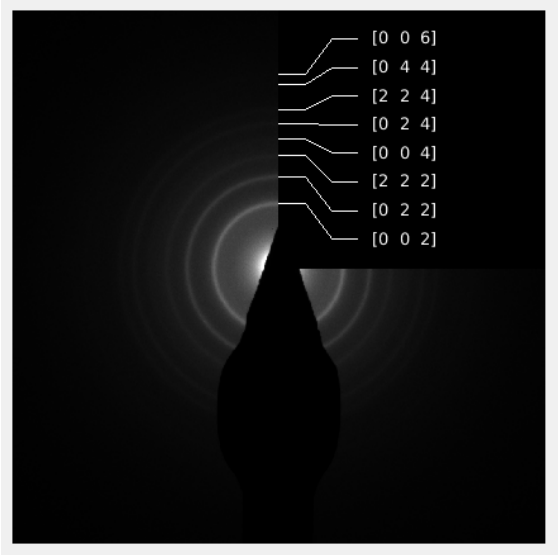


Figure 4.1: Diffraction image

This figure shows the input image and/or some graphical visualization of some results. This particular example shows an identification of diffraction rings and can be obtained using button **Show overview**.

4.3.2 Peak plot

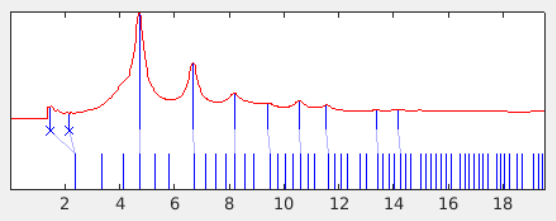


Figure 4.2: Peak plot

The diffraction profile is plotted here once it is known. The profile is a circular average of the image intensity as function of distance from the ring center. The left border of the plot corresponds to the ring center, while the right one corresponds to the image border. Vertical blue lines in the bottom part of the plot stand for the theoretical ring radii specific to the sample material. Vertical blue lines in the upper part (in the profile) represent the ring radii measured in the experimental image. Light-blue lines in between illustrate the assignment between the measured radii and their theoretical counterparts. This plot is interactive. You can click the blue lines corresponding to either theoretical or experimental d-spacing and you should see details in **Cursor** panel and a visualization in the **Diffraction image**.

4.3.3 Input panel

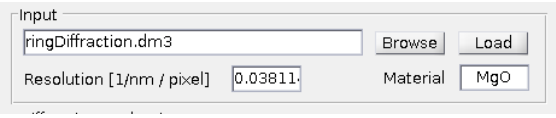


Figure 4.3: Input panel

This panel contains information about the input image.

Browse
This button allows you to find the input image in the directory structure.

Load
Loads given input image.

Resolution
The image resolution can be set manually here.

Material
The sample material can be specified using this field.

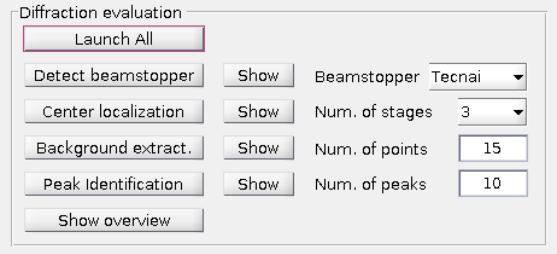


Figure 4.4: Diffraction evaluation panel

4.3.4 Diffraction evaluation panel

The analysis procedure can be controlled using this panel. The whole procedure can be launched at once by single click on the **Launch all** button or it can be performed step by step clicking on the buttons corresponding to individual steps. Partial results of individual steps can be displayed using corresponding **Show** buttons.

Launch all
This button launches all the analysis steps at once.

Detect beamstopper
The algorithm requires the beamstopper to be detected. This can be done manually or automatically for the known beamstoppers. Resulting beamstopper mask is shown once this step is completed. If the mask does not fit the beamstopper correctly, the user shall outline the beamstopper manually. Manual localization can be performed by setting the pop-up menu **Beamstopper** to "Manual" and then clicking the button **Detect beamstopper**.

Beamstopper
This pop-up menu specifies type of the beamstopper for automatic detection or manual localization.

Center localization
This step localizes center of the diffraction rings. This can be done automatically in several stages (see **Num. of stages)** or manually.

Num. of stages
This pop-up menu defines number of stages for the automatic center localization. The higher is the number of stages, the more precise and time consuming the localization is. User can also localize the center manually setting the value to "Manual"

Background extract.
Typically, there is some background in the diffraction image – central parts of the image are brighter compared to the image borders. This button is used to extract the background from the image, which is necessary for precise and reliable ring localization.

Num. of points
The background is approximated by a hyperbolic function touching the diffraction profile from bellow. Number of points, where the hyperbola should touch the diffraction profile is specified here.

Peak identification
This step localizes certain number of the highest peaks in the profile.

Num. of peaks
Number of the highest peaks to be localized (and subsequently crystallographically identified) in the diffraction profile can be specified in this field.

Show overview
Shows an assignment of the plane indices to the diffraction rings into the diffraction view.

4.3.5 Panel for Estimation of material and calib. coef.

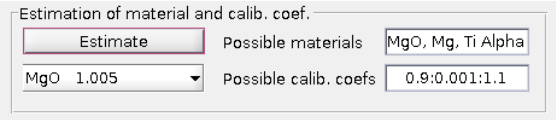


Figure 4.5: Panel for Estimation of material and calib. coef.

If the sample material is not known, the tool can select the most appropriate one from the list given by the user. Similarly, the calibration coefficient can be determined – the user can specify a range of possible values and the algorithm automatically finds the one which best fits the experimental data. Both functionalities can be combined together, so that ringGUI searches for the most appropriate material and calibration coefficient at once.

Possible materials
Comma-separated list of possible sample materials (see **Material** for details).

Possible calilb.coefs
Range of possible calibration coefficients (see **Calib. coef.** for details).

Estimate
Button launching the estimation of the material and/or calibration coefficient.

MgO 1.005 (pop-up menu with estimation results)
Several best-scored combinations of the material and calibration coefficient are stated in this pop-up menu. Selection of particular menu entry automatically sets given sample material and calibration coefficient (calibration coefficient is adjusted, theoretical ring radii are redrawn and assignments to the experimental radii are recalculated).

4.3.6 Peak plot and Diffraction image panels

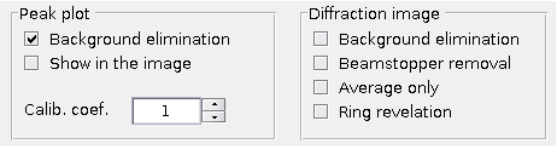


Figure 4.6: Peak plot and Diffraction image panels

These two panels adjust the **Peak plot** and **Diffraction image**.

Background elimination (Peak plot panel)
This checkbox specifies whether to eliminate the background from the **Peak plot** (and from the **Diffraction image** if **Show in the image** is selected).

Show in the image (Peak plot panel)
The checkbox controls whether the diffraction profile is shown in the **Diffraction image**.

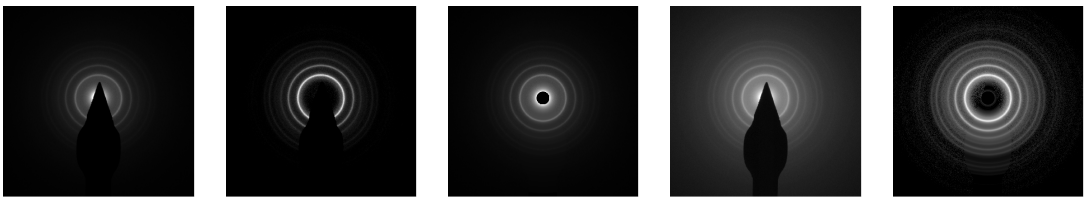
Calib. coef. (Peak plot panel)
This value allows for an adjustment of the camera length calibration inaccuracies. The measured ring radii are multiplied by this coefficient prior to the comparison with the theoretical ones.

Background elimination (Diffraction image panel)
Allows for a removal of the background from the diffraction image (see figure below).

Beamstopper removal (Diffraction image panel)
Removes the beamstopper from the image (see figure below).

Average only (Diffraction image panel)
Shows the intensities calculated from the circular average instead of the input image. This makes the image smoother.

Ring revelation (Diffraction image panel)
Makes the weaker beams more apparent (see figure below).



Original image | Background eliminated | Beamstopper removed | Rings revealed | All together

Figure 4.7: Image enhancement provided by ringGUI

4.3.7 Cursor panel

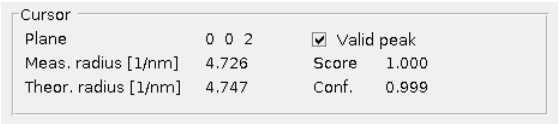


Figure 4.8: Cursor panel

In this panel, one can see the details about the theoretical and experimental ring radii chosen using a mouse-click into the **Peak plot**.

Plane
Miller indices corresponding to the given radius.

Meas radius
Radius measured in the experimental image.

Theor. radius
The theoretical radius specific to the sample material.

Valid peak
This checkbox allows to exclude currently selected peak from the evaluation. Excluded peaks (denoted by small cross in the **Peak plot**) are not displayed in the overview (see **Show overview**) and they are not taken into account during the estimation of material or calibration coefficient (see **Panel for Estimation of material and calib. coef.**.

Score
Score reflecting relative height of the peak.

Conf.
Confidence measure reflecting how the tool is confident, that current peak correspond to a ring in the image.

Chapter 5

How to cite

If you find the software helpful for your research, please cite it. Reference entries and bibtex records of this document and related articles can be found in the main menu entry Help / Citation.

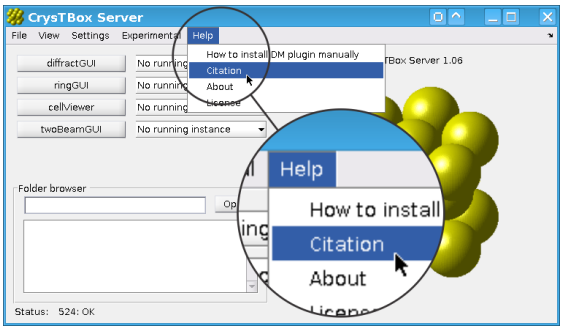


Figure 5.1: Reference entries and bibtex records can be found in Help / Citation.

A reference entry corresponding to this documment is following:

M. Klinger. *CrysTBox - Crystallographic Toolbox*. Institute of Physics of the Czech Academy of Sciences, Prague, 2015. ISBN 978-80-905962-3-8. URL `http://www.fzu.cz/~klinger/crystbox.pdf`

And a bibtex record is following:

```
@book{klinger2015crystboxManual,
  title={CrysTBox - Crystallographic Toolbox},
  author={Klinger, M.},
  isbn={978-80-905962-3-8},
  url={http://www.fzu.cz/~klinger/crystbox.pdf},
  year={2015},
  address = {Prague},
  publisher={Institute of Physics of the Czech Academy of Sciences},
}
```