jems GUI

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Contents

List of Figures

List of Tables

1 Introduction

This document describes jems **G**raphical **U**ser **I**nterface (GUI). The GUI shows little variations depending on the operating system, i.e. MacOSX, Windows or Linux. The GUI of the MacOSX version is introduced in this document.

1.1 Starting jems

On MacOSX, jems is an ordinary application. On *Windows* or *Linux* jems is started using a command file (either .bat or .sh). At startup the **About window** is briefly visible and shows the jems version. Loading the jems application takes several seconds since many classes stored as java classes are translated (compiled) into machine code.

1.2 jems folder

When first started jems create the folder "$\sim /jems$" that contains the following files:

1. **jemsAFF.txt** : copy of the X-ray **A**tomic **F**orm **F**actors. The atomic form factors can be modified and employed in calculations.
2. **jemsCCDCameras.txt** : the **M**odulation **T**ransfer **F**unctions of the camera(s) attached to the microscope.
3. **jemsDefaultCrystal.txt** : the description of the crystal loaded when jems starts.
4. **jemsLicense.txt** : a copy of the jems license created at the time the license code is provided.
5. **jemsMatrixPrecipitateOR.txt** : a list of **O**rientation **R**elationships between matrix and precipitates (Fig. 26c).
6. **jemsMicroscopes.txt** : the characteristics of the microscope defined using the **Parameters** → **Microscope** dialogue (Fig. 108).
7. **jemsPreferences.txt** : the jems running preferences defined using the **Parameters** → **Preferences** dialogue.
8. **jemsRecents.txt** : list of the recently opened **.txt** crystal files.
9. **jemsRecentsCIF.txt** : list of the recently loaded **.cif** files (Fig. 8).

It is recommended to keep "$\sim /jems$" folder free of any other information.

1.3 CCD cameras

The MTF of the CCD cameras are described either by 4 exponential, 4 gaussian, 4 lorentzian or 2 gaussian and 2 lorentzian functions (Fig. 74). The following tags identify the CCD parameters:

- **NA** : name (used as the tab label).
- **LA** : label.
- **PS** : pixel size [μm].
- **RO** : rows number.
- **CO** : columns number.
- **CO** : columns number.
- **MO** : fitting model (0 : exponential, 1 : gaussian, 2 : lorentzian, 3 : mixed).
- **Ai**, **Bi** : fitting coefficients (the A_i coefficients sums up to 1).

A typical set of MTF is shown below[1].

```
NA|Default camera+LA|Default camera+PS|24+RO|1024+CO|1024+MO|4+A1|0.25+A2|0.25+A3|0.25+A4|0.25+B1|0.0+B2|0.0+B3|0.0+B4|0.0+
NA|msc 1K+LA|cm-20+PS|24+RO|1024+CO|1024+MO|1+A1|0.28980445861816406+A2|0.6512896418571472+A3|0.013287605717778206+A4|0.045618306845426 56+B1|0.45493492+B2|0.918
```

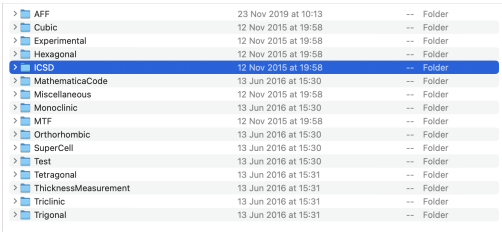
[1]First camera has a perfect uniform MTF, i.e. 1.0 from 0 to Nyquist frequency.

1.4 Data files

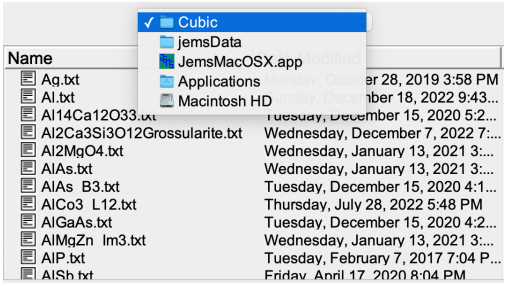
jems contains several data files either in *.txt* or *.cif* formats. Depending on the operating system there are accessible in the folder:

- **MacOSX** : /Applications/JemsMacOSX.app/jemsData.
- **Linux** : ∼/bin/jemsLinux64/jemsLinux/jems/jemsData.
- **Windows** : /Program files/jemsWindows7/jemsWindows/jems/jemsData.

It is recommended to create **working** directories and to save jems data and other files in these directories (one for each crystal file). Loading a *.txt* from a **working** directory makes it the default directory. This makes erasing jems files easier without the risk to delete jems own data files.



(a) jems data files.



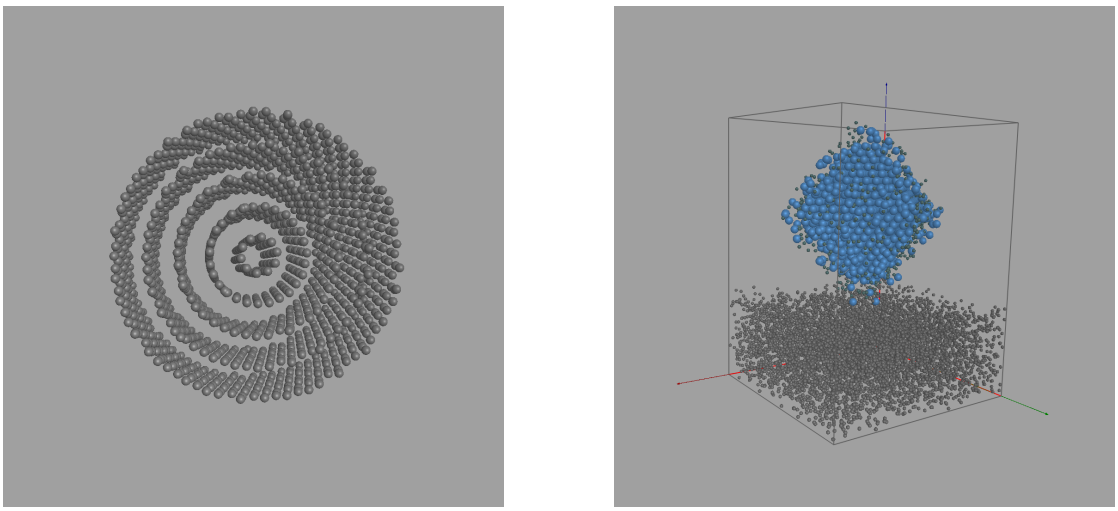
(b) Cubic data files access path (MacOSX version).

Figure 1: jems data files folder.

The data files are mainly organised by crystal system (i.e. cubic, hexagonal, ...). Several other folders contains:

- **AFF** : a backup copy of jemsAFF.txt (to replace jemsAFF.txt in ∼ /*jems*).
- **Experimental** : some experimental images.
- **ICSD** : several .cif files organised by chemical formula.
- **MathematicaCode** : examples of Mathematica code reading jems images.
- **Miscellaneous** : diverse data files (amorphous, graphene).
- **MTF** : a suite of amorphous carbon thin film images for measuring the MTF.
- **SuperCell** : a collection of data files describing super-cells.

- **Test** : several data files for testing jems, in particular carbonNanotube5Walls.txt (Fig. 2a), PtOctahedron.txt (Fig. 2b).
- **ThicknessMeasurement** : images and Al.txt data file for demonstrating thickness measurement using the CBED method.



(a) Carbon nanotube (5 walls).

(b) Pt octahedron super-cell.

Figure 2: Typical super-cells.

1.5 Default crystal

The default crystal is a text file containing the crystal parameters necessary for calculating diffraction patterns and images. Tags are used to name the file and the different crystal parameters. A "|" separates the tag and its value. When jems is first started the $AuCuL_{12}$ structure is put into "$\sim /jems$" folder. Though the crystal files can be directly created and/or modified using a text editor, it is much simpler to use specific jems dialogues (Figs. 11, 17, 19).

The tags are defined as:

- **file** : path to the crystal file.
- **name** : name of the structure.
- **creator** : who created it.
- **date**: when it was created.
- **system** : crystallographic system.
- **superCell** : set eithe to false (unit cell) or true (super cell).
- **HMSymbol** : space-group number and Hermann-Mauguin (short symbol).
- **rps** : **R**egular **P**oint **S**ystem code.
- **lattice** : lattice parameters (a, b, c, α, β, γ).
- **atom** : atom definition (symbol, id, x, y, z, Debye-Waller $[nm^{-2}]$, occupancy, absorption factor[2], AFF set, charge).

```
file|/Users/pierrestadelmann/jems/jemsDefaultCrystal.txt
name|jemsDefaultCrystal
creator|pierrestadelmann
date|Sun Dec 18 08:16:33 CET 2022
system|cubic
superCell|false
HMSymbol|221|24|1|0|0| P m -3 m
rps|0|x    ,   y    ,   z
rps|1|-x    ,  -y    ,   z
rps|2|-x    ,   y    ,  -z
rps|3|x    ,  -y    ,  -z
rps|4|z    ,   x    ,   y
rps|5|z    ,  -x    ,  -y
rps|6|-z    ,  -x    ,   y
rps|7|-z    ,   x    ,  -y
rps|8|y    ,   z    ,   x
rps|9|-y    ,   z    ,  -x
rps|10|y    ,  -z    ,  -x
rps|11|-y    ,  -z    ,   x
rps|12|y    ,   x    ,  -z
rps|13|-y    ,  -x    ,  -z
rps|14|y    ,  -x    ,   z
rps|15|-y    ,   x    ,   z
rps|16|x    ,   z    ,  -y
rps|17|-x    ,   z    ,   y
```

[2]Not used when AFFs specified by Weickenmeier-Kohl tabulation.

```
rps|18|-x    ,  -z    ,  -y
rps|19|x    ,  -z    ,   y
rps|20|z    ,   y    ,  -x
rps|21|z    ,  -y    ,   x
rps|22|-z    ,   y    ,   x
rps|23|-z    ,  -y    ,  -x
lattice|0|0.37426
lattice|1|0.37426
lattice|2|0.37426
lattice|3|90.0
lattice|4|90.0
lattice|5|90.0
atom|0|Au,a,0.000,0.000,0.000,0.005,1.000,0.100,Def,0
atom|1|Cu,c,0.000,0.500,0.500,0.005,1.000,0.050,Def,0
```

1.6 License

The license text file contains information provided by internet. The uniqueID is case sensitive and should be copied/paste from the email. This file is duplicated in the application folder[3]. Below *dd* stands for day, *mmm* stands for month, *ssss* for serial number and *yyyy* for year. *u* indicates that the version ready for Linux, MacOS and Windows operating systems *v* the version number and *b* the build day.

```
date|Sun Dec 18 10:14:49 CET 2022
platform|Mac OS X
host|computer name
version|v.mmmdduyyyybdd
serial|ssss.yyyy
license|License Code
uniqueID|Unique ID
```

[3]This is why the access to application folder must be set to read-write.

1.7 Default microscopes set

The characteristics of the default microscopes' set are shown below. They are separated by a + and followed by a 2 characters tag ending with |. The tags are defined as:

- **NA**| : name (used as the tab label).
- **LA**| : label.
- **AV**| : maximum accelerating voltage [kV].
- **CS**| : 3^{rd} order spherical aberration coefficient [mm].
- **C5**| : 5^{th} order spherical aberration coefficient [mm].
- **CC**| : chromatic aberration coefficient [mm].
- **ES**| : electron energy spread [eV].
- **LS**| : objective lens stability [ppm] (part per million).
- **TM**| : thermal magnetic noise [pm].
- **VS**| : voltage stability [ppm] (part per million).
- **HC**| : electron beam half-convergence [nm^{-1}].

It is possible to directly change these characteristics by editing the *jemsMicroscopes.txt* file, but using the dialogue allows one to plot the microscope transfer function and to check them. The default microscopes' table is loaded using tool button  of the dialogue.

```
NA|CM 20 T+LA|Philips CM 20 twin+AV|200.0+CS|2.0+C5|0.0+CC|2.0+ES|1.6+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|CM 30 T+LA|Philips CM 30 twin+AV|300.0+CS|2.0+C5|0.0+CC|2.0+ES|1.6+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|CM 300 ST+LA|Philips CM 300 super twin+AV|300.0+CS|1.2+C5|0.0+CC|2.0+ES|1.6+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|CM 300 UT-FE+LA|Philips CM 300 ultra twin field emission+AV|300.0+CS|0.7+C5|0.0+CC|1.2+ES|0.8+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Libra 120 HT+LA|Zeiss Libra 120 HT+AV|120.0+CS|2.2+C5|0.0+CC|2.2+ES|1.5+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Libra 200 HT+LA|Zeiss Libra 200 FE-HT+AV|200.0+CS|2.2+C5|0.0+CC|2.2+ES|0.7+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Libra 200 HR+LA|Zeiss Libra 200 FE-HR+AV|200.0+CS|1.2+C5|0.0+CC|1.2+ES|0.7+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Libra 200 Cs-cor.+LA|Zeiss Libra 200 FE Cs-corrected+AV|200.0+CS|0.2+C5|0.0+CC|1.2+ES|0.2+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|HF 2000 FEG+LA|Hitachi 2000 field emission+AV|200.0+CS|1.2+C5|0.0+CC|1.6+ES|0.6+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Jeol 2010+LA|Jeol 2010 LaB6 emission+AV|200.0+CS|1.0+C5|0.0+CC|1.4+ES|1.4+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Jeol 2100F+LA|Jeol 2100 field emission+AV|200.0+CS|1.4+C5|0.0+CC|1.8+ES|0.8+LS|1.0+TM|0.0+VS|1.0+HC|1.0
NA|Jeol 2100F Cs+LA|Jeol 2100 field emission, cs corrected+AV|200.0+CS|0.01+C5|10.0+CC|1.2+ES|0.8+LS|0.1+TM|20.0+VS|0.5+HC|1.0
NA|Jeol 3010+LA|Jeol 3010 LaB6 emission+AV|300.0+CS|0.7+C5|0.0+CC|1.2+ES|1.6+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Jeol 4000 EX+LA|Jeol 4000 LaB6 emission+AV|400.0+CS|1.0+C5|0.0+CC|1.4+ES|1.6+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Topcon 002B+LA|Topcon 002 LaB6 emission+AV|200.0+CS|0.5+C5|0.0+CC|1.2+ES|1.6+LS|5.0+TM|0.0+VS|5.0+HC|1.0
NA|Jeol ARM 200+LA|Jeol 200kV Schottky FEG+AV|200.0+CS|0.001+C5|1.0+CC|1.0+ES|0.7+LS|0.1+TM|20.0+VS|0.5+HC|1.0
NA|Titan 80-300+LA|FEI Titan 80-300 Cs corrected+AV|300.0+CS|-0.03+C5|5.0+CC|1.0+ES|0.6+LS|0.1+TM|20.0+VS|1.0+HC|1.0
NA|ASU 10 MeV source+LA|ASU FEL+AV|10000.0+CS|1.0+C5|0.0+CC|1.0+ES|1.0+LS|1.0+TM|0.0+VS|1.0+HC|1.0
```

2 Main frame

jems main window (Fig. 3) displays 2 panels, the left panel lists the atoms of the structure displayed on the right panel. Atoms of the unit cell generated by the translations of the Bravais lattice are not listed. Popup menus are attached to each panel (see paragraph 2.4).

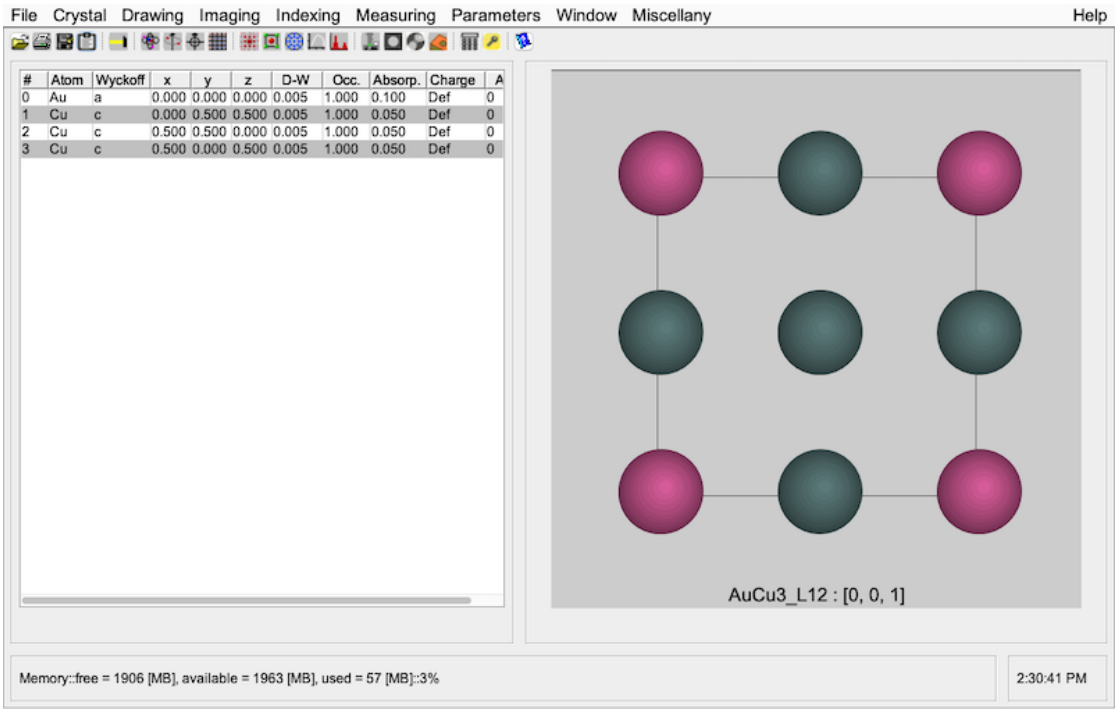


Figure 3: jems main window, MacOSX version.

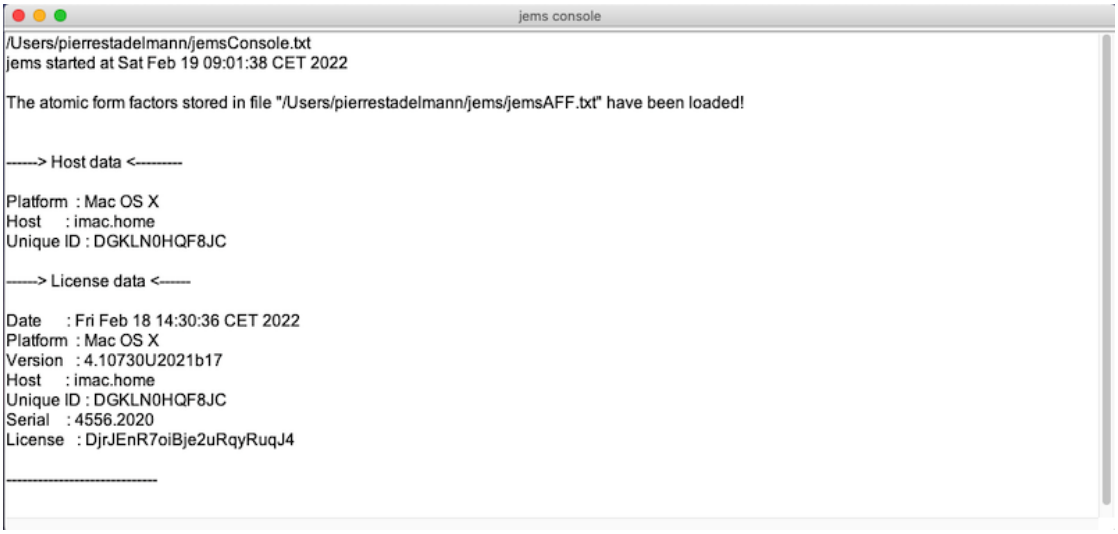
2.1 Console

At startup a scrollable console frame opens that displays information about the user, host and license (Fig. 4a). The console will display more information depending of the debugging options selected in the **Parameters** → **Preferences** dialogue → **Debug** tab (Fig. 4b)[4]. Its content can be copied/paste as text file in any text editing program. The console can be closed if convenient.

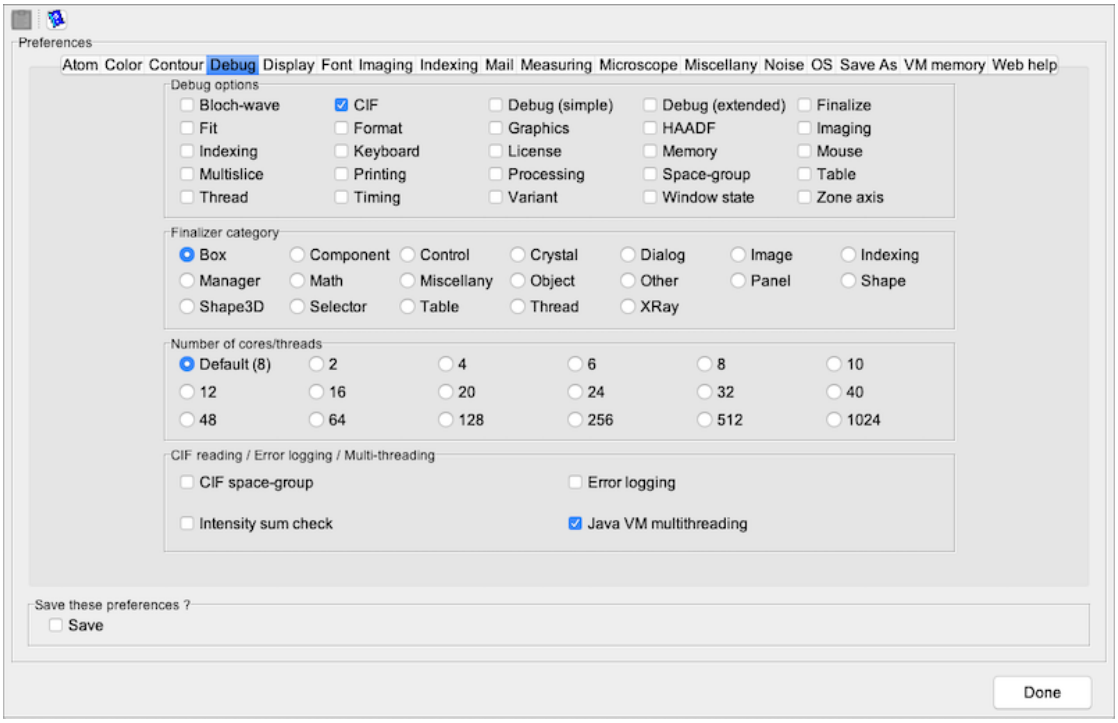
For example, with the **CIF** debug option selected, loading a structure provided as a *.cif file* the console window will display information about the content of the file

[4]Its whole content can be selected and copy/paste into any text editing program.

(not shown here). This information may help detect wrong **CIF** content.



(a) Console frame (MacOSX version).

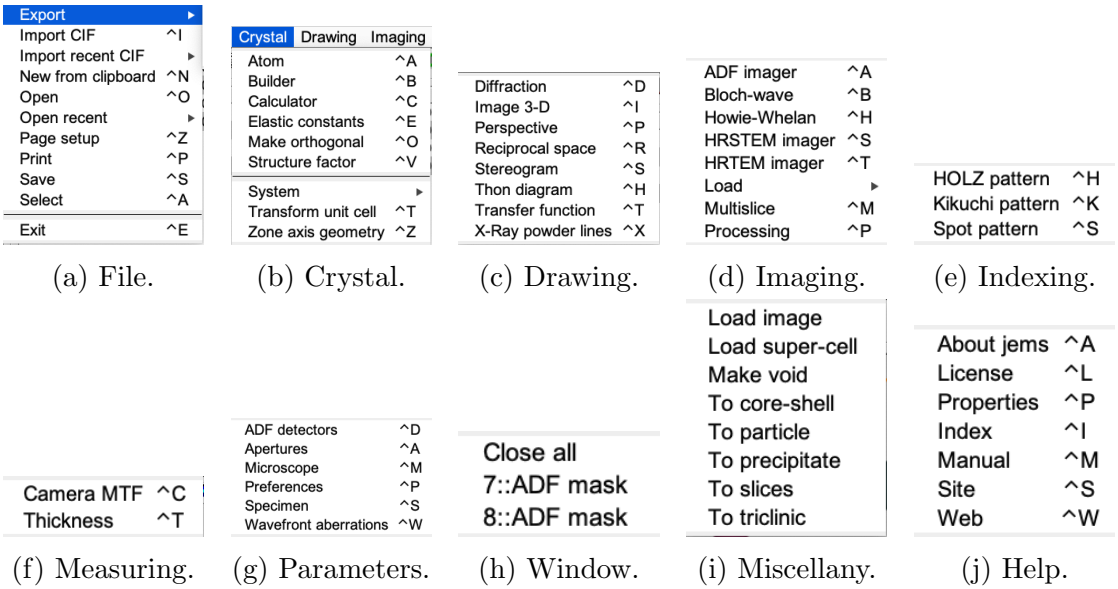


(b) Preferences dialogue, debug panel.

Figure 4: (a) Console and (b) debug panel.

2.2 Menus

The menu bar organises the different menus as usual (Fig. 5). jems student version presents a different menu bar: menu **Miscellany** is missing and several other menus do not offer some menu items found in the licensed version.



(a) File. (b) Crystal. (c) Drawing. (d) Imaging. (e) Indexing.

(f) Measuring. (g) Parameters. (h) Window. (i) Miscellany. (j) Help.

Figure 5: Menus of the menu bar.

2.3 Tool buttons

Most of the tool buttons duplicate a particular menu item in order to access it faster. Only  (**Transfer to clipboard**), that put a copy of the main window (or any window displaying it) in the clipboard, does not duplicate a menu item.

A **tip text** is attached to every tool button and describes its function. The tip text is shown when the mouse or pointer is moved on the tool button. For example the tip text of  is simply "*Transfer to clipboard*".

The tool buttons of the main window allow to:

-  : load a crystal structure in .txt format.
-  : print the atoms table.

- : save the atoms table in .txt format.
- : transfer a frame or dialogue to the clipboard.
- : **Build** a crystal structure (Fig. 11).
- : open the **Atom** dialogue (Fig. 17).
- : open the **R**egular **P**oint **S**ystem (RPS) code dialogue (Fig. 20).
- : open the **Space-group** dialogue (Fig. 19).
- : tabulate the **A**tomic **F**orm **F**actors (AFF) (Fig. 18).
- : plot **S**elected **A**rea **E**lectron **D**iffraction patterns (SAED) (Fig. 22).
- : show **Perspective** views of crystal structures (Fig. 162).
- : plot [u,v,w] and (h,k,l) **Stereographic** projections (Fig. 113).
- : define the **C**ontrast **T**ransfer **F**unction (CTF) and **O**ptical **T**ransfer **F**unction (OTF) (Fig. 97).
- : plot **P**owder pattern (line position) for electron, neutron and X-Ray (Fig. 116).
- : open the **Microscope** dialogue (Fig. 108).
- : open the **Apertures** dialogue (Fig. 79).
- : show the **Wave-front aberrations** dialogue (Fig. 96).
- : show the **Specimen** dialogue (Fig. 84a).
- : open the **Crystallographic calculator** (Fig. 110).
- : open the **Keeper** dialogue (Fig. 90).
- : display a **H**elp file.

The **Help** tool button ( ) is available on each dialogue and frame [5].

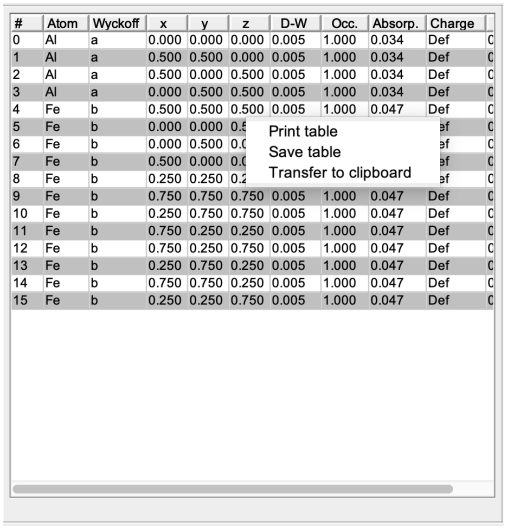
2.4 Popup menus

A double mouse click (or using a touchscreen a double finger or pointer touch) on the left or right panel of the main window displays a popup menu (Fig. 6). Attach

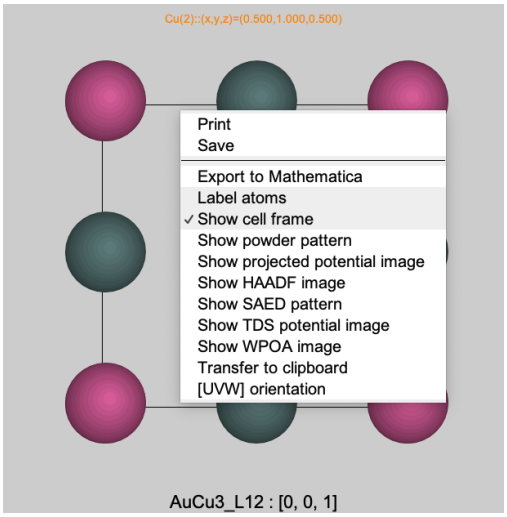
[5] Depending on the dialogue or frame context some of the tool buttons may have a different functionality (described by the tip text)

to a **list** the popup menu allows to *save*, *print* or *transfer* the list (as an image) to the clipboard. Attached to other GUI elements each popup menu item allows to modify the content of the panel or to create new images, etc.

For example the popup menu item **Export to Mathematica** creates a simple Mathematica notebook showing the $AuCu_3$ crystal structure (Fig. 7a). By default the notebook is saved in the default folder, i.e. where the displayed structure is loaded from [6]. As a second example **Show projected potential** generates the image of the projected potential of $AuCu_3$ (Fig. 7b). Note that the toolbar of the image frame contains tools to process the image and that a popup menu is attached to the image (Fig. 7c) allowing to modify the image (Fig. 7d).



(a) Popup menu left panel.

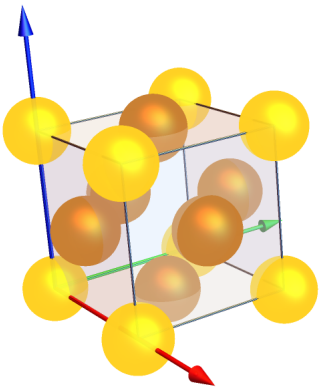


(b) Popup menu right panel.

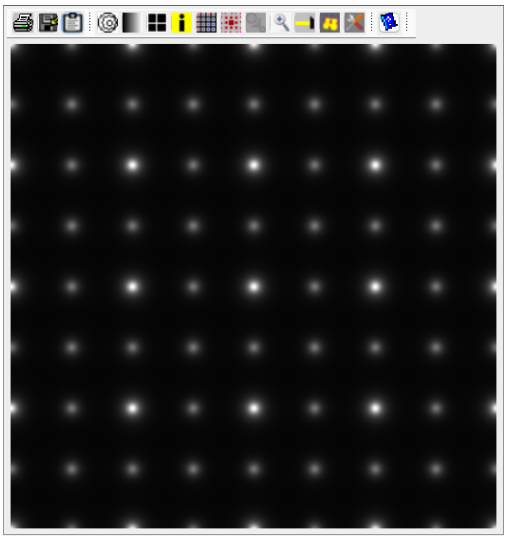
Figure 6: Popup menus attached to the main window left (a) and right (b) panels.

This short document will not described all the simulation and plotting options offered by jems. Only a couple of simulation/plotting frames will be described. The user is urged to refer to these frames in order to figure out how the *not described* frames perform.

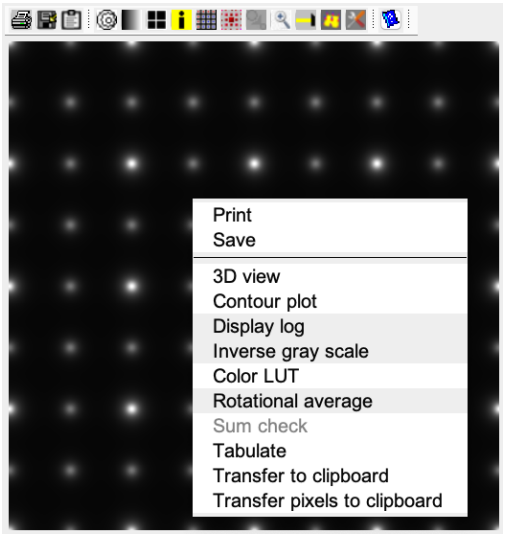
[6] It is always a good idea to create a default folder containing the crystal structure.



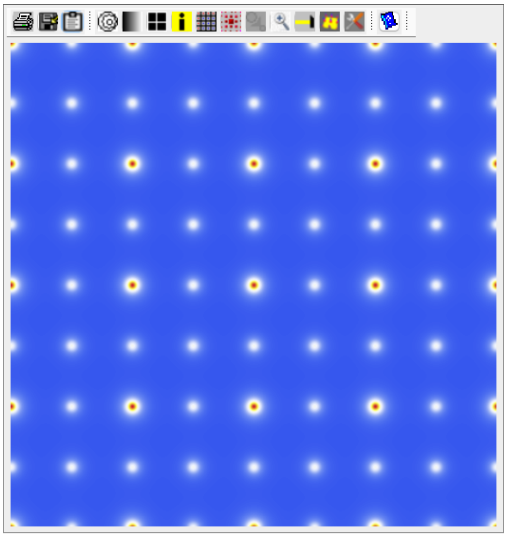
(a) $AuCu_3$ crystal structure displayed using Mathematica (arrows: red x, green y, blue z).



(b) $AuCu_3$ projected potential in [0,0,1] direction.



(c) Popup menu attached to the projected potential image.



(d) Coloured projected potential (temperature map).

Figure 7: Mathematica 3-D view (a) and projected potential (b) of $AuCu_3$. Image popup menu (c) and coloured image (d).

3 Importing crystal structures from CIF files

Menu item **File** → **Import CIF** imports crystal structures defined as **.cif** files provided by databases like the *Crystallography Open Database*, *American Mineralogist Crystal Structure Database* or *Inorganic Crystal Structure Database*.

Fig. 8 shows the dialogue for selecting a crystal structure in a **.cif** file containing 50 related Bismuth ferrates structures.

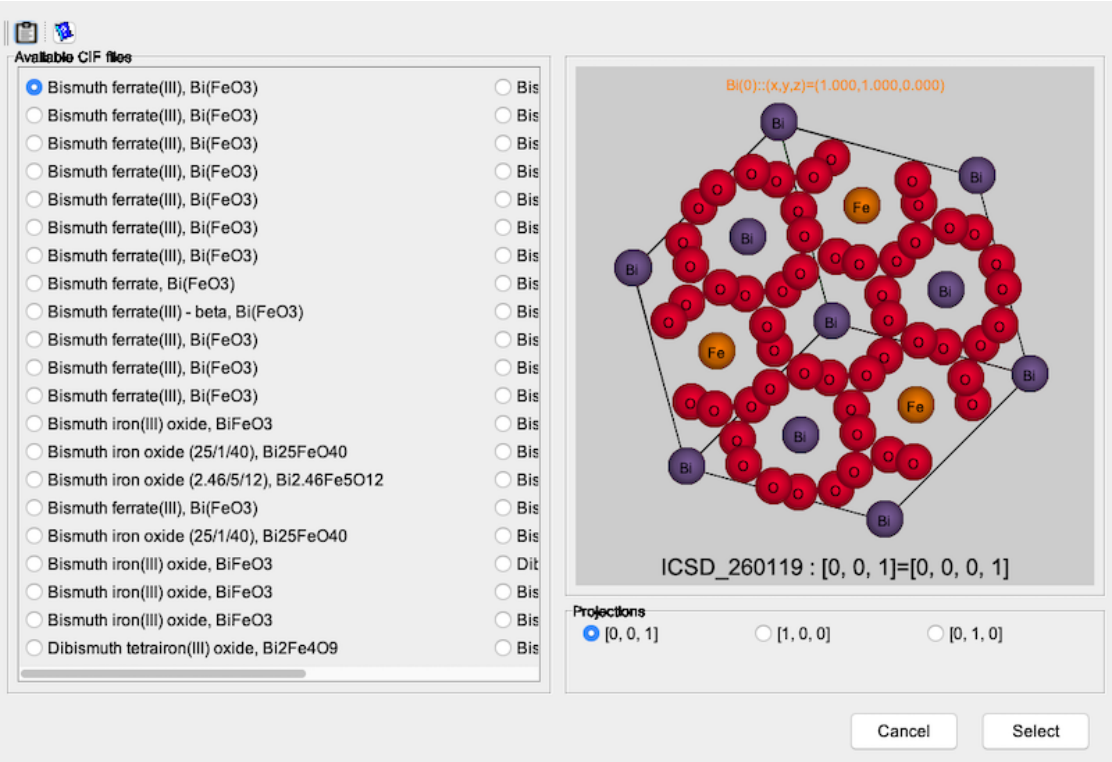
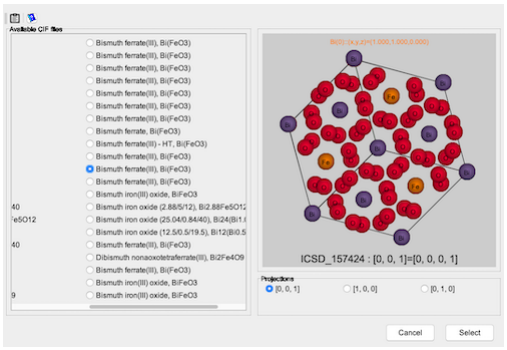


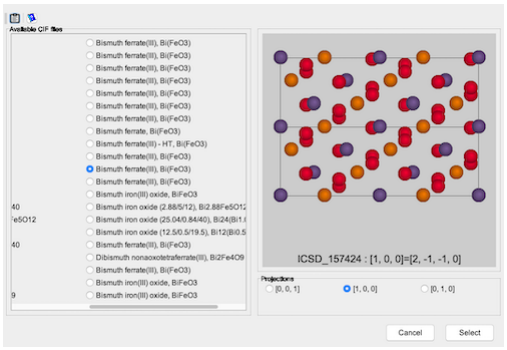
Figure 8: CIF data set selector dialogue.

The selected structure can be observed in [001], [100] or [010] projections. The Select select button selects the structure and closes the dialogue (Fig. 9).

It is then necessary to confirm the **CIF** structure space-group settings since non-conventional settings are not uncommon in crystallographic data bases (Fig. 10).



(a) [001] projection.



(b) [100] projection.

Figure 9: Hexagonal Bismuth ferrate in [001] and [100] projections.

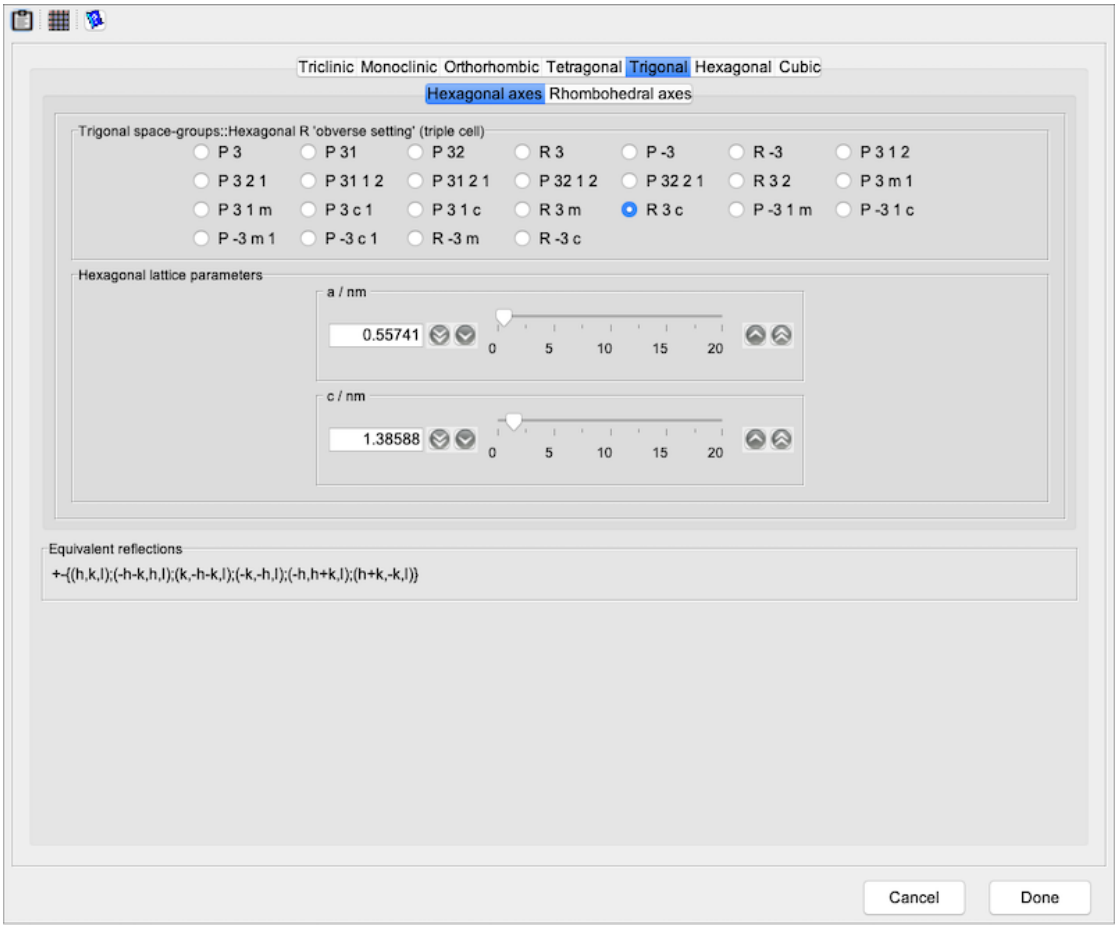


Figure 10: Space-group dialogue to confirm **R 3 c** space-group settings.

4 Crystal builder

The **C**rystal **B**uilder (CB) is started using menu item **Crystal** → **Builder** (Fig. **??**) (or main window's tool button). It opens with the crystal structure displayed in the main window. The CB uses **java3D** and is only available when an **opengl** driver is installed on the computer. The CB allows to build and save crystal structures not distributed with jems.

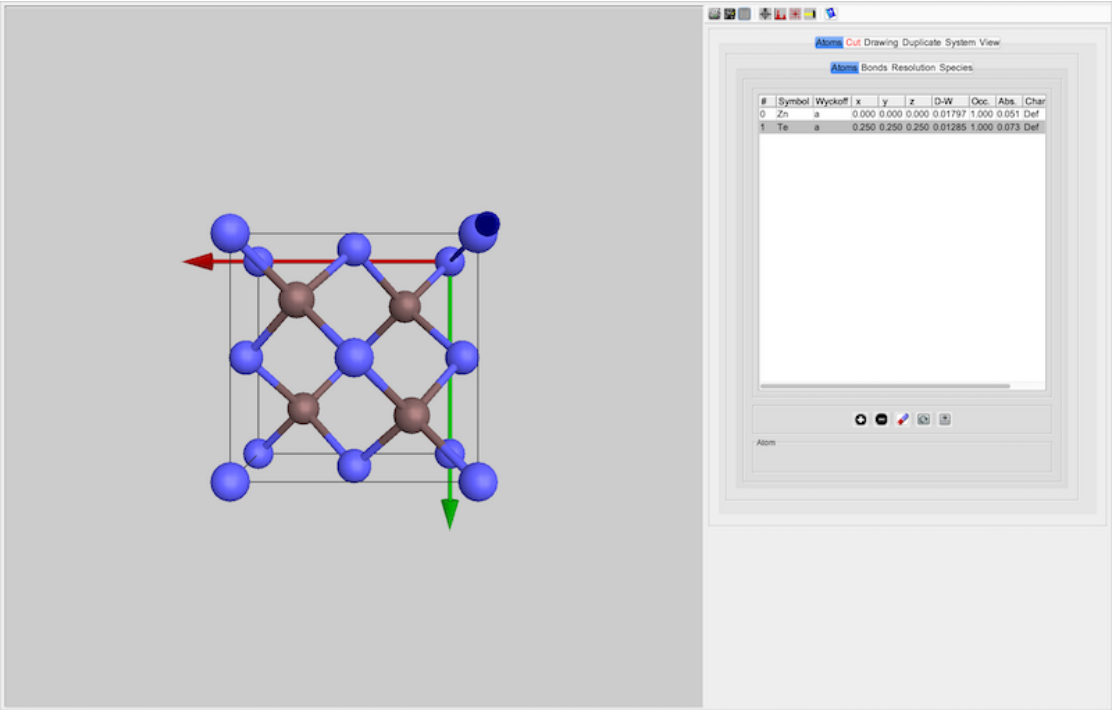


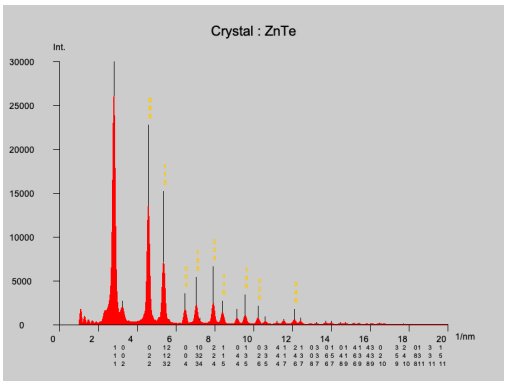
Figure 11: Crystal builder frame.

4.1 Tool buttons

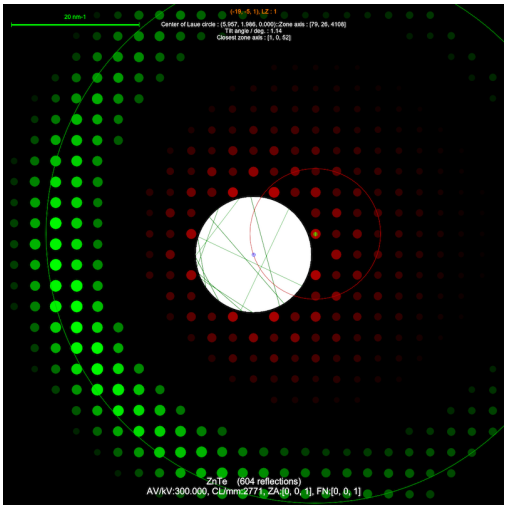
The crystal builder tool buttons allow to:

- : print the crystal structure drawing.
- : save the crystal structure drawing.
- : transfer the frame to the clipboard.
- : open the space-group dialogue (Fig. 19).

-  : plot an ab-initio electron diffraction powder pattern (Fig. 12a).
-  : plot SAED diffraction patterns (Fig. 12b).
-  : duplicate the unit cell $n_x \times n_y \times n_z$ times (Fig. 16c).
-  : display a help file.



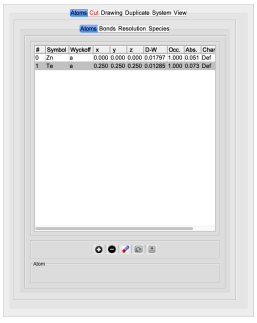
(a) Ab-initio powder pattern of ZnTe a 8x8x8 unit cells crystallite.



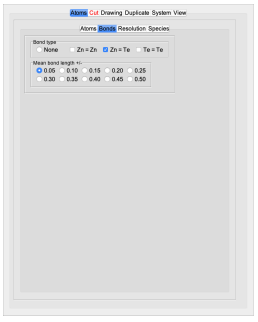
(b) SAED pattern (single scattering).

Figure 12: ZnTe diffraction patterns.

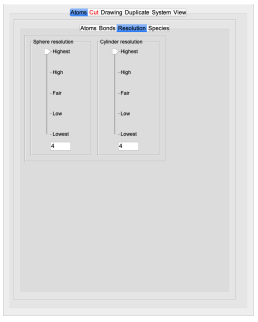
4.2 Tabs



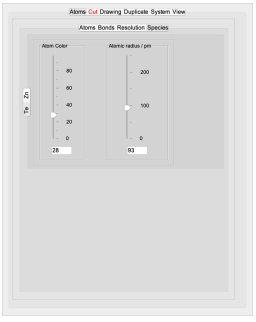
(a) Atoms table.



(b) Bonds selection.



(c) Atoms and bonds resolution.



(d) Atom colour and size selection.

Figure 13: Crystal builder → **Atoms** tabs.

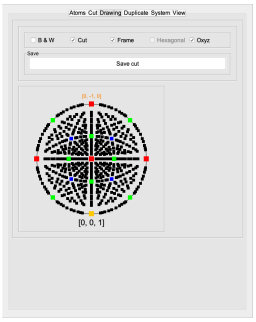
4.3 Atoms table's tool buttons

The tool buttons of the atom table allow to:

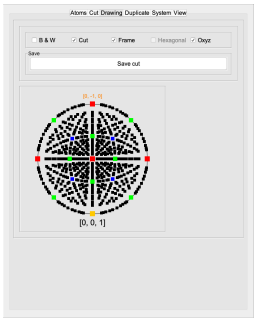
-  : define a new atom position.
-  : delete the selected atom.
-  : erase all the atoms.
-  : modify the selected atom.
-  : save the atoms table as a .txt file[7].

The  and  open the **Atom** dialogue (Fig. 17), see section 4.4.

When an atom of the 3-D drawing is selected (white sphere) it is identified in the **Atom** text field. All the equivalent atoms of the 3-D drawing are identified when an entry of the table is selected (white spheres).



(a) (hkl) cut plane selection.



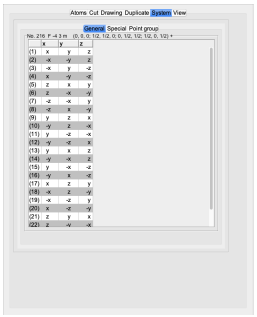
(b) Drawing options and $[uvw]$ viewing direction.

(c) Unit cell duplicating options.

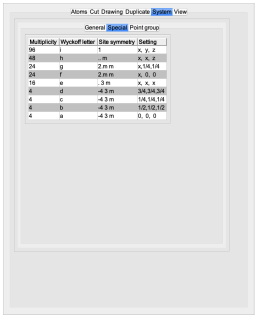
(d) 3-D viewing selection.

Figure 14: Crystal builder → **Cut**, **Drawing**, **Duplicate** & **View** tabs.

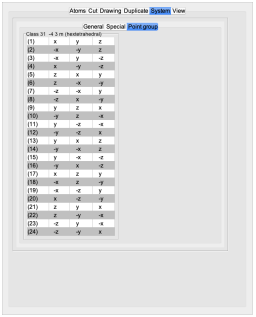
[7]The Wyckoff symbol and AFF source are only saved when the builder frame is closing.



(a) General space-group description.

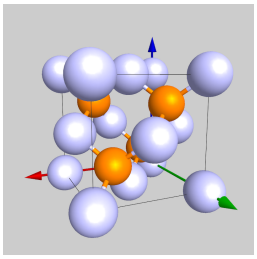


(b) Table of site multiplicity, Wyckoff letter, symmetry and setting.

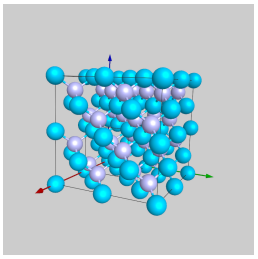


(c) Point group description.

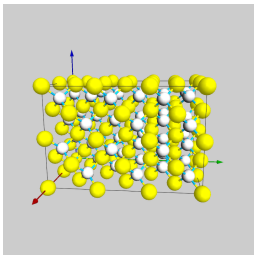
Figure 15: Crystal builder → **System** tabs.



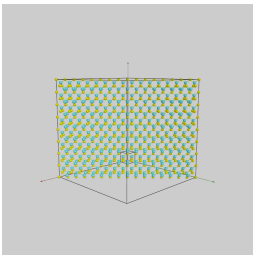
(a) ZnTe unit cell view.



(b) ZnTe view of cell duplicated 2x2x2 times.



(c) ZnTe cell duplicated 2x3x2 times.



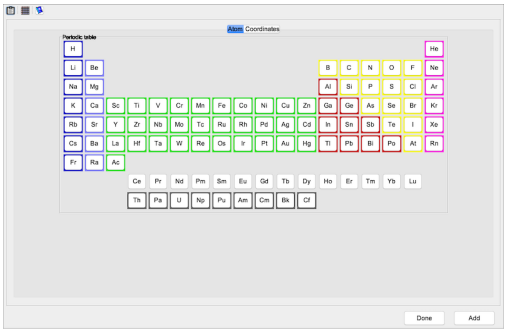
(d) ZnTe view of (110) plane.

Figure 16: Crystal builder allows to build large super-cells.

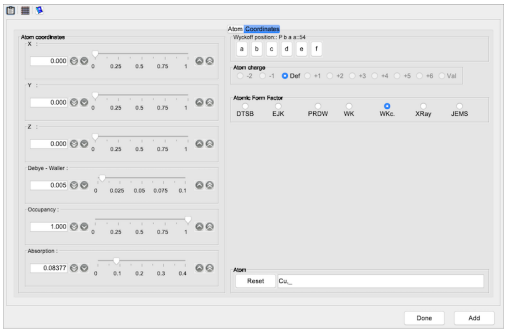
4.4 Crystal builder → Atom dialogue

Figs 17a and 17b show the atom dialogue tabs. It is necessary to first select the atom symbol (**Atom** tab) and then, using the controls of the **Coordinates** tab, to set the fractional atom coordinates (with the help of the Wyckoff position symbol), Debye-Waller temperature factor, occupancy and absorption. When either the Weickenmaier-Kohl **WK** or **WKc.** **A**tomic **F**orm **Factor** (AFF) source is selected the absorption should be set to 0.0 since it is always calculated. The dialogue emits a message when the atom site is already partially or fully occupied. In such a case push the Reset button. The Add and Done buttons updates

the atoms table and closes the dialogue respectively.



(a) Atom selection.



(b) Fractional coordinates can be specified using the Wyckoff (site symmetry) letter.

Figure 17: Atom dialogue.

The tool buttons of the atom dialogue allow to:

-  : transfer the dialogue to the clipboard.
-  : display the AFF tables (Fig. 18). [8, 9, 10, 11]
-  : display a help file.

[8] From Doyle-Turner, Smith-Burge (DTSB), Acta Cryst. **A24** (1968) 390, Acta Cryst. **15** (1962) 182.

[9] Earl J. Kirkland (EJK), Advanced Computing in Electron Microscopy, 1998 Plenum Press, New York.

[10] L. Peng et al. (PRDW), Acta Cryst.**A52** (1996) 257.

[11] A. Weickenmeier and H. Kohl (WK), Acta Cryst. **A47** (1991) 590.

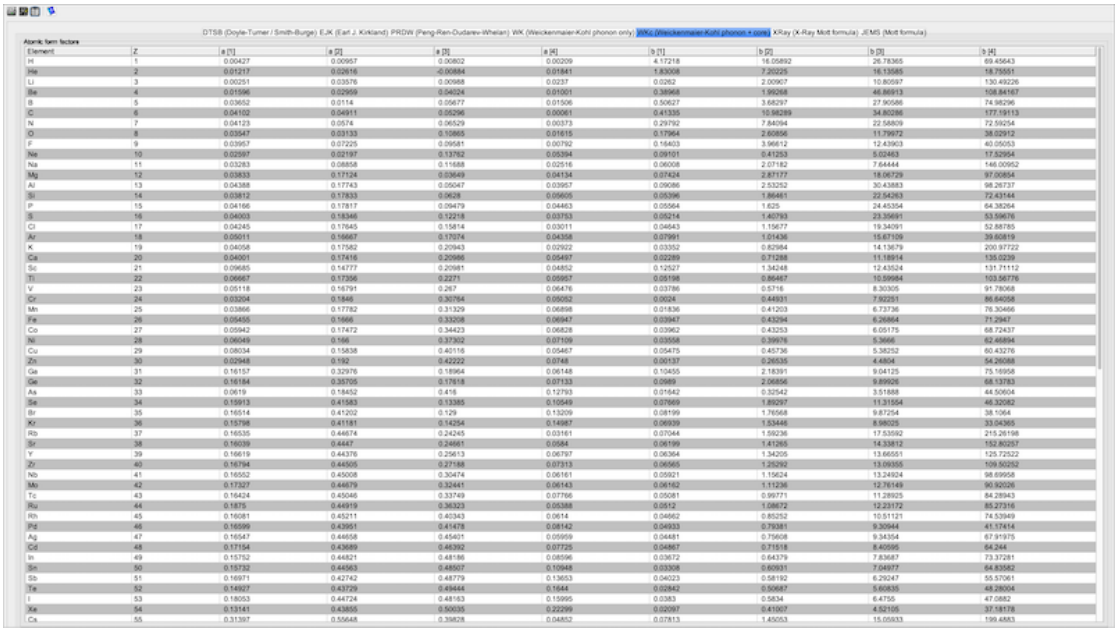
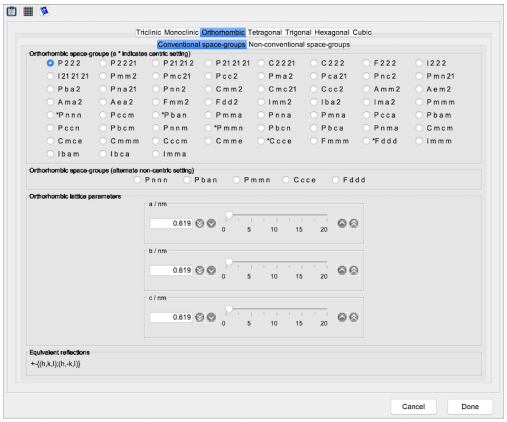


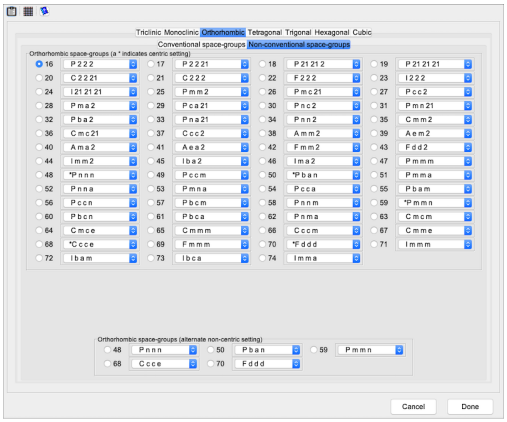
Figure 18: Tables of the **A**tomic **F**orm **F**actors.

4.5 Crystal builder → Space-group dialogue

The **Space-group** dialogue (Fig. 19) defines the space-group and lattice parameters of an orthorhombic unit cell. The conventional and non-conventional space-groups are organised by crystal system (from triclinic to cubic). The tab of the conventional **orthorhombic** system displays also the lattice parameters' controls and the non-conventional one the alternate groups that depend on the **permutation** of the a, b, c lattice parameters.



(a) Conventional **Orthorhombic** space-groups.



(b) Non-conventional **Orthorhombic** space-groups.

Figure 19: Space-group dialogue (orthorhombic unit cell).

The tool buttons of the space-group dialogue allow to:

- : transfer the dialogue to the clipboard.
- : display the space-group general and special positions as well as its point-group (Fig. 15a).
- : display a help file.

4.6 Regular Point System code dialogue

The symmetry operations of the space-group and the lattice parameters are also entered using the RPS code dialogue (menu item **Crystal** → **System** → **RPS code** or tool button only available from the main jems window (Fig. 20) [12].

The tool buttons of the RPS code dialogue allow to:

- : print the RPS code table.
- : save the RPS code table.
- : transfer the dialogue frame to the clipboard.

[12]It is always simpler to define the space-group using the space-group dialogue since special positions (site symmetry, i.e. Wyckoff letter) allow a safer and faster setting of the fractional coordinates of the atoms position.

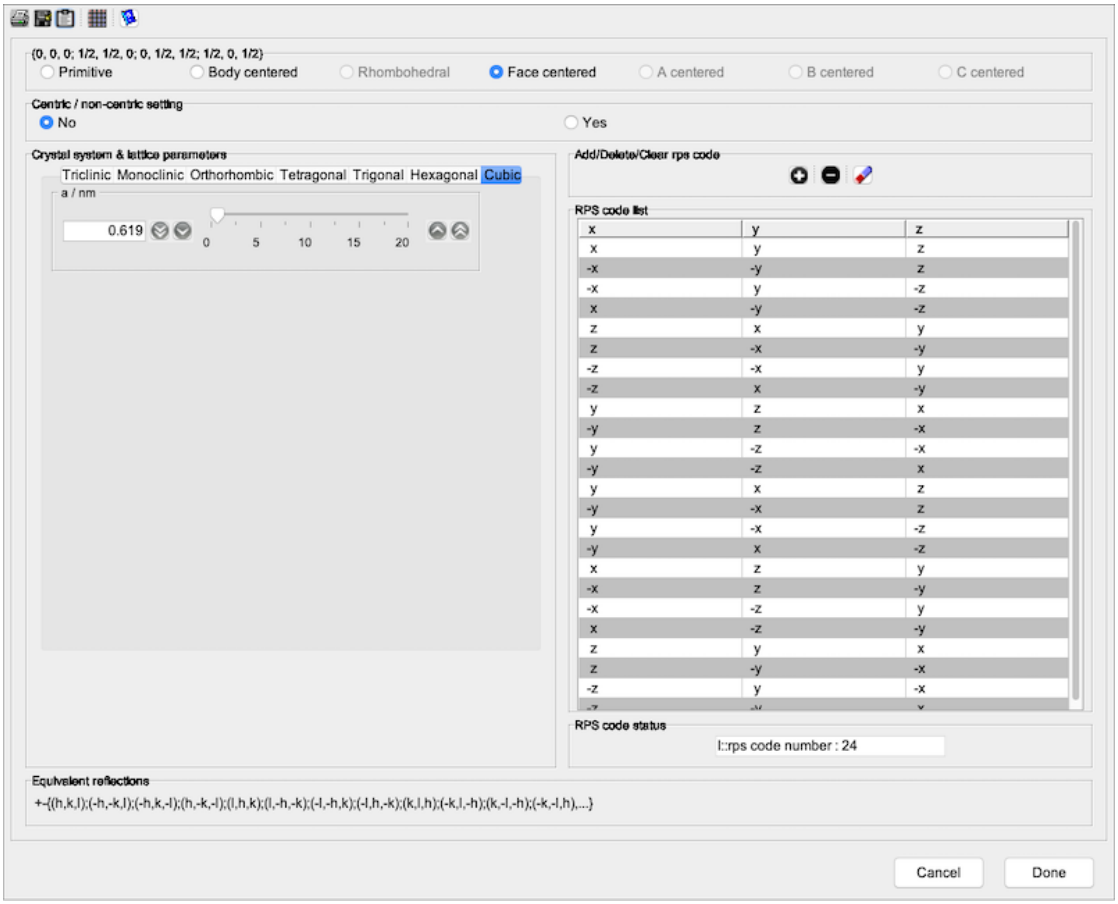


Figure 20: RPS code dialogue for entering the regular point system code.

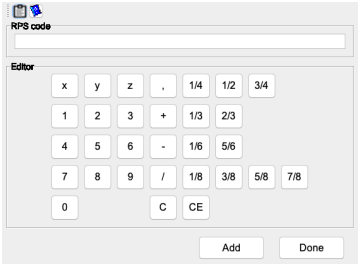
- : display the space-group general positions as well as its point-group when identified (Figs 15a, 15c).
- : display a help file.

This dialogue permits to define pretty strange unit cells since the validity of the RPS code for a given crystal system is not checked (Fig. 21).

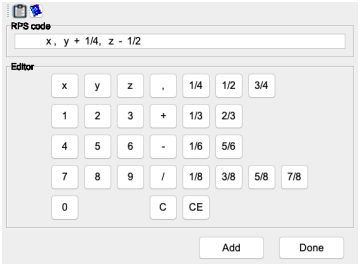
The tool buttons of the RPS code table allow to:

- : add a new RPS code.
- : delete the selected RPS code.
- : erase all RPS codes (except (x, y, z)).

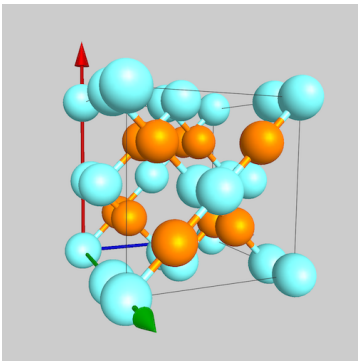
The ⊕ tool button opens the RPS code editor dialogue (Fig. 21a). The Add adds a new code and Done closes the dialogue and update the list of RPS codes (Fig. 21b). The modified unit cell can be a bit unusual since jems does not check the validity of the new RPS code (Fig. 21c). Nevertheless the RPS code editor is useful to define similar unit cells of different crystal systems [13].



(a) RPS code editor dialogue.



(b) Using the Editor keys (or entering the code directly) to define a new code (x, y + 1/4, z - 1/2).



(c) jems does not check the new code validity → 3-D view of the updated unit-cell.

Figure 21: RPS code editor.

[13] For example in case of phase transformation.

5 SAED patterns

Plotting **S**elected **A**rea **E**lectron **D**iffraction patterns (SAED) is activated by either the **Drawing** → **Diffraction** menu item or the tool button . The SAED frame (Fig. 22) shows the SAED pattern of the crystal structure shown in (Fig. 3) along the selected [uvw] zone axis.

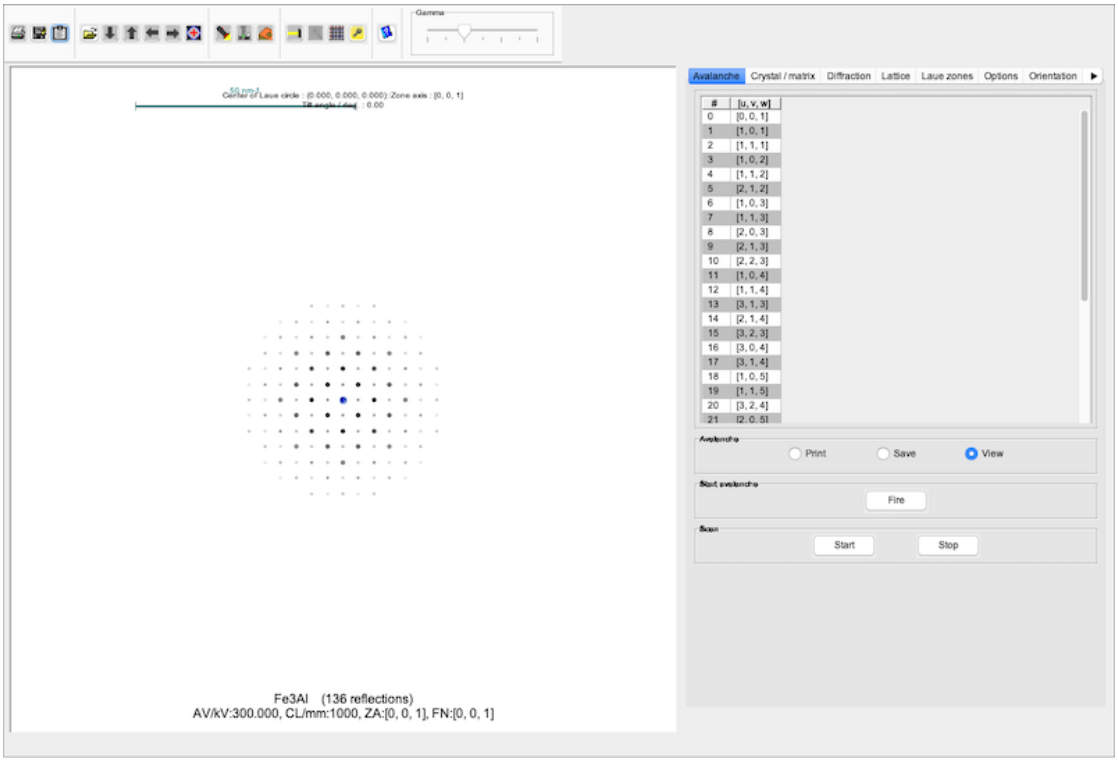


Figure 22: SAED patterns frame.

5.1 Tool buttons

The tool buttons of the SAED frame allow to:

- : print the SAED pattern.
- : save the SAED pattern.
- : transfer the frame to the clipboard.
- : load an experimental SAED pattern.

-  : move the **C**enter of the **L**aue **C**ircle (CLC) down.
-  : move the CLC up.
-  : move the CLC left.
-  : move the CLC right.
-  : reset the CLC to (0,0,0) reflection.
-  : search the closest zone axis.
-  : open the **Microscope** dialogue (Fig. 108).
-  : open the **Specimen** dialogue (Fig. 84a).
-  : start/stop the precession mode.
-  : start/stop magnifying the experimental SAED pattern (Fig. 23).
-  : tabulate the plotted reflections (Fig. 24).
-  : open the **Keeper** dialogue (Fig. 90).
-  : open the associated help dialogue.

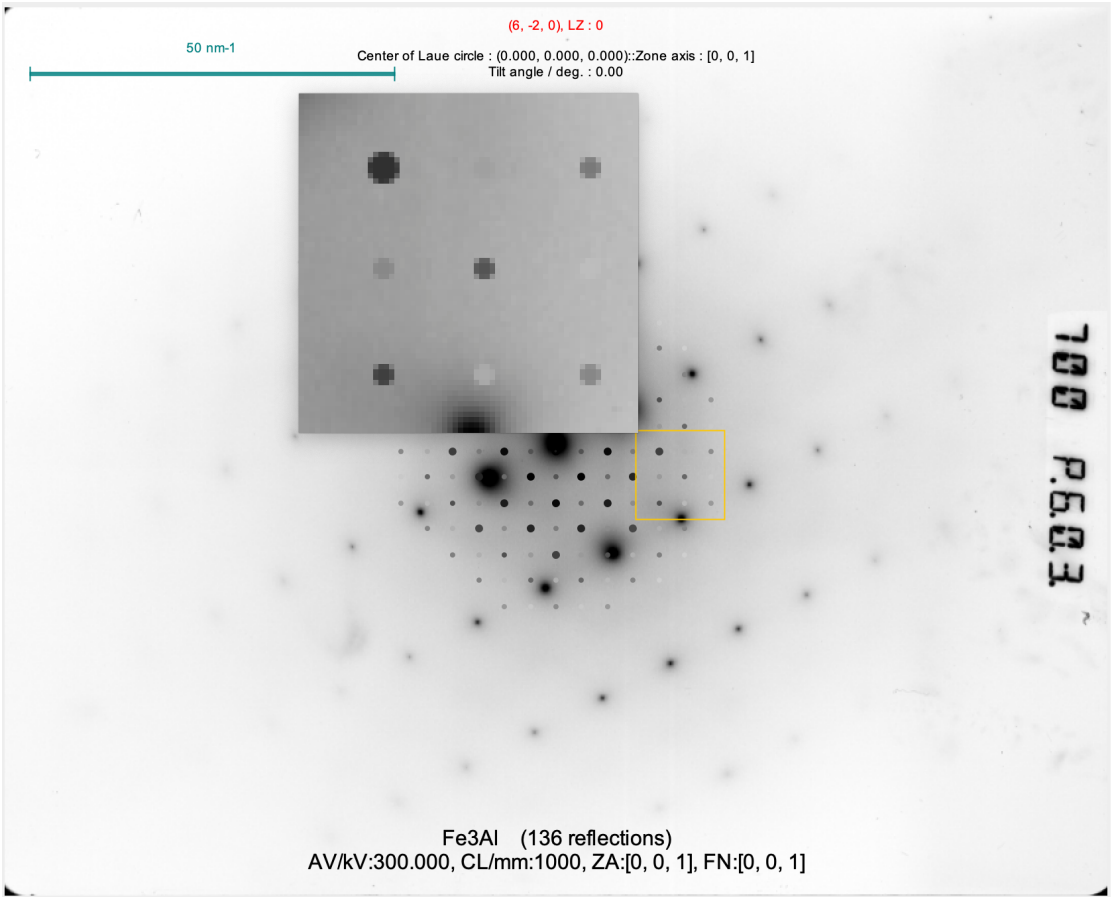
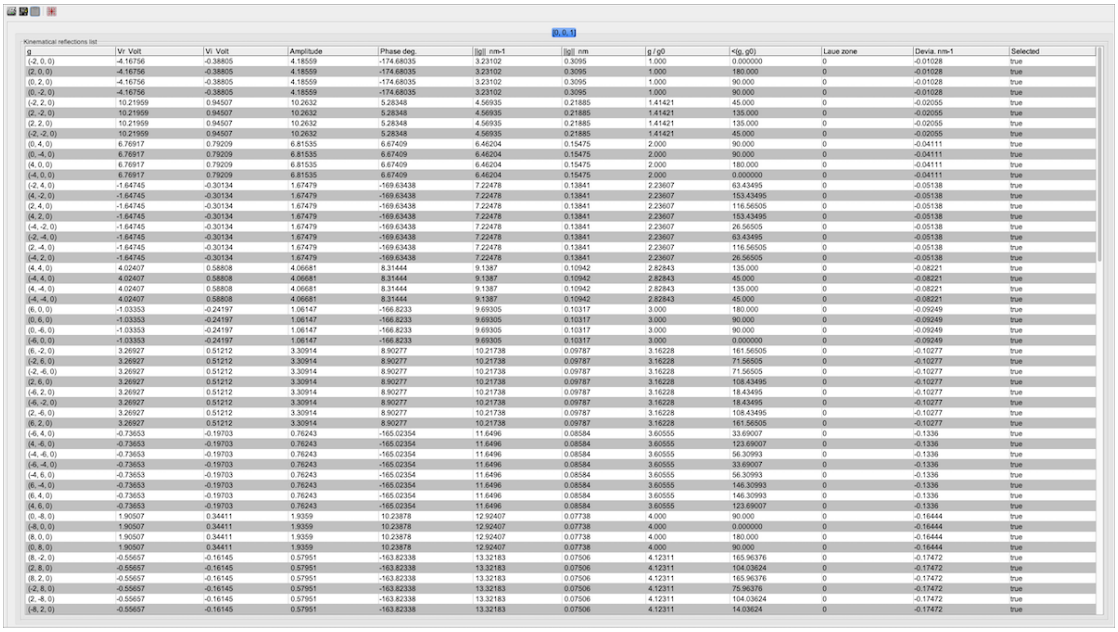


Figure 23: Experimental SAED with a magnified area (yellow square).


Kinematical reflections list

g	Vr. Volt	Vi. Volt	Amplitude	Phase deg.	|g| nm-1	|g| nm	g / g0	∠(g, g0)	Laue zone	Devia. nm-1	Selected
(-2, 0, 0)	-4.16756	-0.38805	4.18559	-174.68035	3.23102	0.3095	1.000	0.000000	0	-0.01028	true
(2, 0, 0)	-4.16756	-0.38805	4.18559	-174.68035	3.23102	0.3095	1.000	180.000	0	-0.01028	true
(0, 2, 0)	-4.16756	-0.38805	4.18559	-174.68035	3.23102	0.3095	1.000	90.000	0	-0.01028	true
(0, -2, 0)	-4.16756	-0.38805	4.18559	-174.68035	3.23102	0.3095	1.000	90.000	0	-0.01028	true
(-2, 2, 0)	10.21959	0.94507	10.2632	5.28348	4.56935	0.21885	1.41421	45.000	0	-0.02055	true
(2, -2, 0)	10.21959	0.94507	10.2632	5.28348	4.56935	0.21885	1.41421	135.000	0	-0.02055	true
(2, 2, 0)	10.21959	0.94507	10.2632	5.28348	4.56935	0.21885	1.41421	135.000	0	-0.02055	true
(-2, -2, 0)	10.21959	0.94507	10.2632	5.28348	4.56935	0.21885	1.41421	45.000	0	-0.02055	true
(0, 4, 0)	6.76917	0.79209	6.81535	6.67409	6.46204	0.15475	2.000	90.000	0	-0.04111	true
(0, -4, 0)	6.76917	0.79209	6.81535	6.67409	6.46204	0.15475	2.000	90.000	0	-0.04111	true
(4, 0, 0)	6.76917	0.79209	6.81535	6.67409	6.46204	0.15475	2.000	180.000	0	-0.04111	true
(-4, 0, 0)	6.76917	0.79209	6.81535	6.67409	6.46204	0.15475	2.000	0.000000	0	-0.04111	true
(-2, 4, 0)	-1.64745	-0.30134	1.67479	-169.63438	7.22478	0.13841	2.23607	63.43495	0	-0.05138	true
(4, -2, 0)	-1.64745	-0.30134	1.67479	-169.63438	7.22478	0.13841	2.23607	153.43495	0	-0.05138	true
(2, 4, 0)	-1.64745	-0.30134	1.67479	-169.63438	7.22478	0.13841	2.23607	116.56505	0	-0.05138	true
(4, 2, 0)	-1.64745	-0.30134	1.67479	-169.63438	7.22478	0.13841	2.23607	153.43495	0	-0.05138	true
(-4, 2, 0)	-1.64745	-0.30134	1.67479	-169.63438	7.22478	0.13841	2.23607	26.56505	0	-0.05138	true
(2, -4, 0)	-1.64745	-0.30134	1.67479	-169.63438	7.22478	0.13841	2.23607	63.43495	0	-0.05138	true
(2, -4, 0)	-1.64745	-0.30134	1.67479	-169.63438	7.22478	0.13841	2.23607	116.56505	0	-0.05138	true
(-4, 2, 0)	-1.64745	-0.30134	1.67479	-169.63438	7.22478	0.13841	2.23607	26.56505	0	-0.05138	true
(4, 4, 0)	4.02407	0.58808	4.06681	8.31444	9.1387	0.10942	2.82843	135.000	0	-0.08221	true
(4, 4, 0)	4.02407	0.58808	4.06681	8.31444	9.1387	0.10942	2.82843	45.000	0	-0.08221	true
(4, -4, 0)	4.02407	0.58808	4.06681	8.31444	9.1387	0.10942	2.82843	135.000	0	-0.08221	true
(-4, -4, 0)	4.02407	0.58808	4.06681	8.31444	9.1387	0.10942	2.82843	45.000	0	-0.08221	true
(6, 0, 0)	-1.03353	-0.24197	1.06147	-166.8233	9.69305	0.10317	3.000	180.000	0	-0.09249	true
(0, 6, 0)	-1.03353	-0.24197	1.06147	-166.8233	9.69305	0.10317	3.000	90.000	0	-0.09249	true
(0, -6, 0)	-1.03353	-0.24197	1.06147	-166.8233	9.69305	0.10317	3.000	90.000	0	-0.09249	true
(-6, 0, 0)	-1.03353	-0.24197	1.06147	-166.8233	9.69305	0.10317	3.000	0.000000	0	-0.09249	true
(6, -2, 0)	3.26927	0.51212	3.30914	8.90277	10.21738	0.09787	3.16228	161.56505	0	-0.10277	true
(2, 6, 0)	3.26927	0.51212	3.30914	8.90277	10.21738	0.09787	3.16228	71.56505	0	-0.10277	true
(-2, -6, 0)	3.26927	0.51212	3.30914	8.90277	10.21738	0.09787	3.16228	71.56505	0	-0.10277	true
(2, 6, 0)	3.26927	0.51212	3.30914	8.90277	10.21738	0.09787	3.16228	108.43495	0	-0.10277	true
(-6, 2, 0)	3.26927	0.51212	3.30914	8.90277	10.21738	0.09787	3.16228	18.43495	0	-0.10277	true
(6, -2, 0)	3.26927	0.51212	3.30914	8.90277	10.21738	0.09787	3.16228	18.43495	0	-0.10277	true
(2, -6, 0)	3.26927	0.51212	3.30914	8.90277	10.21738	0.09787	3.16228	108.43495	0	-0.10277	true
(6, 2, 0)	3.26927	0.51212	3.30914	8.90277	10.21738	0.09787	3.16228	161.56505	0	-0.10277	true
(-6, 4, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	33.69007	0	-0.1336	true
(6, -6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	123.69007	0	-0.1336	true
(-6, -6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	56.30993	0	-0.1336	true
(-6, 6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	33.69007	0	-0.1336	true
(-6, 6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	56.30993	0	-0.1336	true
(6, -6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	146.30993	0	-0.1336	true
(6, 6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	146.30993	0	-0.1336	true
(6, 6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	123.69007	0	-0.1336	true
(0, -8, 0)	1.90507	0.34411	1.9359	10.23878	12.92407	0.07738	4.000	90.000	0	-0.16444	true
(-8, 0, 0)	1.90507	0.34411	1.9359	10.23878	12.92407	0.07738	4.000	0.000000	0	-0.16444	true
(8, 0, 0)	1.90507	0.34411	1.9359	10.23878	12.92407	0.07738	4.000	180.000	0	-0.16444	true
(0, 8, 0)	1.90507	0.34411	1.9359	10.23878	12.92407	0.07738	4.000	90.000	0	-0.16444	true
(8, -2, 0)	-0.55657	-0.16145	0.57951	-163.82338	13.32183	0.07506	4.12311	165.96376	0	-0.17472	true
(2, 8, 0)	-0.55657	-0.16145	0.57951	-163.82338	13.32183	0.07506	4.12311	104.03624	0	-0.17472	true
(8, 2, 0)	-0.55657	-0.16145	0.57951	-163.82338	13.32183	0.07506	4.12311	165.96376	0	-0.17472	true
(-2, 8, 0)	-0.55657	-0.16145	0.57951	-163.82338	13.32183	0.07506	4.12311	75.96376	0	-0.17472	true
(2, -8, 0)	-0.55657	-0.16145	0.57951	-163.82338	13.32183	0.07506	4.12311	104.03624	0	-0.17472	true
(-8, 2, 0)	-0.55657	-0.16145	0.57951	-163.82338	13.32183	0.07506	4.12311	14.03624	0	-0.17472	true

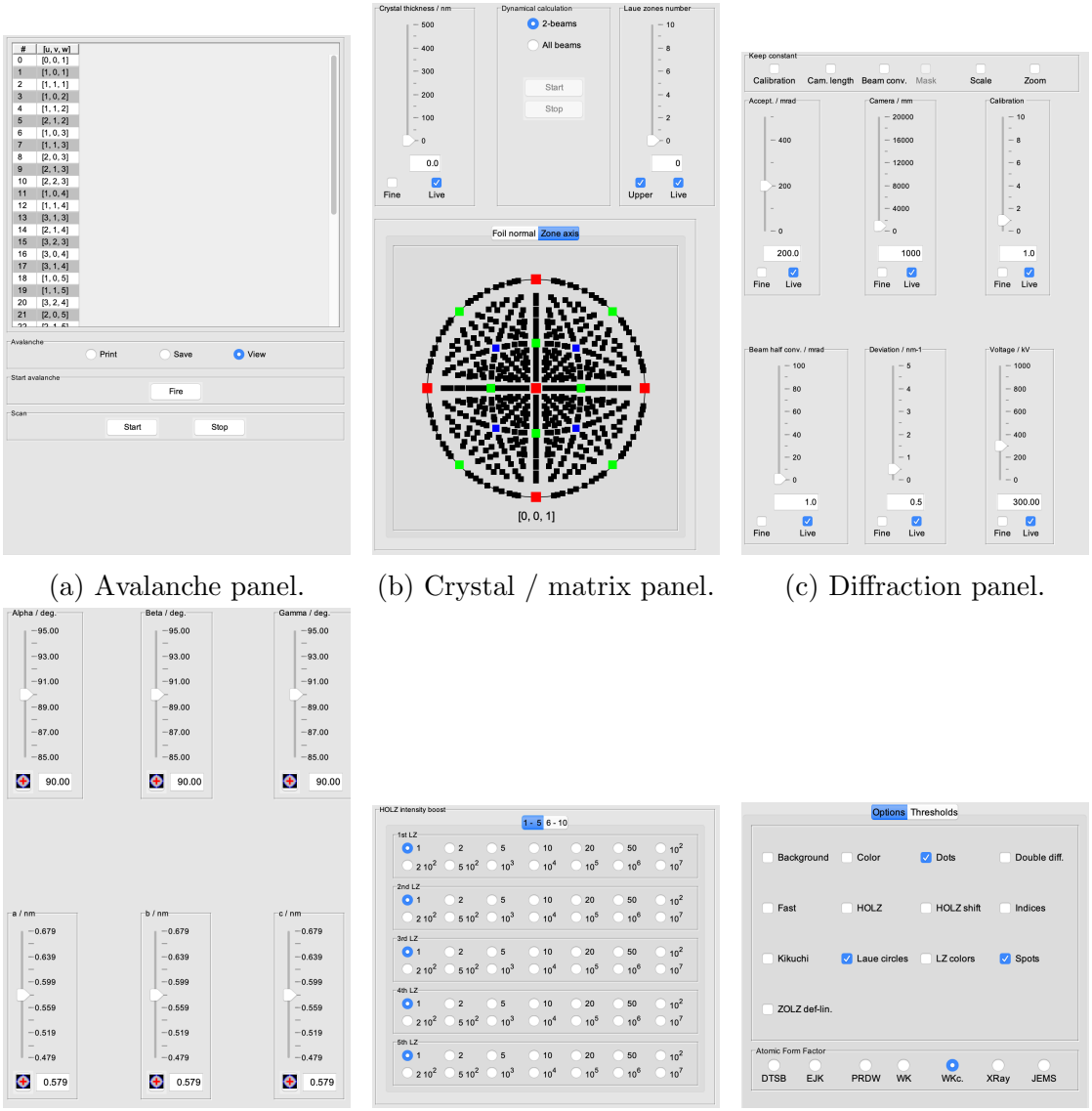
Figure 24: Table of the plotted reflections.

5.2 Tabs

All the controls necessary to draw SAED patterns are grouped in tabs that contains controls to:

- **Avalanche**: allows selecting a single or a range of [u,v,w] zone axis directions to plot, print or save as a .pdf booklet (Fig. 25a).
- **Crystal / matrix**: change the crystal thickness, perform dynamical calculations (Bloch-wave approach), select the Laue zones to plot or change the foil normal and zone axis (Fig. 25b).
- **Diffraction**: change the acceptance angle, the camera length, the calibration, the beam convergence, the deviation (number of reflections) and the accelerating voltage (Fig. 25c).
- **Lattice**: change the lattice parameters (Fig. 25d).
- **Laue zones**: boost the reflections intensity of the Laue zones (Fig. 25e).
- **Options**: select plot options (i.e. background, colour, etc) (Fig. 25f).
- **Oeientation**: set the relative orientation of the experimental and calculated patterns (Fig. 26a).

- **Process**: perform some image processing operations on the loaded experimental SAED pattern (Fig. 26b) [14].
- **Variant**: plot epitaxial or twinned patterns (Fig. 26c).

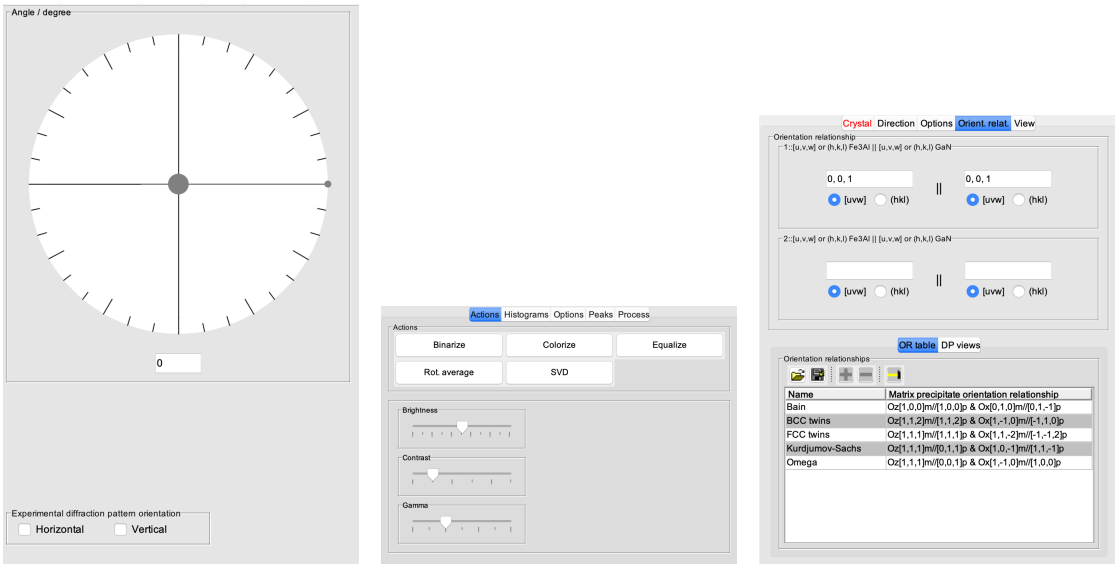


(a) Avalanche panel. (b) Crystal / matrix panel. (c) Diffraction panel.

(d) Lattice panel. (e) Laue zones panel. (f) Options panel.

Figure 25: First 6 tabs of SAED plotting controls.

[14] Only available when an experimental SAED pattern is loaded.



(a) Orientation panel. (b) Process panel. (c) Variant panel.

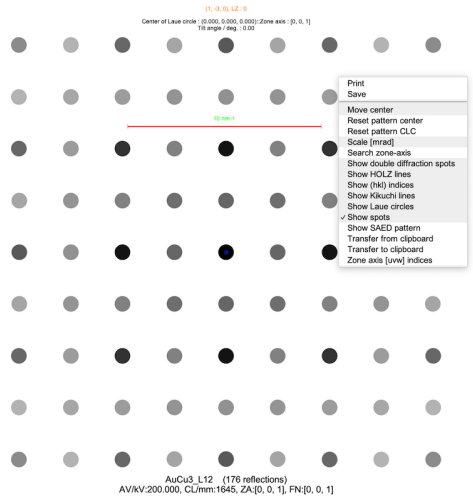
Figure 26: Last 3 tabs of SAED plotting controls.

5.3 Popup menu

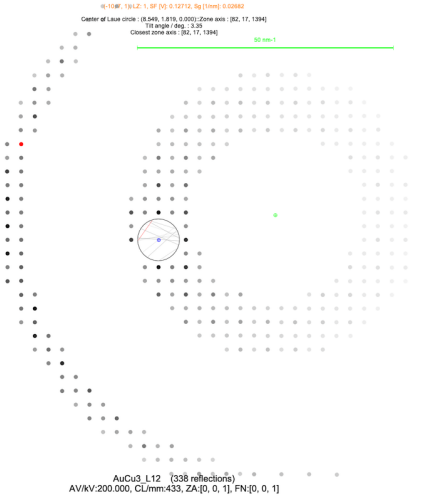
The popup menu attached to the SAED drawing duplicates several options of the **Options** tab (Fig. 27a).

Popup menu item **Move center** when selected allows to move the center of the diffraction pattern by dragging the *green cross*. When unselected the CLC is moved (also dragging the green cross), and the crystal is tilted away from the $[u, v, w]$ zone axis direction [15]. The *blue cross* marks the diffraction patttern center, i.e. the center of the $(0, 0, 0)$ reflection.

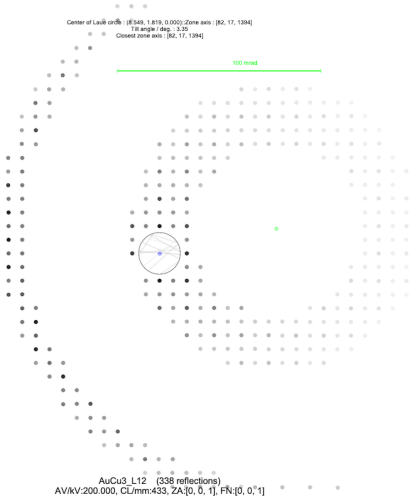
[15]The crystal orientation is always defined by the $[u, v, w]$ zone axis indices and the (h, k, l) of the CLC, the CLC being the projection of the Ewald center on the Zeroth Order Laue Zone (ZOLZ).



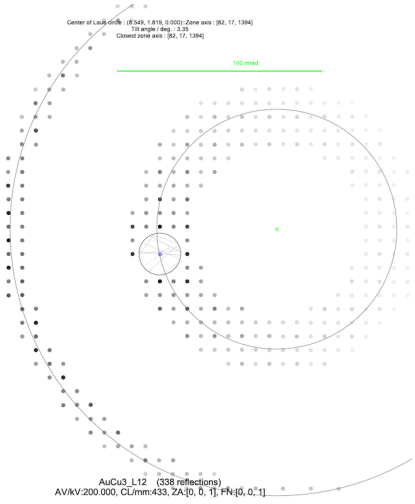
(a) SAED popup menu → Move center selected.



(b) SAED drawing with HOLZ reflections and lines.



(c) SAED drawing with HOLZ reflections and lines.



(d) SAED drawing with HOLZ reflections and lines and Laue circles.

Figure 27

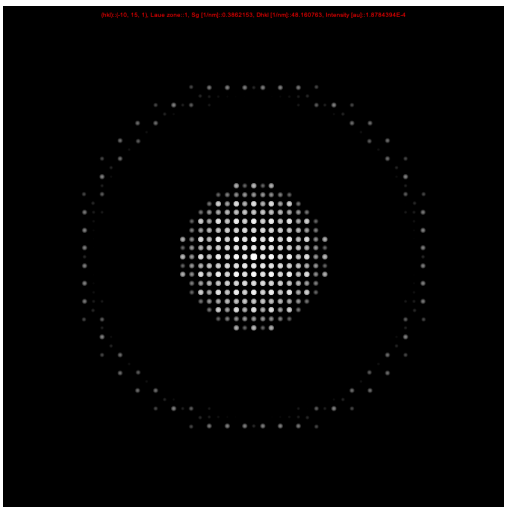
Popup menu item **Show HOLZ lines** displays the First Order Laue Zone (FOLZ) reflections and corresponding lines of the $(0, 0, 0)$ reflection zoomed 10 times. A mouse click on any HOLZ line highlights in red the HOLZ line and its associated reflection (Fig. 27b).

Popup menu item **Scale** $[mrad]$ when selected defines the scale in $[mrad]$ instead of $[nm^{-1}]$ (Fig. 27c).

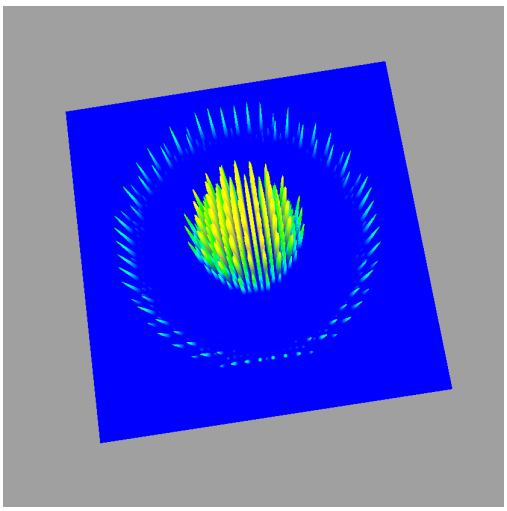
Popup menu item **Show Laue circles** when selected displays the Laue circles (Fig. 27d).

Popup menu item **Show Kikuchi lines** when selected displays the Kikuchi lines.

Popup menu item **Show SAED pattern** opens a frame with a SAED pattern image (Fig. 28a) and a 3-D view can be created using the popup menu attached to the image (Fig. 28b).



(a) SAED image (intensity log scale, FOLZ reflections intensity x 100).



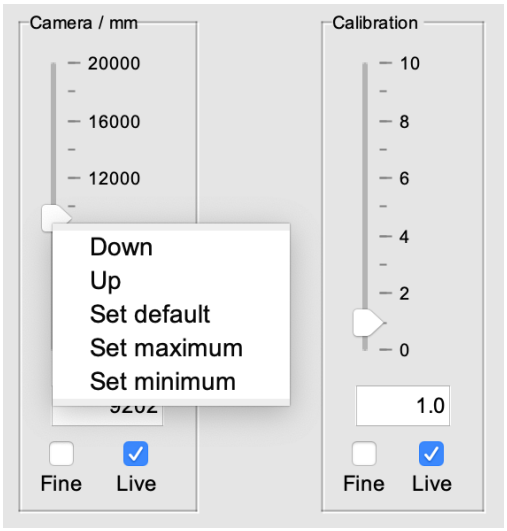
(b) SAED 3-D view.

Figure 28: SAED images

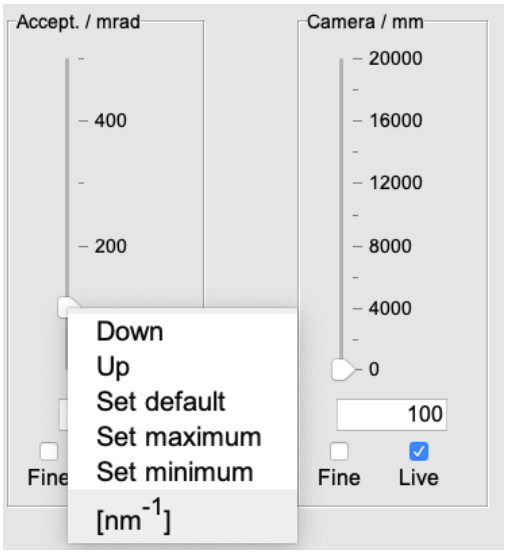
5.4 Sliders of Diffraction tab

Sliders in jems allow to modify parameters of drawings and images. Most sliders have a popup menu of type shown on Fig. 29a. The **Live** check box when selected forces the slider to update immediately the drawing or image. When unselected the update happens when the pointer leaves the slider. For lengthly updates it is good practice to unselect it. The **Fine** check box decreases the range of the slider. It is always possible to enter directly a value (within the selected range). Hit the **Return** keyboard key to confirm the entered value.

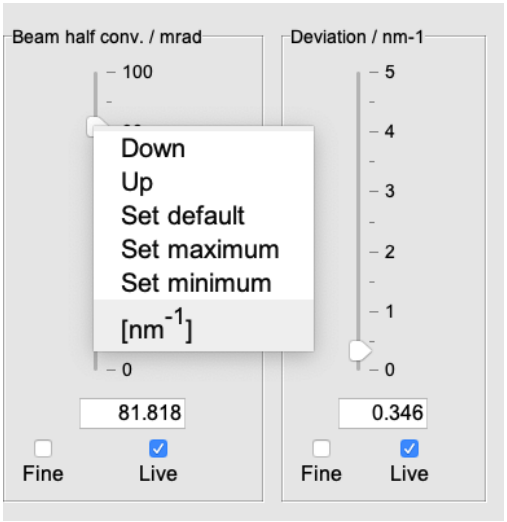
Sliders of parameters provided in $[nm^{-1}]$ can be modified to accept values in $[mrad]$ (Figs 29b, 29c).



(a) Camera length slider and its popup menu.



(b) Acceptance angle slider and its popup menu.



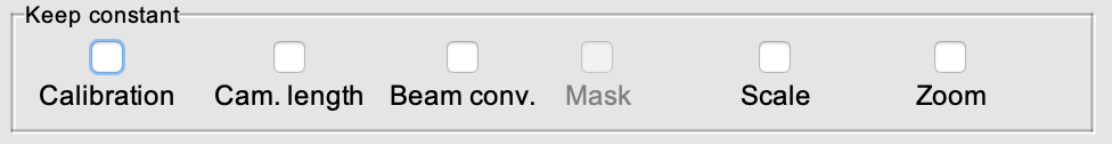
(c) Beam half convergence slider and its popup menu.

Figure 29: Typical SAED drawing sliders.

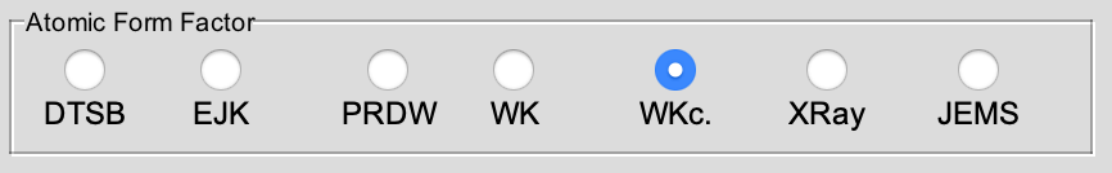
5.5 Other SAED parameters

Check boxes of Fig. 30a allow keeping constant a selection of drawing parameters when changing crystal structure or $[u, v, w]$ zone axis direction.

The source of the **A**tomic **F**orm **F**actors (AFF) is selected using the radio buttons of Fig. 30b. The source is described by a little tip text.



(a) Check boxes fixing selected parameters.



(b) Radio buttons selecting the AFF source.

Figure 30: SAED 2-D image and 3-D view.

5.6 SAED Bloch-wave calculation

The reflections intensity can be calculated when multiple scattering effects are included (dynamical calculation). This can be done either in the 2-beams approximation or all beams condition with or without HOLZ reflections included (Fig. 31). The calculation accepts a few hundred reflections and the intensity of the reflections is tabulated for thicknesses up to $500nm$. Remember that the calculation time is proportional to the third power of the number **n** of reflections (n^3). The number of reflections is selected using the **Deviation** slider that includes reflections at a distance to the Ewald sphere smaller than *"Deviation"* (Fig. 29c).

The **Start** button starts the dynamical calculation and the **Crystal thickness** slider changes the crystal thickness. A mouse click on a (h, k, l) reflection (except $(0, 0, 0)$) displays its intensity and phase (modulo 2π) as a function of crystal thickness (Fig. **??**). Mathematica tables and plots can then be created as well as text files (Figs 33a, 33b).

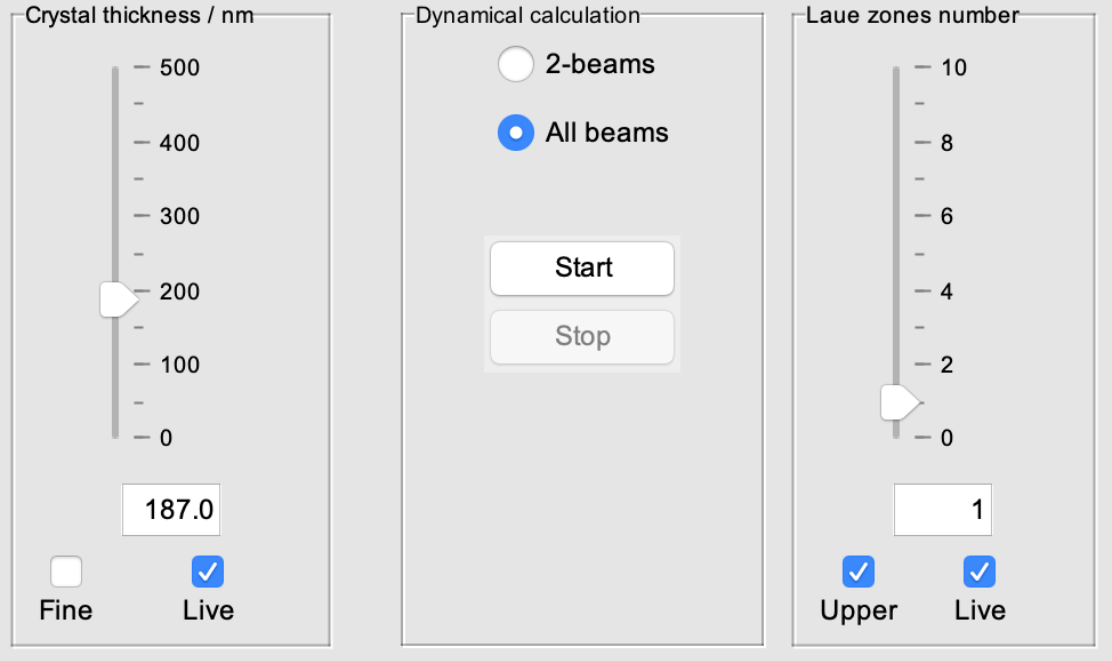


Figure 31: Dynamical SAED calculation controls.

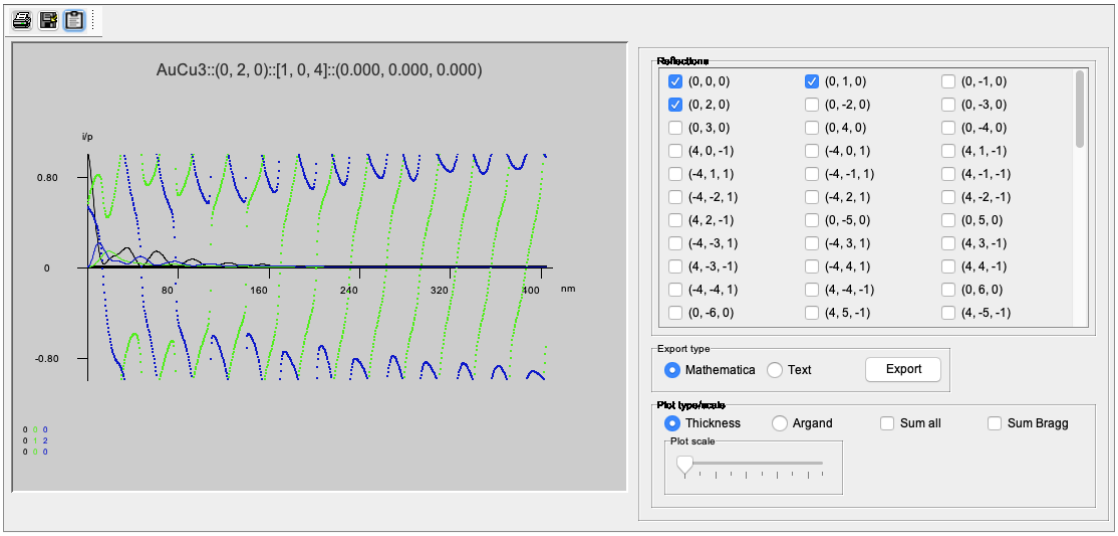
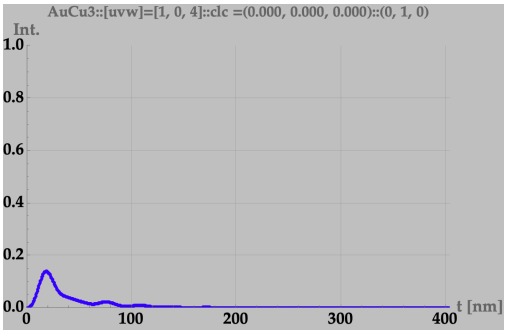
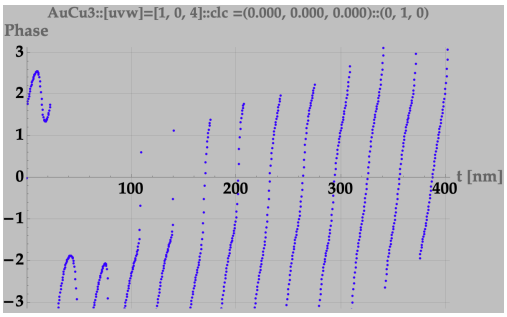


Figure 32: Plot of the intensity/phase of reflections as a function of crystal thickness.



(a) Mathematica intensity plot of $(0, 1, 0)$ reflection.



(b) Mathematica phase plot of $(0, 1, 0)$ reflection.

Figure 33: Mathematica plots of the $(0, 1, 0)$ reflection intensity and phase (modulo 2π).

5.7 SAED precession calculation

SAED precession calculations are performed by first tilting the crystal a few degrees out of perfect zone axis direction and then starting the precession using  tool button. The deviation should be set to a low value ($\sim 0.1\,[nm-1]$) since all the reflections are put into **Bragg** conditions during the precession. Precession calculations that include multiple scattering (dynamical diffraction) are performed using **Imaging** $\rightarrow$ **Bloch-wave** $\rightarrow$ **CBED** (sec. **??**).

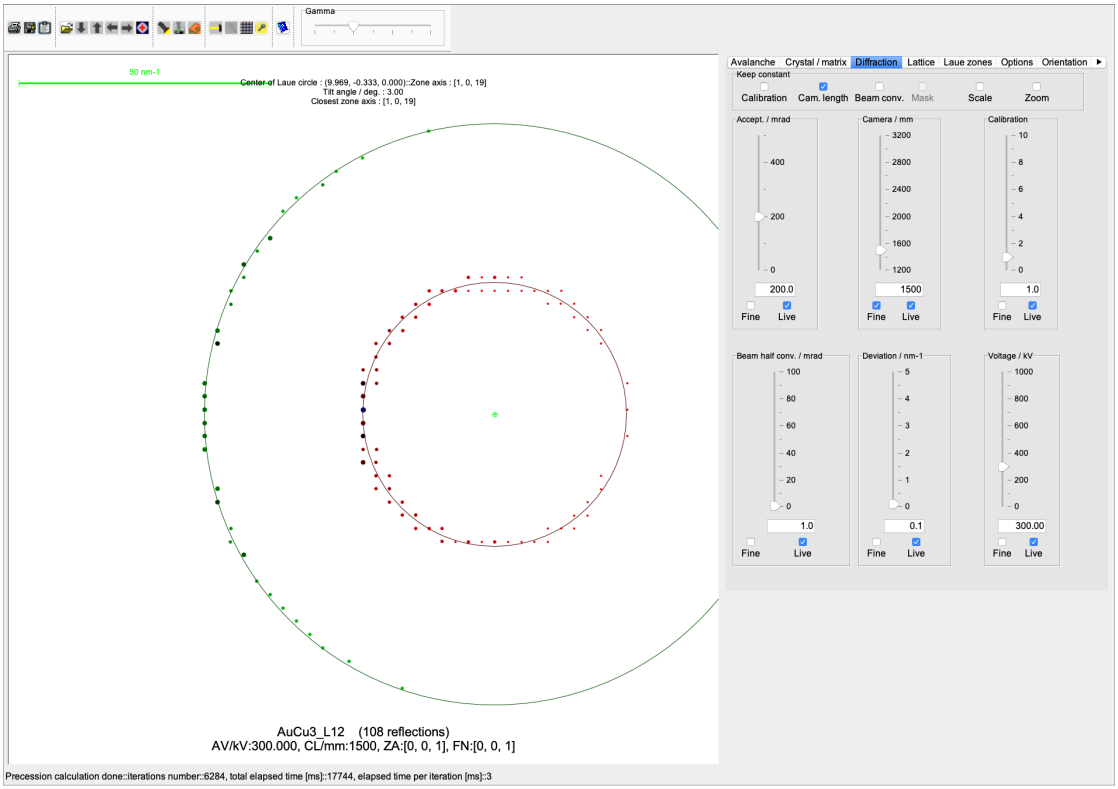
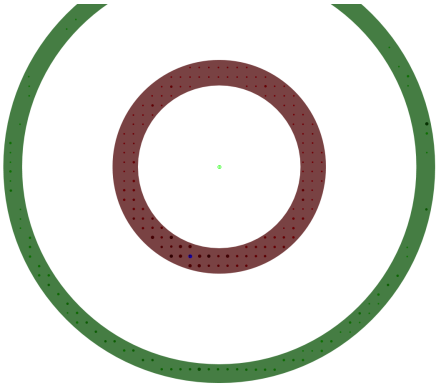
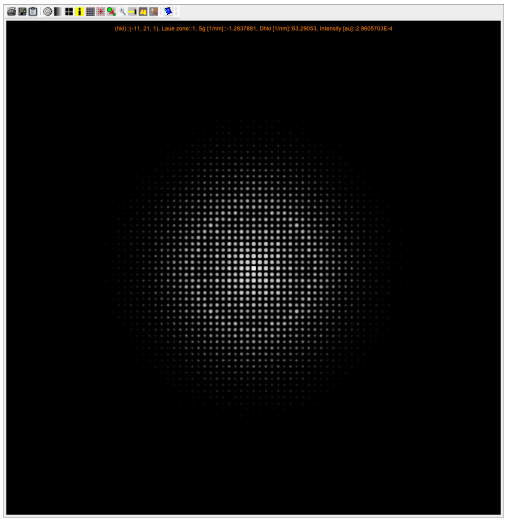


Figure 34: SAED precession settings, camera length 2000 $[mm]$, deviation 0.1 $[nm^{-1}]$, tilt 3.0 $[deg]$.



(a) SAED precession rotation, ZOLZ & FOLZ.



(b) Precession image (log scale).

Figure 35: SAED precession.

6 Bloch-wave calculations

Bloch-wave calculations is activated by **Imaging** → **Bloch-wave** menu item. The Bloch-wave frame (Fig. 36) allows to calculate CBED, LACBED and HREM images.

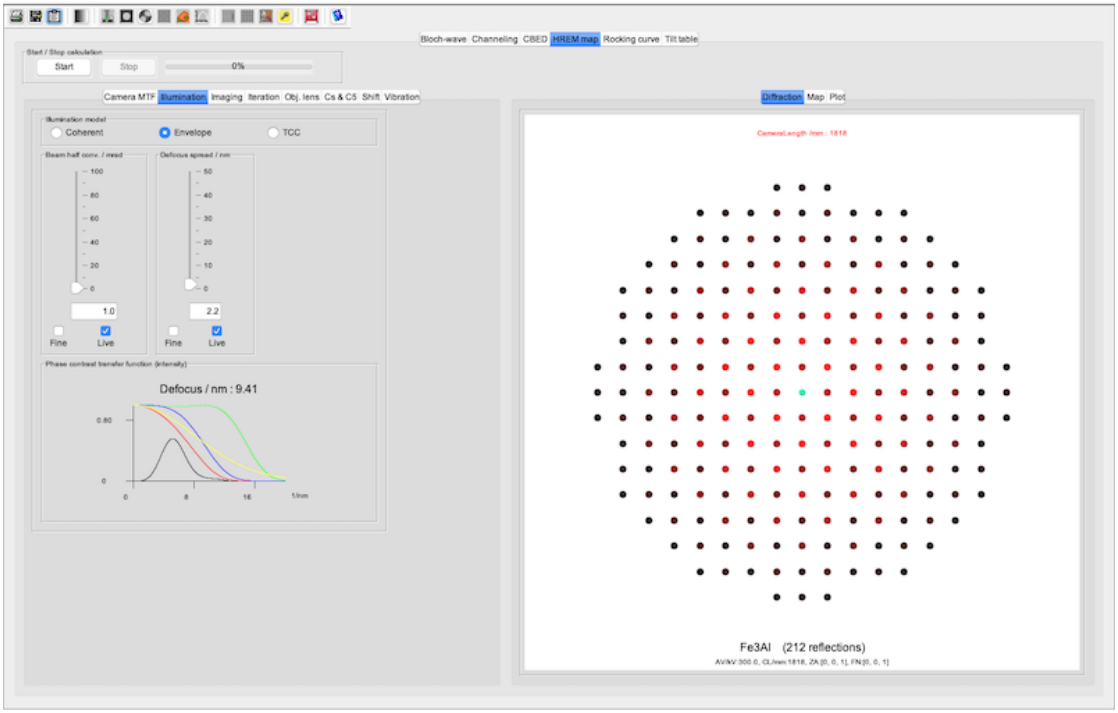


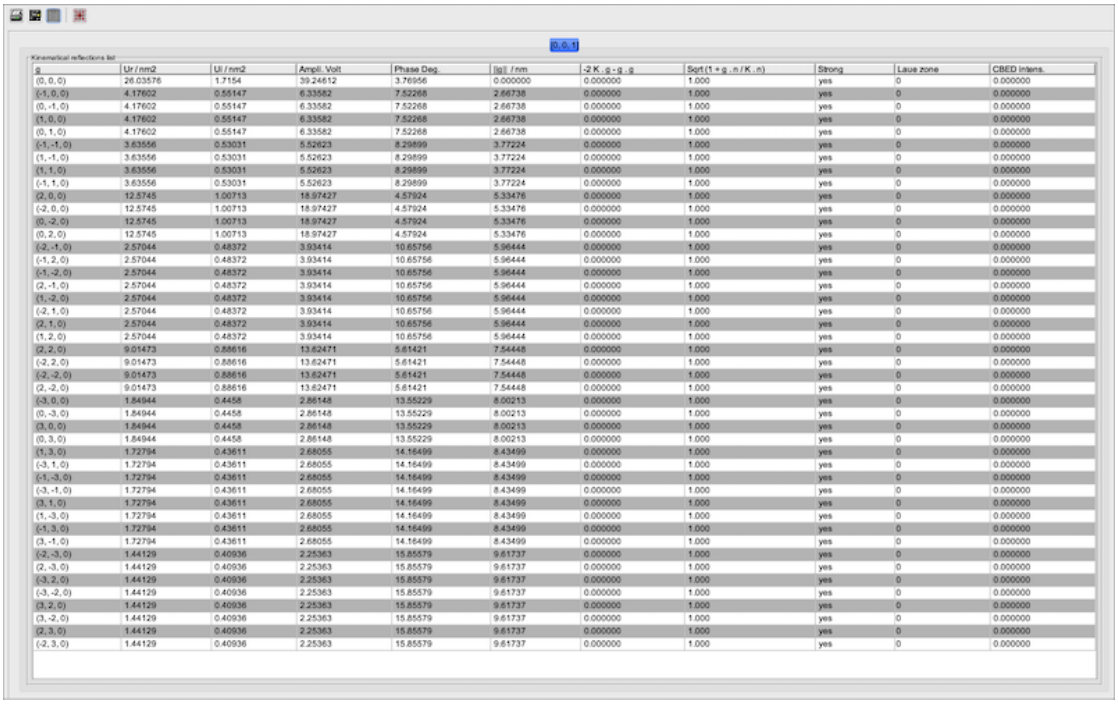
Figure 36: Bloch-wave calculations frame.

6.1 Tool buttons

The tool buttons of the Bloch-wave frame allow to:

- : print the plot or image.
- : save the crystal structure in .txt format.
- : transfer a frame image to the clipboard.
- : set the default gray LUT.
- : open the **Microscope** dialogue (Fig. 108).
- : open the **Apertures** dialogue (Fig. 79).

-  : open the **Wave-front aberrations** dialogue (Fig. **??**).
-  : control the holography biprism (when holography mode is enabled).
-  : open the **Specimen** dialogue (Fig. 84a).
-  : open the **Transfer function** frame (Fig. 97).
-  : start/stop the SAED precession.
-  : tabulate the (h, k, l) reflections (Fig. 37).
-  : open the toolbox with context dependent controls.
-  : open the **Keeper** dialogue (Fig. 90).
-  : reset the wave-front aberrations and imaging conditions.
-  : open the associated help dialogue.



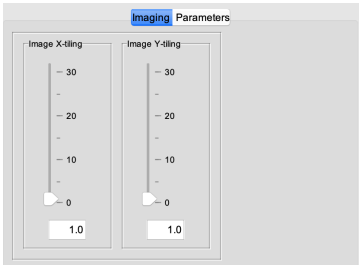
g	Ur / nm2	UI / nm2	Ampli. Volt	Phase Deg.	|g| / nm	-2 K . g - g . g	Sqrt (1 + g . n / K . n)	Strong	Laue zone	CBED Intens.
(0, 0, 0)	26.03576	1.7154	39.24612	3.76956	0.000000	0.000000	1.000	yes	0	0.000000
(-1, 0, 0)	4.17602	0.55147	6.33582	7.52268	2.66738	0.000000	1.000	yes	0	0.000000
(0, -1, 0)	4.17602	0.55147	6.33582	7.52268	2.66738	0.000000	1.000	yes	0	0.000000
(1, 0, 0)	4.17602	0.55147	6.33582	7.52268	2.66738	0.000000	1.000	yes	0	0.000000
(0, 1, 0)	4.17602	0.55147	6.33582	7.52268	2.66738	0.000000	1.000	yes	0	0.000000
(-1, -1, 0)	3.63556	0.53031	5.52623	8.29899	3.77224	0.000000	1.000	yes	0	0.000000
(1, -1, 0)	3.63556	0.53031	5.52623	8.29899	3.77224	0.000000	1.000	yes	0	0.000000
(1, 1, 0)	3.63556	0.53031	5.52623	8.29899	3.77224	0.000000	1.000	yes	0	0.000000
(-1, 1, 0)	3.63556	0.53031	5.52623	8.29899	3.77224	0.000000	1.000	yes	0	0.000000
(2, 0, 0)	12.5745	1.00713	18.97427	4.57924	5.33476	0.000000	1.000	yes	0	0.000000
(-2, 0, 0)	12.5745	1.00713	18.97427	4.57924	5.33476	0.000000	1.000	yes	0	0.000000
(0, -2, 0)	12.5745	1.00713	18.97427	4.57924	5.33476	0.000000	1.000	yes	0	0.000000
(0, 2, 0)	12.5745	1.00713	18.97427	4.57924	5.33476	0.000000	1.000	yes	0	0.000000
(-2, -1, 0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	yes	0	0.000000
(-1, 2, 0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	yes	0	0.000000
(-1, -2, 0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	yes	0	0.000000
(2, -1, 0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	yes	0	0.000000
(1, -2, 0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	yes	0	0.000000
(-2, 1, 0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	yes	0	0.000000
(2, 1, 0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	yes	0	0.000000
(1, 2, 0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	yes	0	0.000000
(2, 2, 0)	9.01473	0.88616	13.62471	5.61421	7.54448	0.000000	1.000	yes	0	0.000000
(-2, 2, 0)	9.01473	0.88616	13.62471	5.61421	7.54448	0.000000	1.000	yes	0	0.000000
(-2, -2, 0)	9.01473	0.88616	13.62471	5.61421	7.54448	0.000000	1.000	yes	0	0.000000
(2, -2, 0)	9.01473	0.88616	13.62471	5.61421	7.54448	0.000000	1.000	yes	0	0.000000
(-3, 0, 0)	1.84944	0.4458	2.86148	13.55229	8.00213	0.000000	1.000	yes	0	0.000000
(0, -3, 0)	1.84944	0.4458	2.86148	13.55229	8.00213	0.000000	1.000	yes	0	0.000000
(3, 0, 0)	1.84944	0.4458	2.86148	13.55229	8.00213	0.000000	1.000	yes	0	0.000000
(0, 3, 0)	1.84944	0.4458	2.86148	13.55229	8.00213	0.000000	1.000	yes	0	0.000000
(-3, 3, 0)	1.72794	0.43611	2.68055	14.16499	8.43499	0.000000	1.000	yes	0	0.000000
(-3, 1, 0)	1.72794	0.43611	2.68055	14.16499	8.43499	0.000000	1.000	yes	0	0.000000
(-1, -3, 0)	1.72794	0.43611	2.68055	14.16499	8.43499	0.000000	1.000	yes	0	0.000000
(-3, -1, 0)	1.72794	0.43611	2.68055	14.16499	8.43499	0.000000	1.000	yes	0	0.000000
(3, 1, 0)	1.72794	0.43611	2.68055	14.16499	8.43499	0.000000	1.000	yes	0	0.000000
(1, -3, 0)	1.72794	0.43611	2.68055	14.16499	8.43499	0.000000	1.000	yes	0	0.000000
(-1, 3, 0)	1.72794	0.43611	2.68055	14.16499	8.43499	0.000000	1.000	yes	0	0.000000
(3, -1, 0)	1.72794	0.43611	2.68055	14.16499	8.43499	0.000000	1.000	yes	0	0.000000
(-2, -3, 0)	1.44129	0.40936	2.25363	15.85579	9.61737	0.000000	1.000	yes	0	0.000000
(2, -3, 0)	1.44129	0.40936	2.25363	15.85579	9.61737	0.000000	1.000	yes	0	0.000000
(-3, 2, 0)	1.44129	0.40936	2.25363	15.85579	9.61737	0.000000	1.000	yes	0	0.000000
(-3, -2, 0)	1.44129	0.40936	2.25363	15.85579	9.61737	0.000000	1.000	yes	0	0.000000
(3, 2, 0)	1.44129	0.40936	2.25363	15.85579	9.61737	0.000000	1.000	yes	0	0.000000
(2, -2, 0)	1.44129	0.40936	2.25363	15.85579	9.61737	0.000000	1.000	yes	0	0.000000
(2, 3, 0)	1.44129	0.40936	2.25363	15.85579	9.61737	0.000000	1.000	yes	0	0.000000
(-2, 3, 0)	1.44129	0.40936	2.25363	15.85579	9.61737	0.000000	1.000	yes	0	0.000000

Figure 37: Reflections table.

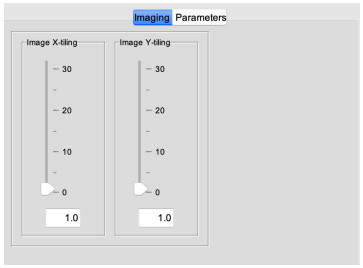
6.2 Tabs

The controls of the parameters for the different Bloch-wave calculations are grouped in the following tabs in order to calculate:

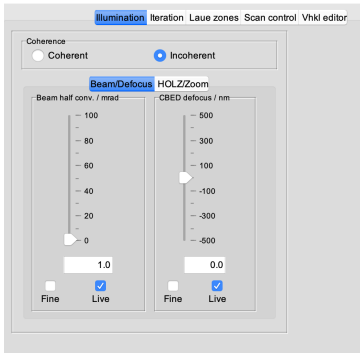
- **Bloch-wave**: Bloch-wave images (Fig. 38a).
- **Channeling**: channeling images (Fig. 38b).
- **CBED**: CBED, LACBED and dynamical precession patterns (Fig. 38c).
- **HREM map**: maps of HREM images (Fig. 38d).
- **Rocking curve**: rocking curves (Fig. 38e).
- **Tilt table**: tables of tilted HREM maps (Fig. 38f).



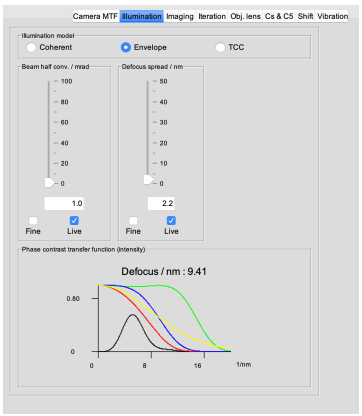
(a) Bloch-wave panel.



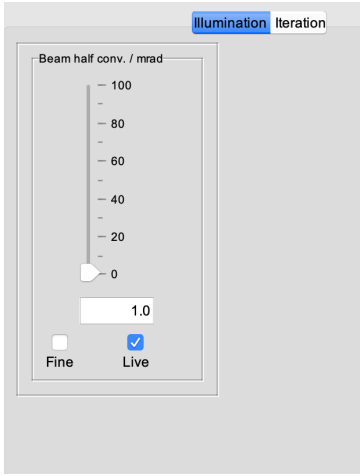
(b) Channeling panel.



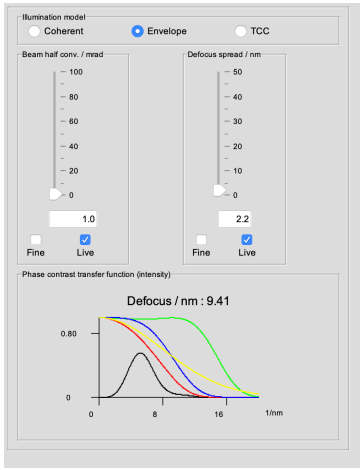
(c) CBED panel.



(d) HREM map panel.



(e) Rocking curve panel.



(f) Tilt table panel.

Figure 38: Tabs of the different Bloch-wave calculations.

6.3 HREM images map calculations using the Bloch-wave method

In order to calculate a HREM images map (Fig. 39) [16] by the **B**loch-**W**ave (BW) approach, it is necessary to define the:

- The image formation model. The **"Coherent"** model assumes a coherent illumination, **"Envelope"** introduces the attenuation envelopes due to partial coherence and **"TCC"** uses **T**ransmission **C**ross **C**oefficients.
- Camera length $[nm]$ and number of reflections (set using the context sensitive tool box button ).
- Illumination and image formation model (Fig. 40a).
- Imaging conditions, defocus $[nm]$ and image dimension (Figs 40c, 40d) [17].
- Crystal thickness $[nm]$, images map, AFF and HRTEM imager (Figs 40e, 40f, 40g, 40h).
- 2-fold astigmatism $[nm]$, 2^{nd} order coma $[nm]$, 3-fold astigmatism $[nm]$ and objective aperture diameter $[nm^{-1}]$ (Fig. 41a).
- Defocus $[nm]$, 3^{nd} and 5^{th} spherical aberrations $[mm]$ (Fig. 41b).
- Image shift $[nm]$ and phase shift $[deg]$ (Fig. 41c) [18].
- Specimen drift, **T**hermal **M**agnetic noise (TM noise) and specimen vibration (Figs 42a, 42b).

Note that the transfer function *intensity* is plotted on Figs 40a, 40b, 40c[19]. The popup menu associated with the plot allows to identify the transferred spacial frequencies (Fig. 40b). The line colours are:

- **Red**: transfer function including attenuation due to partial spatial and temporal coherence as well as **T**hermal **M**agnetic noise (TM).
- **Yellow**: thermal magnetic noise [20].

[16] The thickness step in HRTEM calculations by the Bloch-wave method is not necessarily a multiple of the unit cell thickness.

[17] When placing the pointer (mouse) on the transfer function drawing, the defocus is modified using the keyboard arrow keys ↑ and ↓

[18] The phase shift control is active when a beam stop is inserted in the back focal plane of the objective lens  (apertures dialogue).

[19] The intensity plot is intended to identify the reflections transferred by the objective lens (lines are indexed when aimed).

[20]  cancels the TM noise as well all other aberrations (except the spherical aberrations).

- **Green**: partial spatial coherence (beam convergence).
- **Blue**: partial temporal coherence (defocus spread).

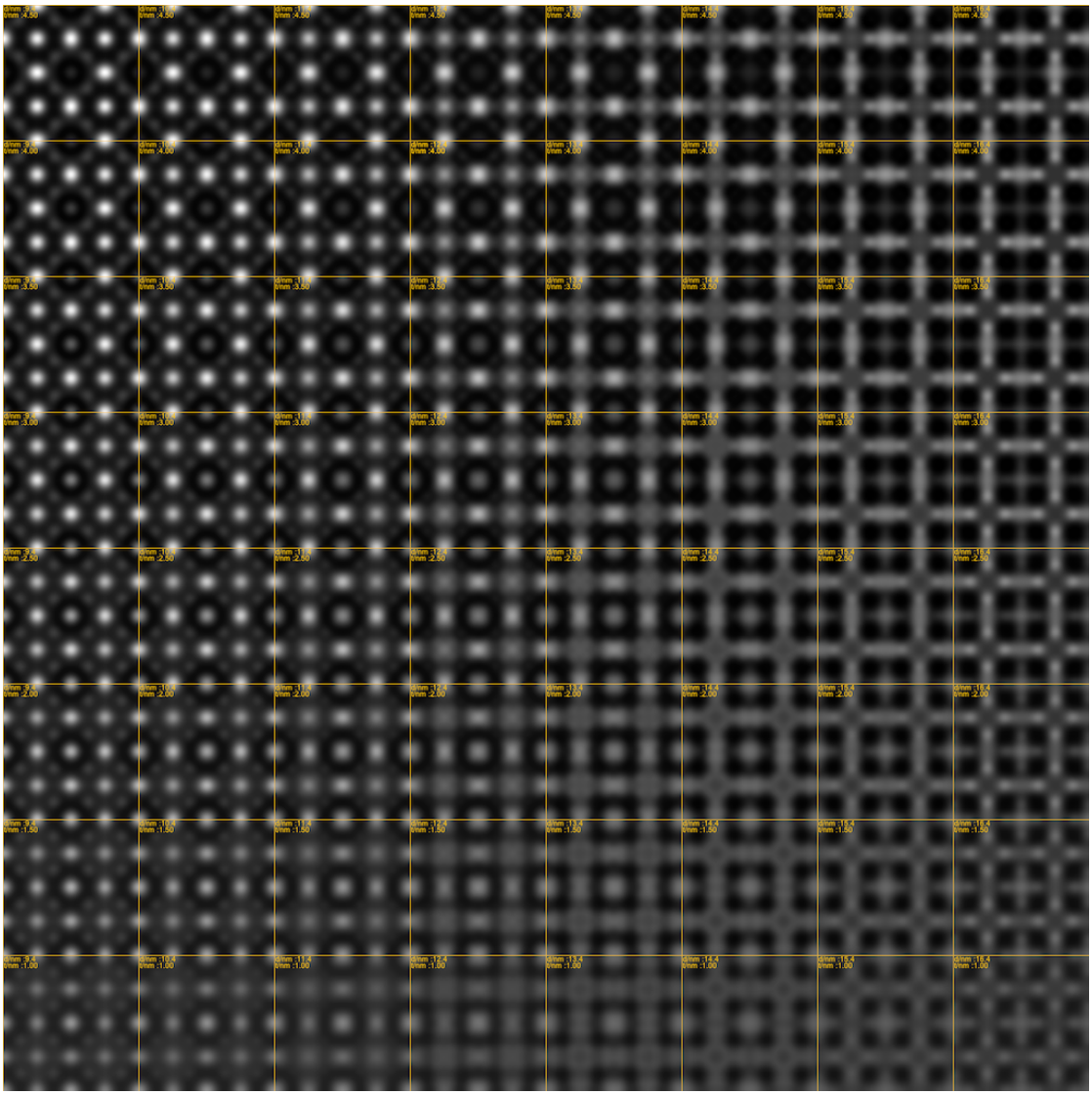
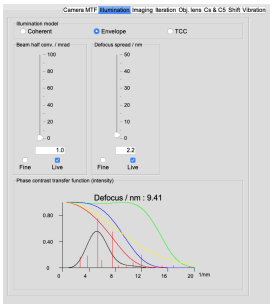
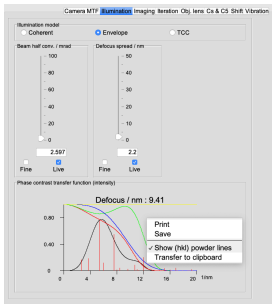


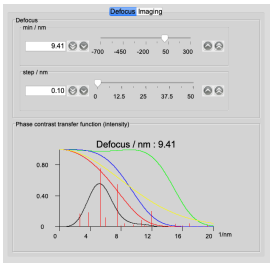
Figure 39: $AuCu_3$ (8×8) HREM images map with decreasing defocus (horizontally) and increasing thickness (vertically).



(a) Illumination and imaging model.

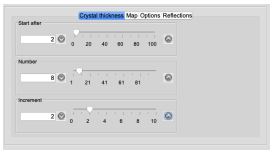


(b) Popup menu associated with the transfer function drawing (intensity).



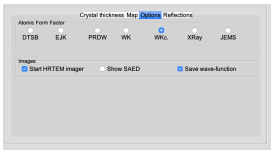
(c) Starting defocus $[nm]$ (minimum), defocus step $[nm]$.

(d) Defocus series size and duplication of unit cell image.

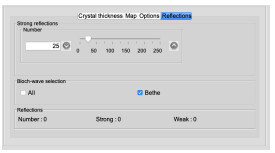


(e) Minimum crystal thickness $[nm]$, number of iterations, thickness increment $[nm]$.

(f) Plot and map options.



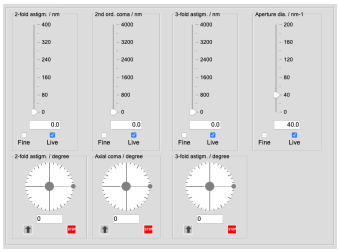
(g) HREM map iteration options.



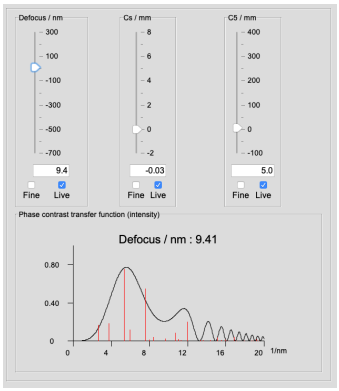
(h) Reflections number and Bethe approximation.

Figure 40: Controls the illumination, defocus, specimen thickness values, number of *strong* reflections and introduces Bethe approximation.

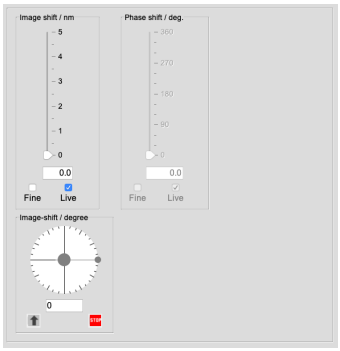
When the wave-functions are saved (as .ems) images and the **"Start HRTEM imager"** is selected (Fig. 40g) a frame is activated that allows to introduce in the HRTEM image calculations all wave-front aberrations (up to order 8) as well as beam tilt and objective aperture center among others (**??**).



(a) Objective lens aberrations $[nm]$ and objective aperture size $[nm^{-1}]$

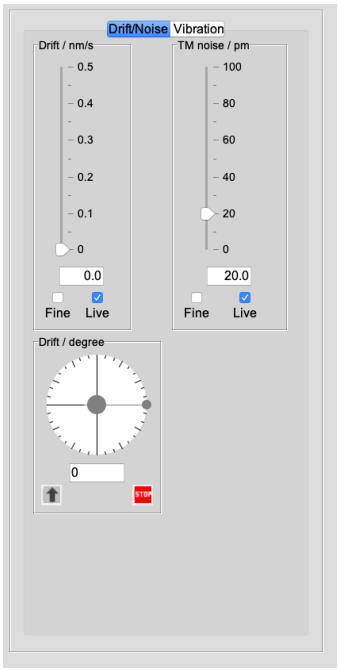


(b) Defocus $[nm]$ 3^{rd} and 5^{th} order spherical aberrations $[mm]$.

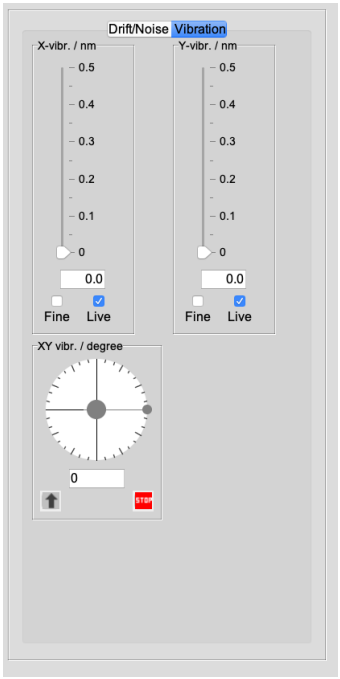


(c) Image shift $[nm]$ and phase shift $[deg]$.

Figure 41



(a) Image drift $[nms^{-1}$]and **T**hermal **Magnetic** noise $[pm]$.



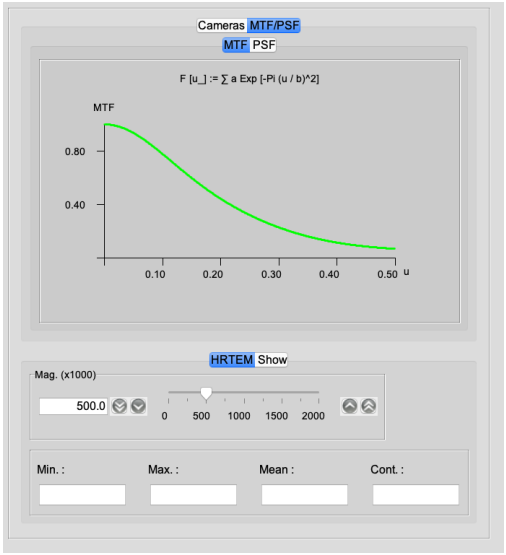
(b) Specimen vibration $[nm]$.

Figure 42

When the MTF of the camera **M**odulation **T**ransfer **F**unction (MTF) has been measured it is possible to introduce its effect in the HRTEM image simulation. This requires to enable the **Plot** → **Image** check box (**Iteration** → **Map** →**Plot** → **Image**). When HRTEM image calculation is completed select the panel (**HREM map** → **Plot**) [21] (Figs 44a, 44a, 45a, 45a).

The HRTEM imaging parameters used by the image displayed on the **Plot** panel can be changed interactively. As an example select the **Obl. lens** tab and modify the 3-fold astigmatism and its orientation (Figs 46c, 46f, 46e, 46f).

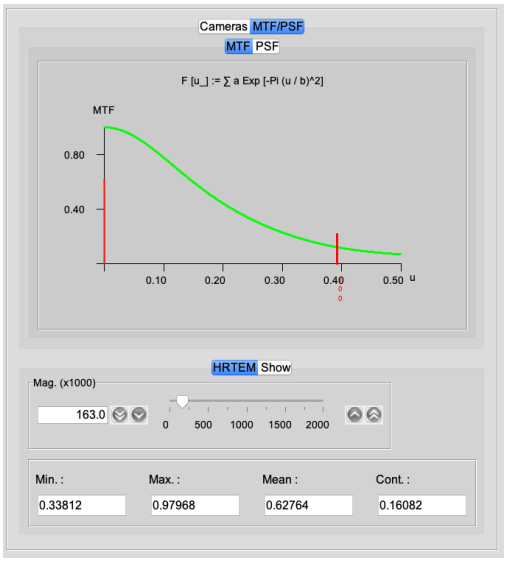
(a) Table of cameras with magnification controls.



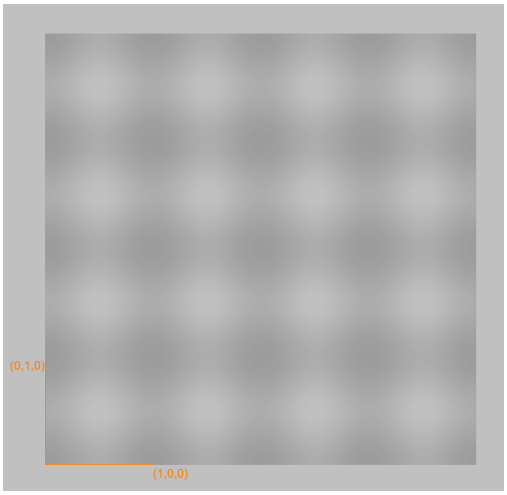
(b) MTF of a 1024 x 1024, 24 μm pixel size camera.

Figure 43: Controls to introduce the camera MTF in the HRTEM simulations.

[21] To start the calculation either the **Diffraction** or **Map** tab must be selected

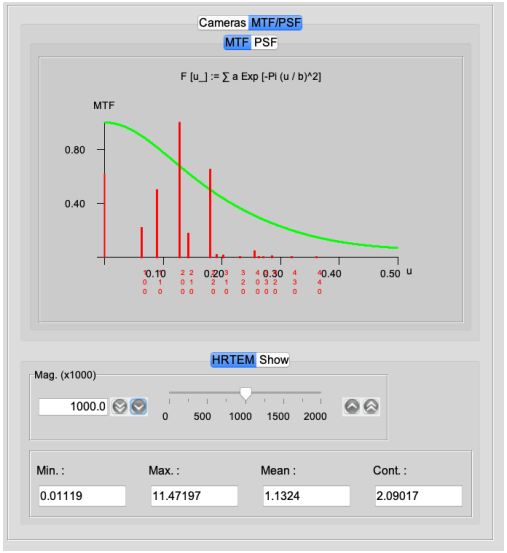


(a) At **low** magnification the camera transfers only **low** spatial image frequencies.

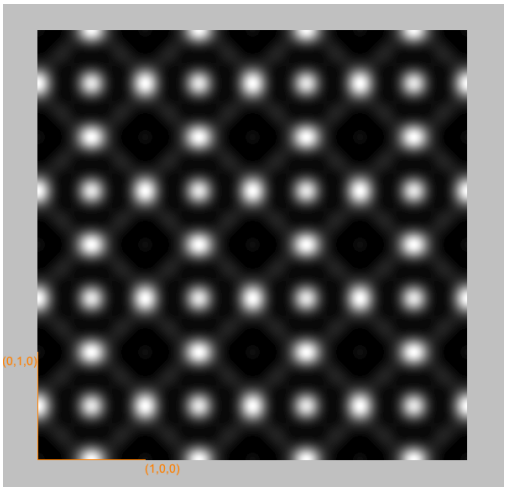


(b) At **low** magnification the contrast and resolution of the image are **low**.

Figure 44: Low magnification.



(a) At **high** magnification the camera transfers **high** spatial image frequencies.



(b) At **high** magnification the contrast and resolution of the image are **high**.

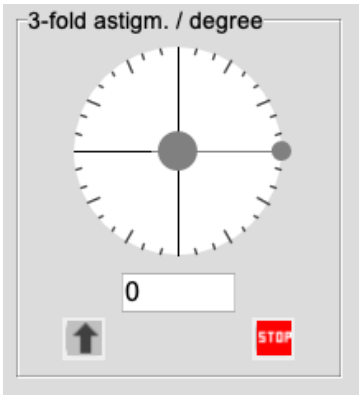
Figure 45: High magnification.

By default 2 MTF are listed in the MTF table:

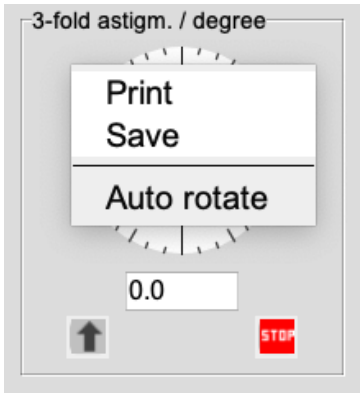
- a camera with a constant MTF of value 1.0.
- a 1024 x 1024 camera of 24 μm pixel size.

As an example select the **Obj. lens** tab and modify the 3-fold astigmatism and its orientation (Figs 46b, 46a, 46c, 46d, 46e, 46f) [22].

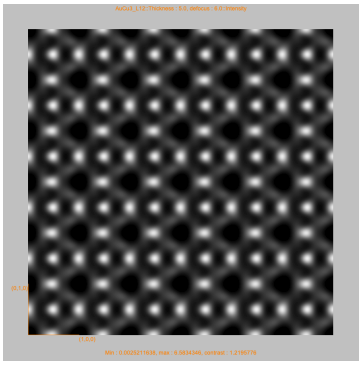
[22] A popup menu is associated with the image in order to transfer it to the clipboard.



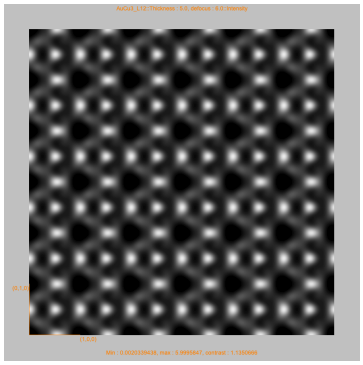
(a) 3-fold astigmatism orientation control (a value is set by dragging the needle or clicking on a graduation).



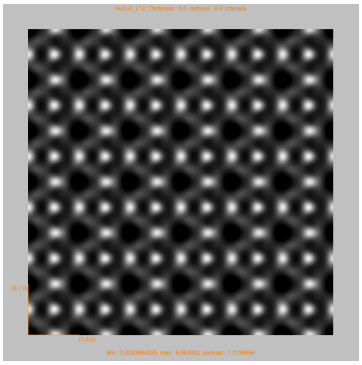
(b) 3-fold astigmatism orientation control and associated popup menu. **Auto rotate** popup menu item changes continuously the orientation.



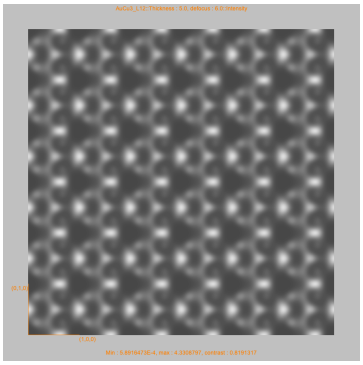
(c) 300nm 3-fold astigmatism oriented at 0°.



(d) 300nm 3-fold astigmatism oriented at 60°.



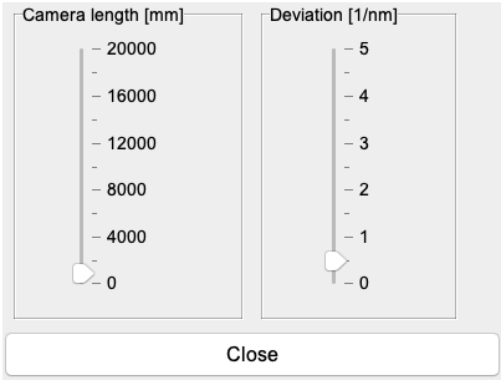
(e) 600nm 3-fold astigmatism oriented at 0°.



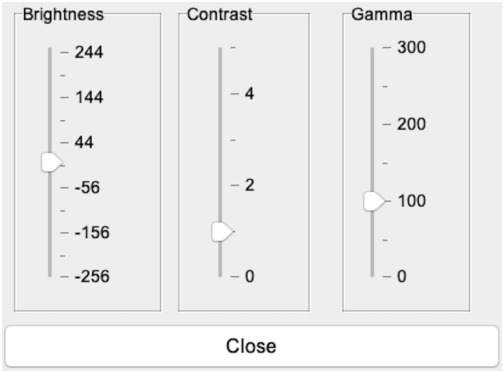
(f) 600nm 3-fold astigmatism oriented at 60°.

Figure 46: Effect of 3-fold astigmatism on HRTEM images.

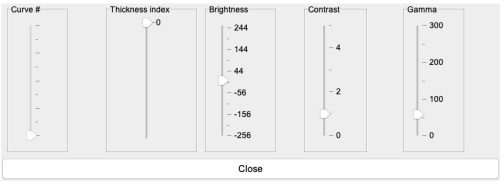
The contrast of the plotted HRTEM image is modified using the controls provided in context specific tools boxes  (Figs 47a, 47b, 47c).



(a) Tool box of **Diffraction** context to change the camera length and the number of reflections (deviation control).



(b) Tool box of **Map** context to change the image contrast.

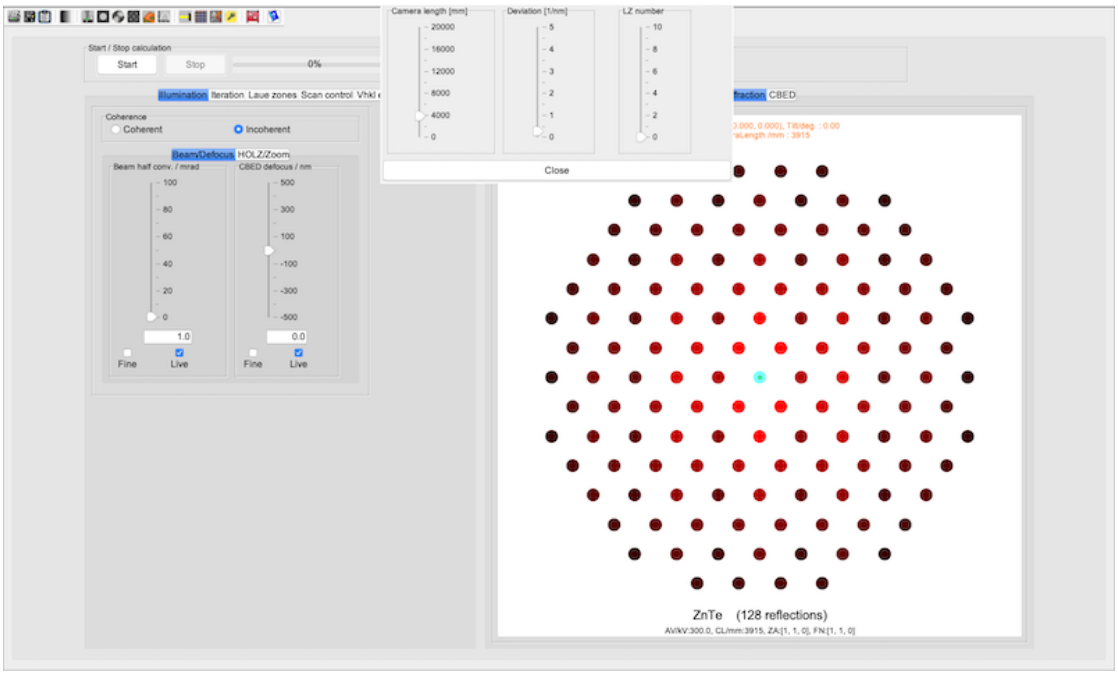


(c) Tool box of **Plot** context to change the plotted curve (intensity versus thickness of (h, k, l) reflections), the crystal thickness, and the image contrast.

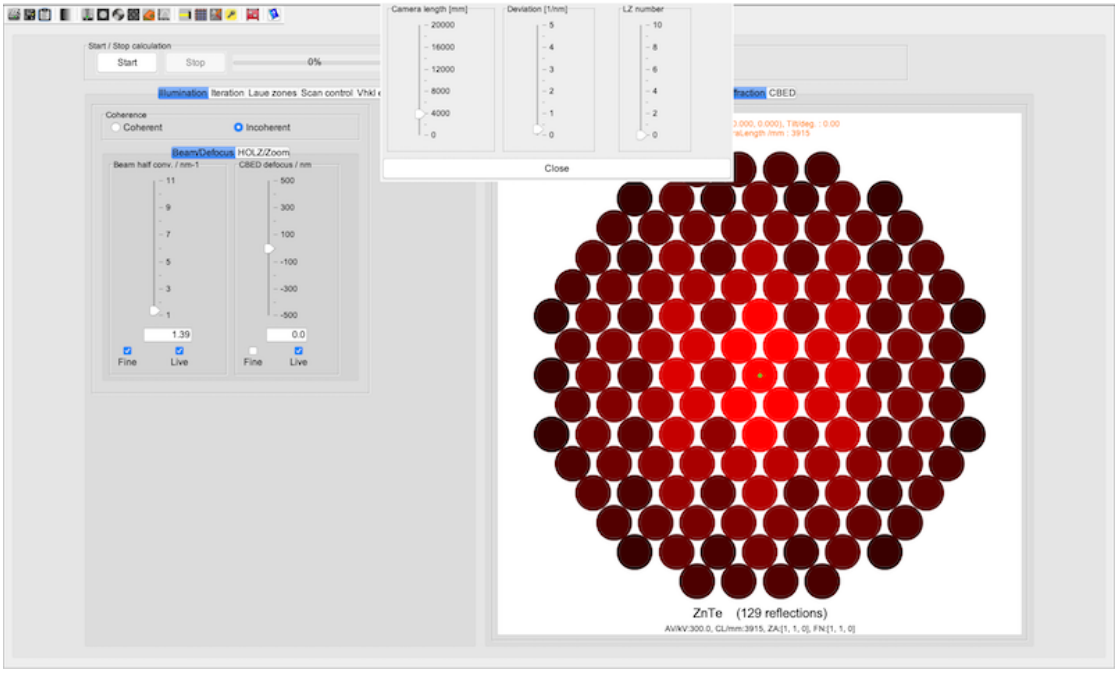
Figure 47: Tool boxes of **Diffraction** (a), **Map** (b) and **Plot** (c) contexts.

6.4 CBED patterns calculation using the Bloch-wave method

Fig. 48a displays the main tab for calculating **C**onvergent **B**eam **E**lectron **D**iffraction (CBED) patterns. The camera length, deviation and Laue zones controls of the toolbox are activated using  tool button. The convergence of the incident electron beam is set by the Beam half conv [*mrad*] control. Its popup menu allows to set it in $[nm-1]$ (Fig. 48b). The **CBED defocus** control makes possible to calculate coherent CBED.



(a) CBED calculation by the Bloch-wave method.



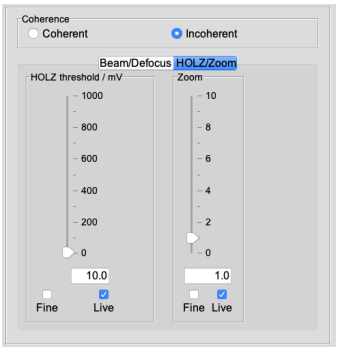
(b) Illumination control ($[nm-1]$) set to have just touching reflections.

Figure 48: ZnTe $[1,1,0]$ CBED pattern calculation.

The CBED calculations are controlled using sliders, check boxes or radio buttons distributed in the following tabs:

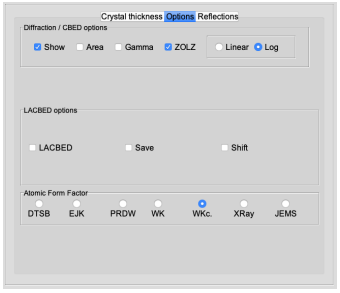
- **Illumination**: Figs 49a, 49b.
- **Iteration**: Figs 49c, 49d, 49e.
- **Laue zones**: Fig 49f.
- **Scan control**: Figs 50a, 50b.
- **Vhkl editor**: Fig. 50c.

(a) Beam half-conv $[mrad]$ or $[nm-1]$ and CBED defocus $[nm]$ controls.

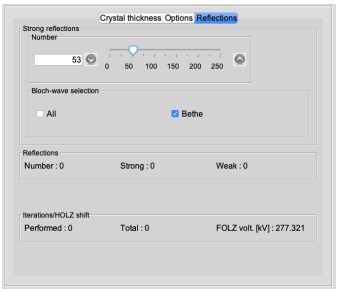


(b) HOLZ threshold $[mV]$ and Zoom controls.

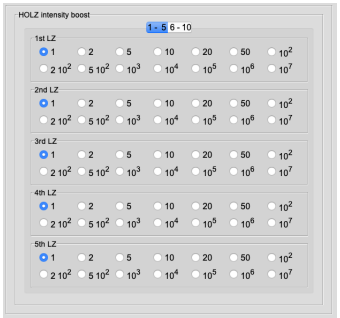
(c) Defines the minimum thickness $[nm]$, the number of thickness steps and the increment of the steps. The thickness step minimum is $1\,nm$.



(d) Defines CBED options to **Show** the progress of the calculation, scan a rectangular area instead of the circular area delimited by the $(0,0,0)$ spot, to fix the gamma for all the series of CBED patterns, displays the ZOLZ lines and uses a linear or logarithmic intensity scale.

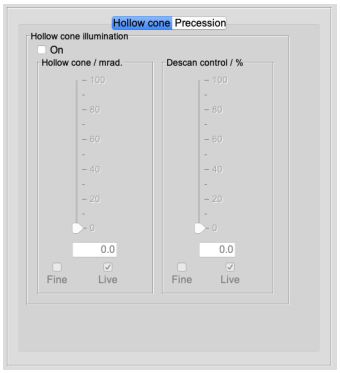


(e) Sets the minimum number of the strong reflections. When the **Bethe** checkbox is enabled a weak reflection is selected, its effect is introduced introduced in the calculation using the Bethe perturbation approximation.

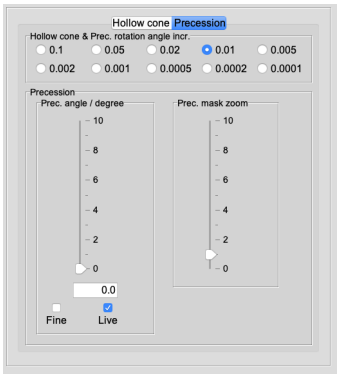


(f) Boosts the intensity of the HOLZ reflections and lines shown on the Diffraction plot.

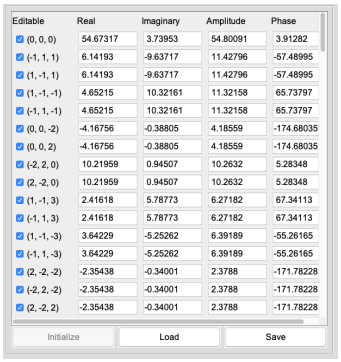
Figure 49: CBED controls tabs.



(a) Simulates **Hollow cone illumination**.

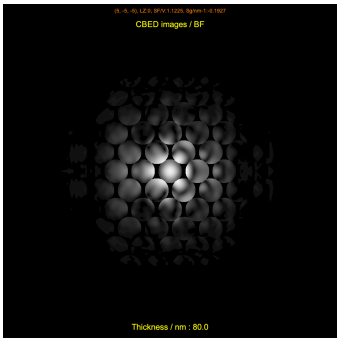


(b) Defines the dynamical precession parameters: rotation increment, precession angle [*degree*] and the size of the intensity integration area.

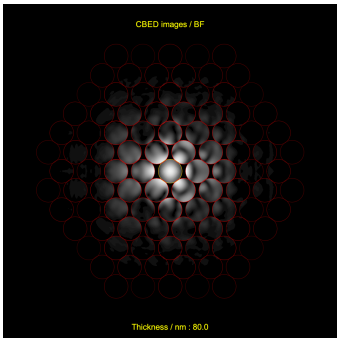


(c) Allows to set the structure factor of selected reflections.

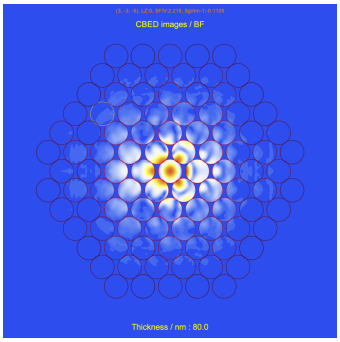
Figure 50: CBED controls tabs.



(a) 80 *nm*, ZnTe [110]. Vertical symmetry plane is missing to ZnTe polarity (thickness and contrast settings provided by the toolbox.

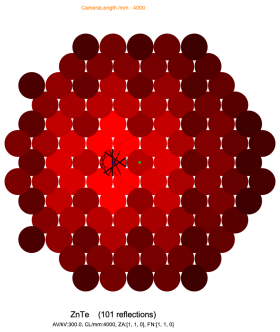


(b) 80 *nm*, ZnTe [110], indexed reflections (using the toolbox).

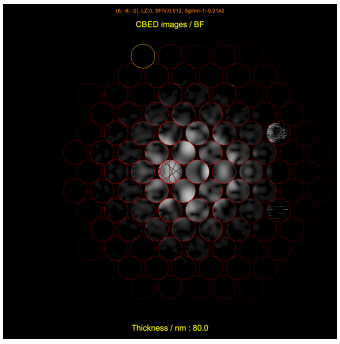


(c) 80 *nm*, ZnTe [110], reflections are indexed & colour LUT (using the popup menu).

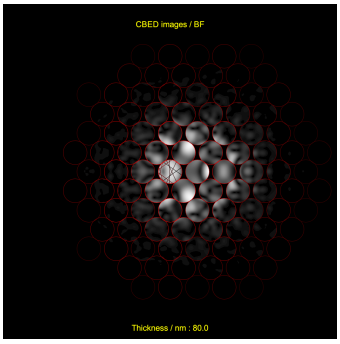
Figure 51: CBED patterns.



(a) SAED ZnTe [110] & CLC (002).



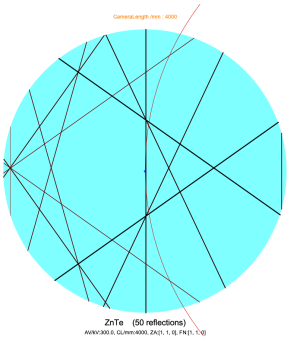
(b) 80 nm, ZnTe [110] & CLC (002), strong reflections & Bethe approximation.



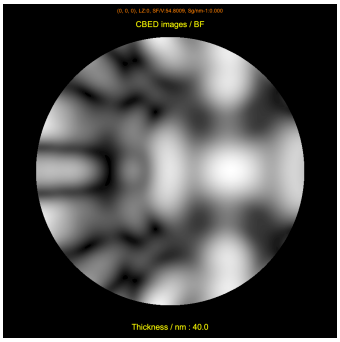
(c) 80 nm, ZnTe [110] & CLC (002), all reflections.

Figure 52: Tilted CBED patterns.

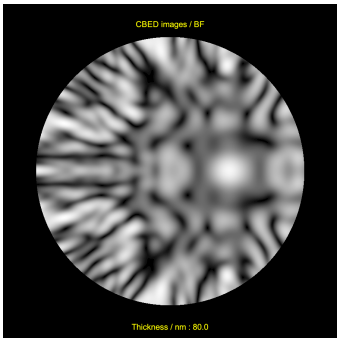
6.5 Large Angle CBED (LACBED)



(a) SAED ZnTe [110] & CLC (002).



(b) LACBED 40 nm, ZnTe [110] & CLC (002), all reflections.



(c) LACBED 80 nm, ZnTe [110] & CLC (002), all reflections.

Figure 53: LACBED patterns, (001) reflection (bright field).

6.6 CBED precession

6.7 CBED follow cone

7 Multislice calculations

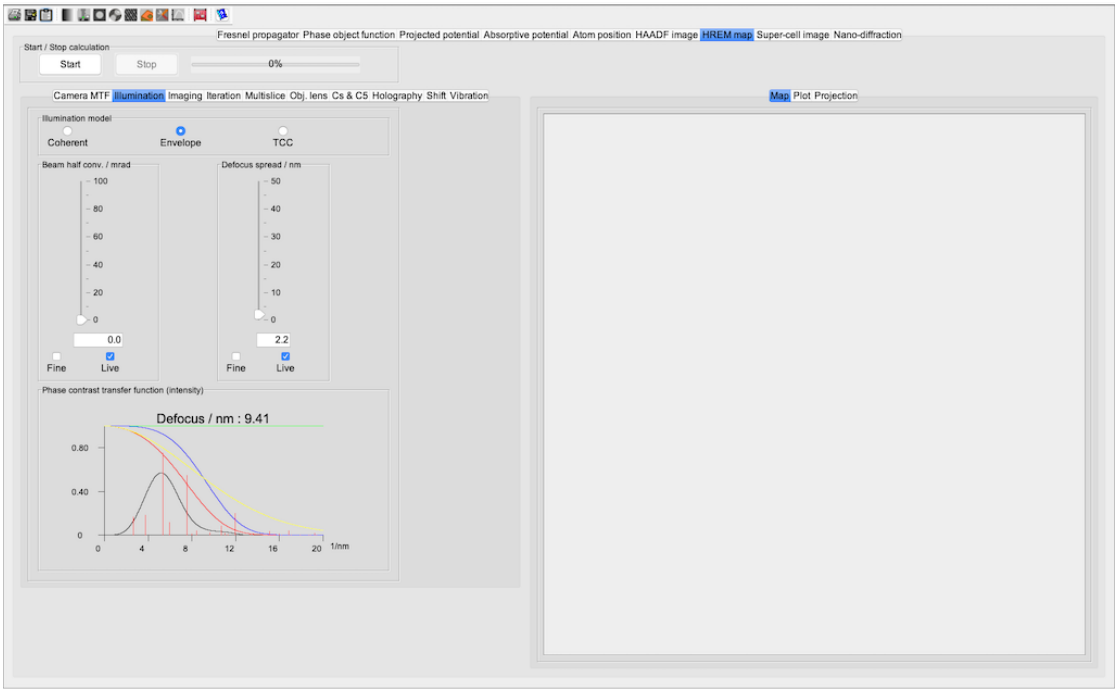


Figure 54: Multislice frame.

7.1 Tool buttons

The tool buttons of the multislice frame allow to:

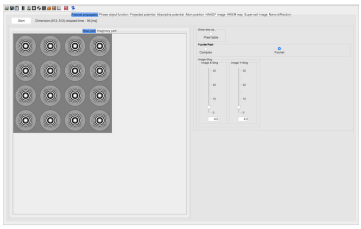
- : print the plot or image.
- : save the crystal structure in .txt format.
- : transfer a frame image to the clipboard.
- : set the default gray **LUT**.
- : open the microscope dialogue (Fig. 84a).
- : control the size and (h,k,l) center of the apertures (Fig. 79).
- : open the **Wave-front aberrations** dialogue (Fig. 96).
- : control the holography biprism (when holography mode is enabled).
- : show the **Specimen** dialogue (Fig. 84a).

-  : open **Map**, **Plot**, **Projection** tabs controls.
-  : open the **Transfer function** frame (Fig. 97).
-  : reset the wave-front aberrations and imaging conditions.
-  : open the associated help dialogue.

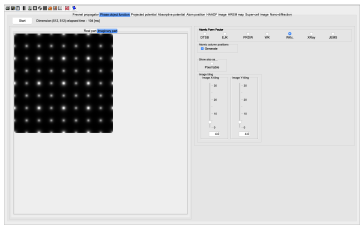
7.2 Tabs

The controls of the parameters for the different Bloch-wave calculations are grouped in the following tabs in order to calculate:

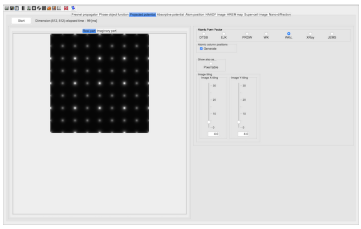
- **Fresnel propagator**: the propagation of the wave-function from slice to slice (Fig. 55a).
- **Phase object function**: the interaction of the wave-function with a slice (Fig. 55b).
- **Projected potential**: the projected potential of a slice (Fig. 55c).
- **Absorptive potential**: the absorptive potential (Fig. 55d).
- **Atom position**: the atoms position (scaled to the projected potential size) (Fig. 55e).
- **HAADF image**: **H**igh **A**ngle **A**nnular **D**ark **F**ield images of a stack of super-cells (Fig. 55f).
- **HREM map**: HREM images map (Fig. 55i).
- **Super-cell image**: HREM images of a stack of super-cells (Fig. 56a).
- **Nano diffraction**: CBED patterns of a stack of super-cells (Fig. 56d).



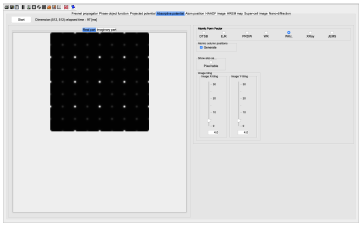
(a) Fresnel propagator between slices (4 x 4) unit cells.



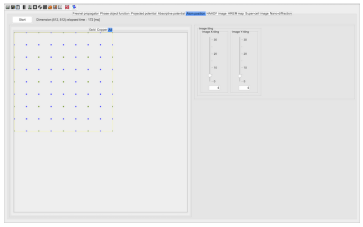
(b) Phase object function of a slice (4 x 4) unit cells..



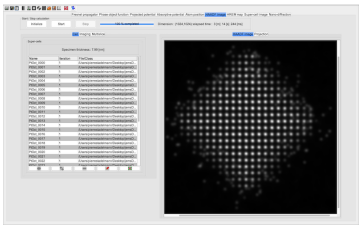
(c) Projected potential of a slice (4 x 4) unit cells..



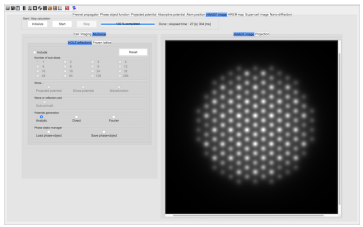
(d) Absorptive potential of a slice (4 x 4) unit cells.



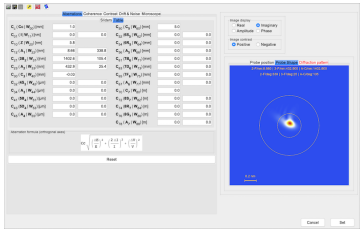
(e) Atom position in a slice (4 x 4) unit cells.



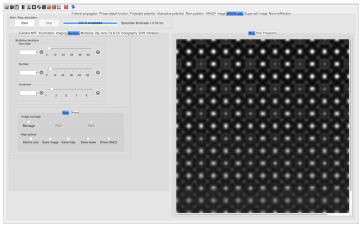
(f) HAADF image.



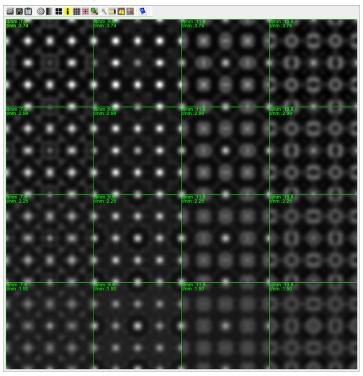
(g) HAADF probe dialogue.



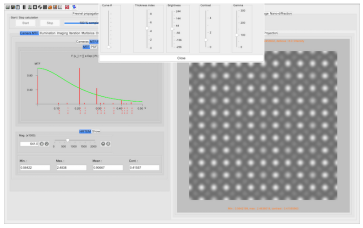
(h) Wave-front aberrations (up to order 8).



(i) HREM image maps (2 x 2 unit cells, 4 x 4 images).

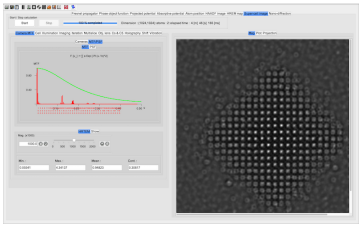


(j) HREM image maps (2 x 2 unit cells, 4 x 4 images, labelled with defocus, thickness & atomic columns position).

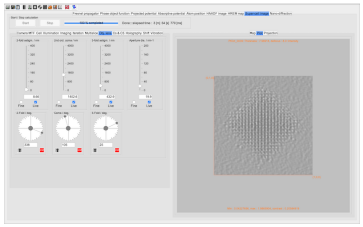


(k) HREM image viewed in **Plot** tab (using **Iteration** → **Options** → **Others** & Plot → Image). The thickness and contrast of the displayed image are changed using the controls appearing when the tool button is pushed.

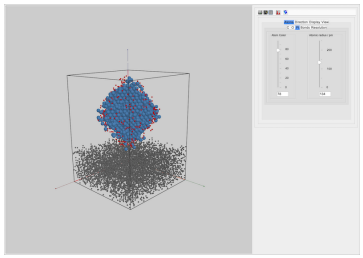
Figure 55: Tabs of multislice calculations frame.



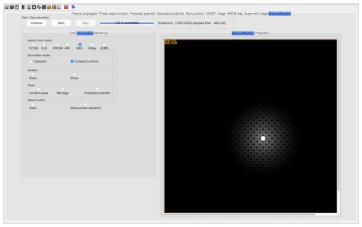
(a) Super-cell HRTEM images (with the camera MTF panel).



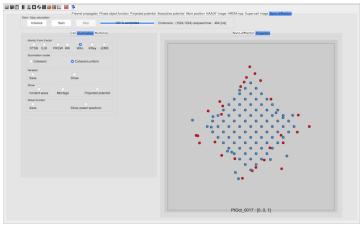
(b) Super-cell **Plot** tab that enables to vary imaging conditions, in particular aberrations. Thickness is set using the tool button.



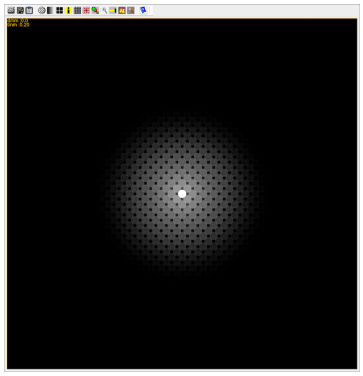
(c) Super-cell model generated from the stack of cells (**Cell** → tool button).



(d) Nano-diffraction tab.



(e) Nano-diffraction pattern, projected model.



(f) CBED nano-diffraction calculated by the multislice method.

Figure 56: Tabs of multislice calculations frame (continued).

The images and maps dimension (width, height) are set in the **Parameters** → **Preferences** → **Imaging** tab, where the size of the GUI panels is also defined. Recommended typical values (depending of the PC or Laptop screen resolution) are:

- 1024 for **Maximum dimension of reduced images**.
- 1024 for **Maximum image dimension**.
- 4096 for **Maximum map dimension**.

The other setting that sets the HREM image dimension is the **Pixel size of high resolution images** $[nm]$. As an example selecting a pixel size of 0.01 $[nm]$ means that the projected potential of a 1×1 $[nm^2]$ unit cell will be sampled with a step size of maximum $[0.01]\,nm$ and then its maximum dimension will be 128×128

pixels. For a 10×10 $[nm^2]$ super-cell the projected potential dimension will be 2048×2048 pixels. For such large cells a 0.02 $[nm]$ pixel size is recommended (depending on the computer).

Images or maps larger than their specified maximum dimension will be reduced automatically.

7.3 HREM images map calculations using the multislice method

The HREM map controls are placed in tabs that are almost identically organised as found in the Bloch-wave HREM calculation with the exception of the **Multislice** → **HOLZ reflections** tab (Fig. 57a). Some of the controls are put in a sub-tab **Multislice** → **Frozen lattice** tab (Fig. 57b).

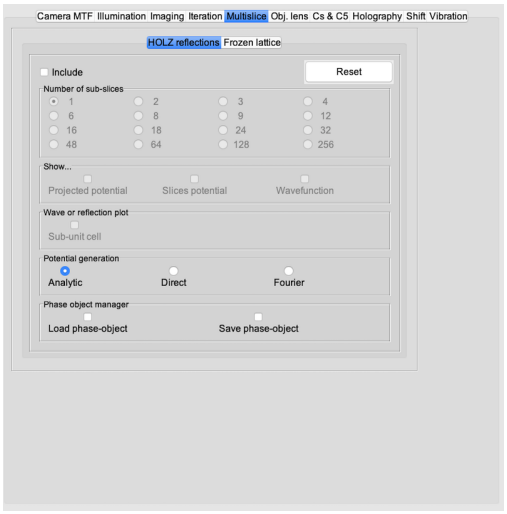
The **Multislice** offers 3 different ways to generate the projected potential of any crystal slice:

- **Analytic** analytical calculation, slightly slower than **Direct**.
- **Direct** atoms potential is calculated and patched at its fractional (x, y) image coordinates. It is faster than **Fourier** or **Analytic** methods but can produce artefacts (eliminated with checkbox **Frozen lattice** → **Enable** which introduces lattice vibrations (Einstein model)).
- **Fourier** done in Fourier space. Most precise and most time consuming.

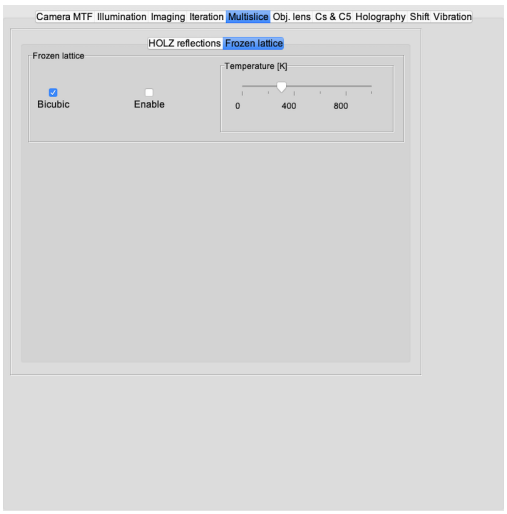
The HOLZ reflections can only be included in the multislice calculations when the crystal is cut into slices thinner than the unit cell thickness [23].

The Reset button erases the **P**hase **O**bject **F**unction (POF). The POF images can be saved for futur use or loaded in order to redo a calculation.

[23] Only orthogonal cells can be sliced. To create an orthogonal cell use menu item **Crystal** → **Make orthogonal** or **Crystal** → **Transform unit cell**.



(a) **Multislice** → **HOLZ reflections** tab controlling the generation of the projected potential of the crystal slices.



(b) **Multislice** → **Frozen lattice** tab controlling atom displacement and potential interpolation.

Figure 57: **HREM** → **Multislice** tabs.

7.4 HAADF image calculations using the multislice method

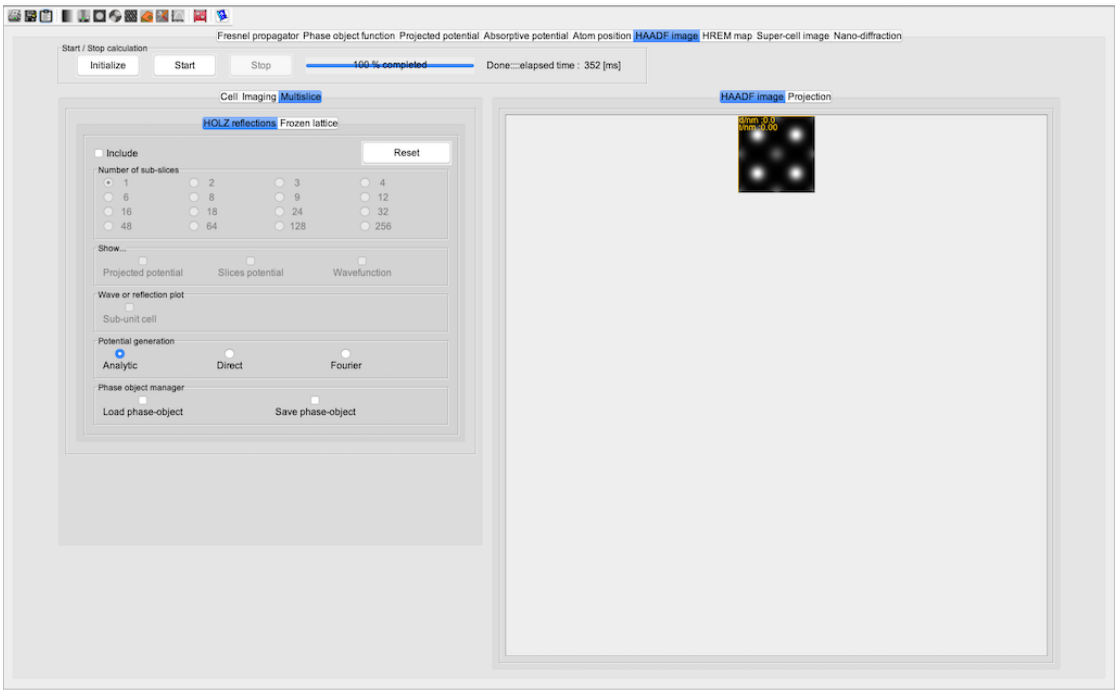


Figure 58: HAADF image calculation.

8 HRTEM imager

The HRTEM imager is shown on Fig. 59. It allows to introduce in the HRTEM image simulation wave-front aberrations up to order 8, the effects of crystal or beam tilt as well as *"out of center"* objective aperture or beam stop (Zernike phase contrast). The calculations are interactive, i.e. a change of any imaging parameters can be seen in real time in the **Image** panel. The **left** part of the HRTEMImager frame controls the simulation of the images and the **right** part displays either the HRTEM image, the **C**ontrast **T**ransfer **F**unction (CTF) or the **W**ave-**F**unction (WF).

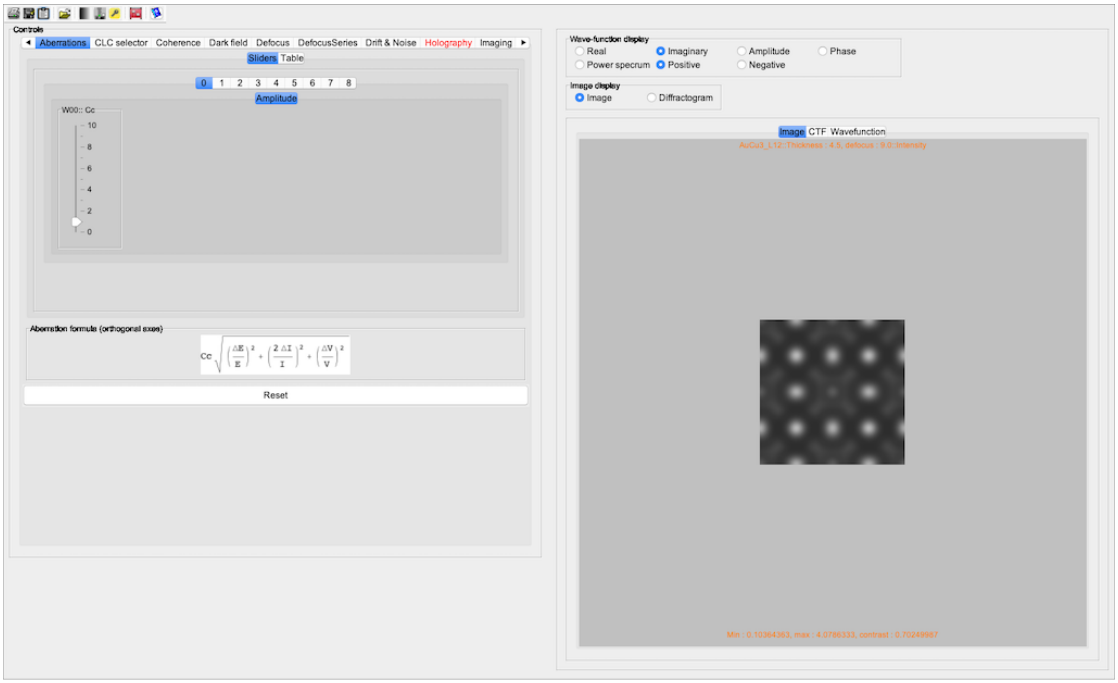


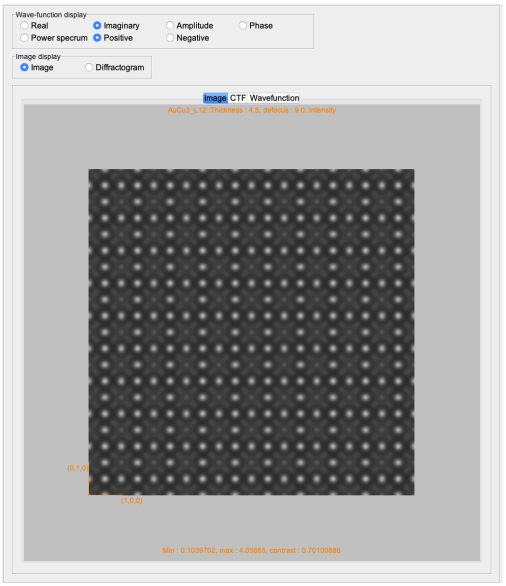
Figure 59: HRTEM imager frame (activated with the largest crystal thickness).

8.1 Tool buttons

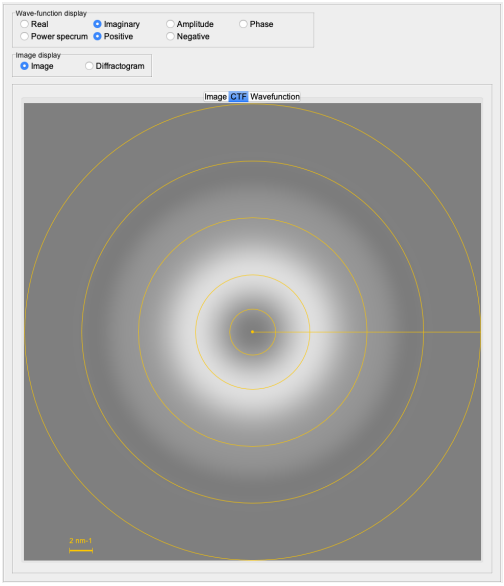
The tool buttons of the HRTEM imager allow to:

-  : print the image, CTF or wave-function.
-  : save the image, CTF or wave-function

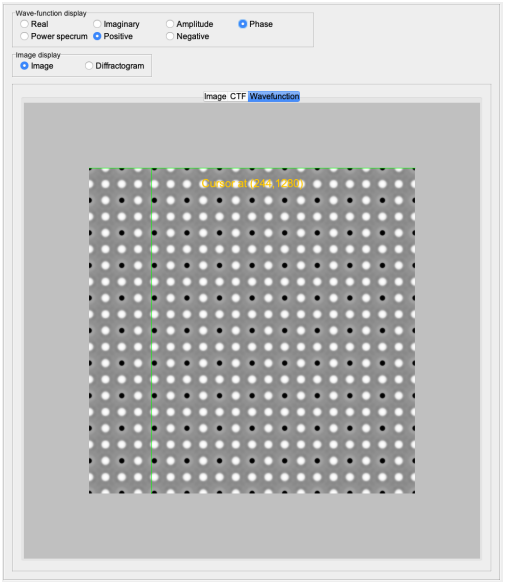
-  : transfer the HRTEM frame to the clipboard.
-  : open a wave-function (.ems file).
-  : set the default gray LUT.
-  : open the **Microscope** dialogue (Fig. 108).
-  : open the **Keeper** dialogue (Fig. 90).
-  : reset the aberrations.
-  : open the associated help dialogue.



(a) Image tab (the image is displayed as 10×10 $AuCu_3$ unit cells).



(b) CTF tab (imaginary part of the transfer function).



(c) Tab displaying the **"Phase"** of the wave-function.

Figure 60: HRTEM imager, right tabs.

8.2 Tabs

The imaging controls are organised in several tabs aimed at:

- **Camera MTF**: introducing the camera MTF (Figs 43a, 43b), see sec. 6.3.
- **Aberrations**: including aberrations up to order 8 in the image simulation [24] (Figs. 61a, 61b) [25].
- **CLC selector**: controling to tilt the incident beam (**green cross**), to set the reflection number and specimen thickness [26] (Figs 61c, 61d).
- **Coherence**: changing the coherence of the illumination (61e).
- **Dark field**: setting dark field condition, i.e. move the (0,0,0) reflection away from the optical axis of objective lens (Figs 62a, 62b).
- **Defocus**: setting the defocus [27] (Fig. 62c).
- **Defocus series**: generating series of defocused images (to be saved as .ems or .jpg and a little .html page) [28](Fig. 62d).
- **Drift & Noise**: introducing image specimen drift and poisson noise (Fig. 63a).
- **Holography**: generating HRTEM hologram images (Figs 63c), 63d).
- **Imaging**: adjusting image brightness, contrast, gamma as well as image tiling x & y and noise level (63f).
- **Objective aperture**: defining the size and position of the objective aperture as well as the beam stop size and phase shift to simulate Zernike phase contrast (Figs 64a, 64b) [29].

[24]The maximum aberration order is defined in **Parameters** → **Preferences** → **Imaging** → **Others** tab.

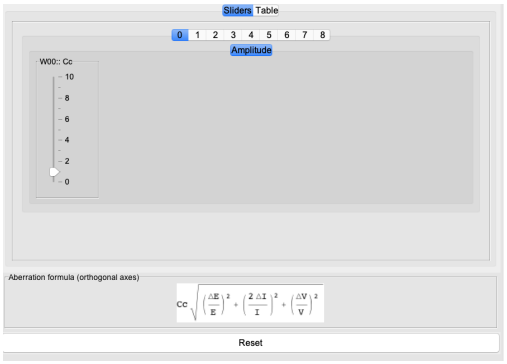
[25]The label of the spherical aberration refers to the geometric aberration notation C_{30} (Krivanek) or C_3 (Haider) and the wave-front aberration W_{40}).

[26]The crystal thickness can only be modified interactively when the wave-function has been calculated by the **Bloch-wave** approach. When the **multislice** approach has been employed it is necessary to load the wave-function.

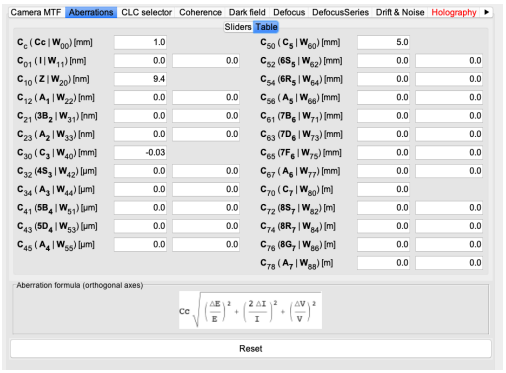
[27]When placing the pointer (mouse) on the transfer function drawing, the defocus is modified using the keyboard arrow keys ↑ and ↓.

[28]The defocus series can be loaded and imaged using menu item **Imaging** → **Load** → **Stack**.

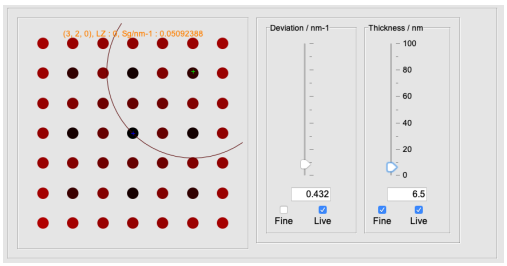
[29]The **Stretch** option increases the image contrast.



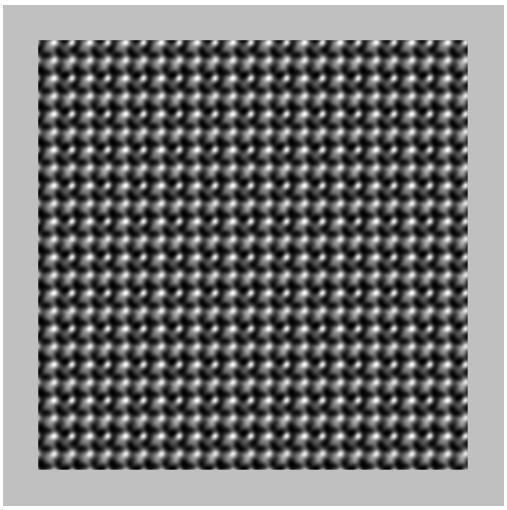
(a) Aberrations are defined using sliders.



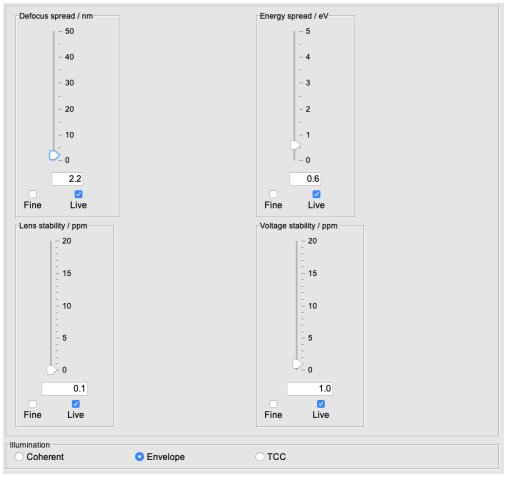
(b) Table of aberrations with Krivanek, Haider and wave-front notations.



(c) CLC, deviation (reflections number) and crystal thickness settings.

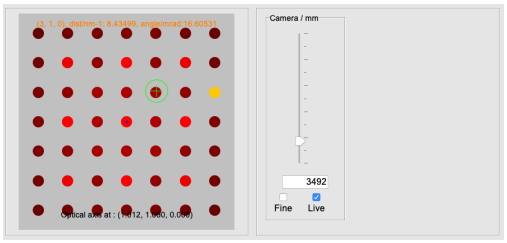


(d) Tilted crystal (i.e. CLC (h, k, l) indices set by the **green cross** position).

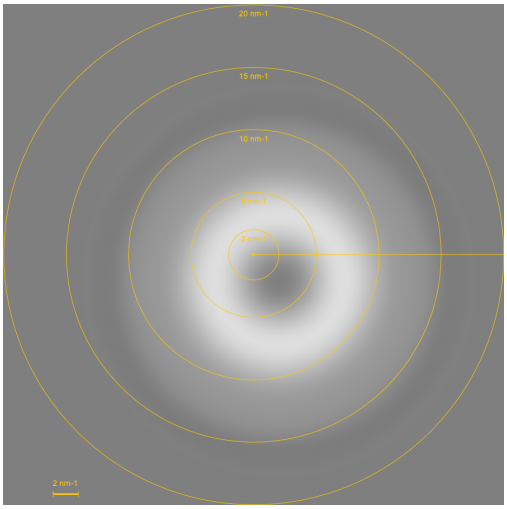


(e) Illumination coherence.

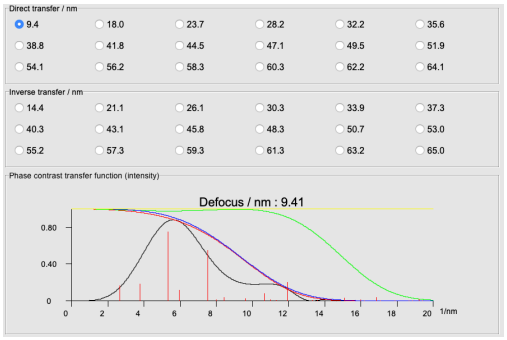
Figure 61: **Aberrations**, **CLC** and **Coherence** tabs.



(a) Dark field condition.



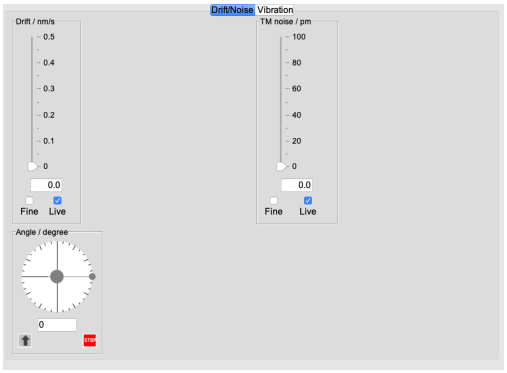
(b) CTF in dark field condition.



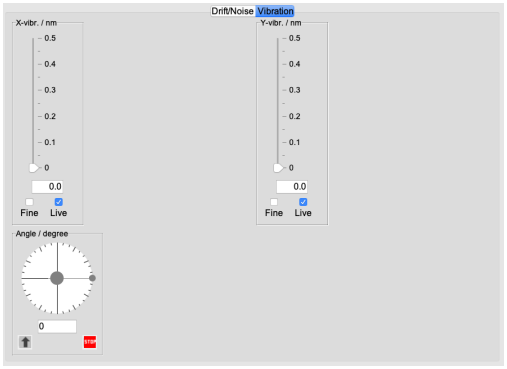
(c) Defocus setting.

(d) Defocus series can be saved in .ems or .jpg format.

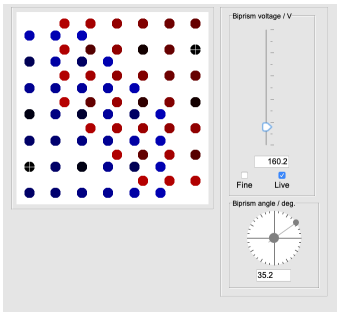
Figure 62: **Dark field**, **Defocus** and **Defocus series** tabs.



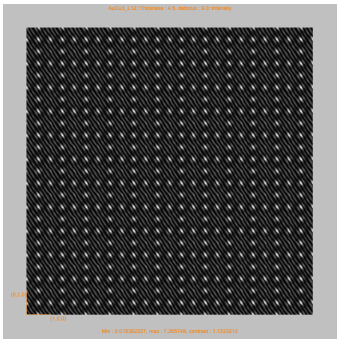
(a) Drift & Noise.



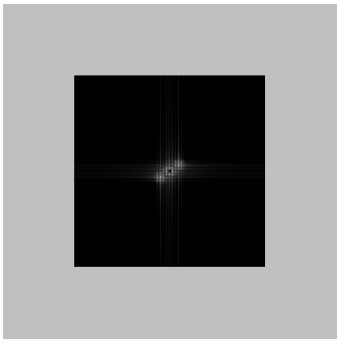
(b) Vibration.



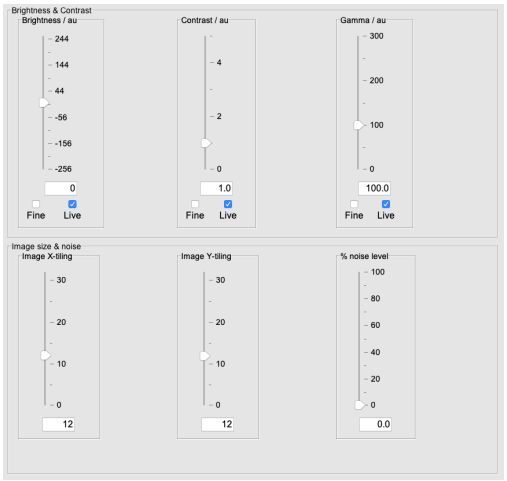
(c) Biprism voltage and orientation.



(d) HRTEM image in holography mode.

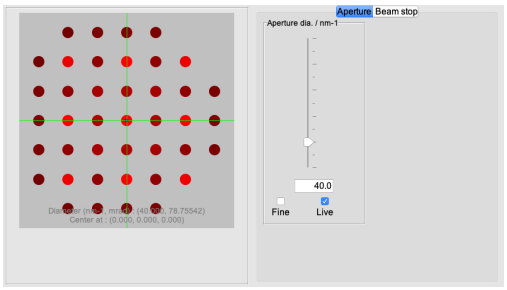


(e) Diffractogram of holography HRTEM image in holography mode.

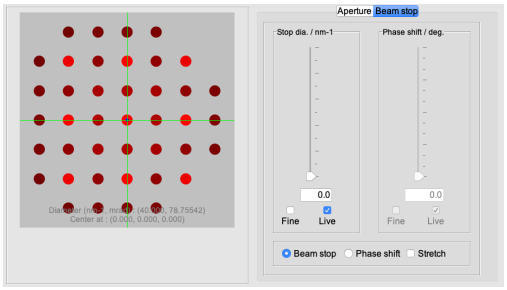


(f) Image brightness, contrast, gamma as well as tiling and poisson noise level.

Figure 63: **Drift/Noise**, **Holography** and **Imaging** tabs.



(a) Objective aperture diameter $[nm^{-1}]$.



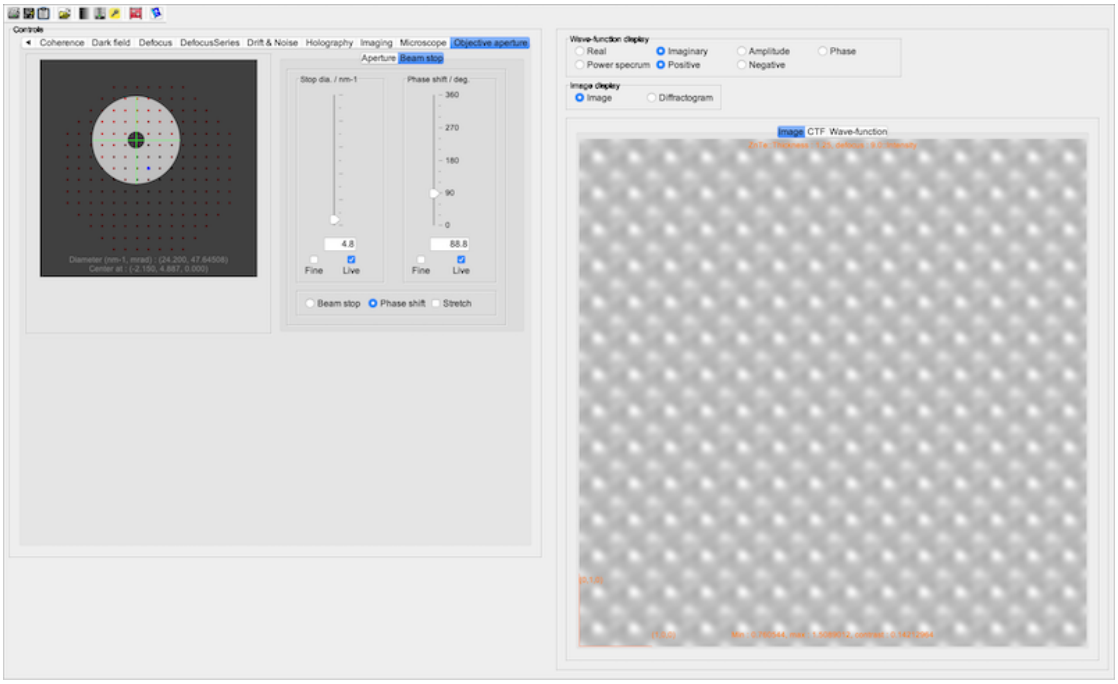
(b) Beam stop $[nm^{-1}]$ for Zernike phase contrast imaging (**??**).

Figure 64: **Objective aperture and beam stop & phase shift** $[deg]$ tabs.

The wave-front aberration W_{ij} defines the i^{th} power of the radial angle and the j^{fold} azimutal angle [30].

[30] The chromatic aberration is W_{00}.

8.3 Zernike phase contrast



(a) HRTEM imager allows to move, resize the objective aperture or the beam stop and shift the blocked reflection(s) interactively.

Figure 65: HRTEM imager, objective aperture settings.

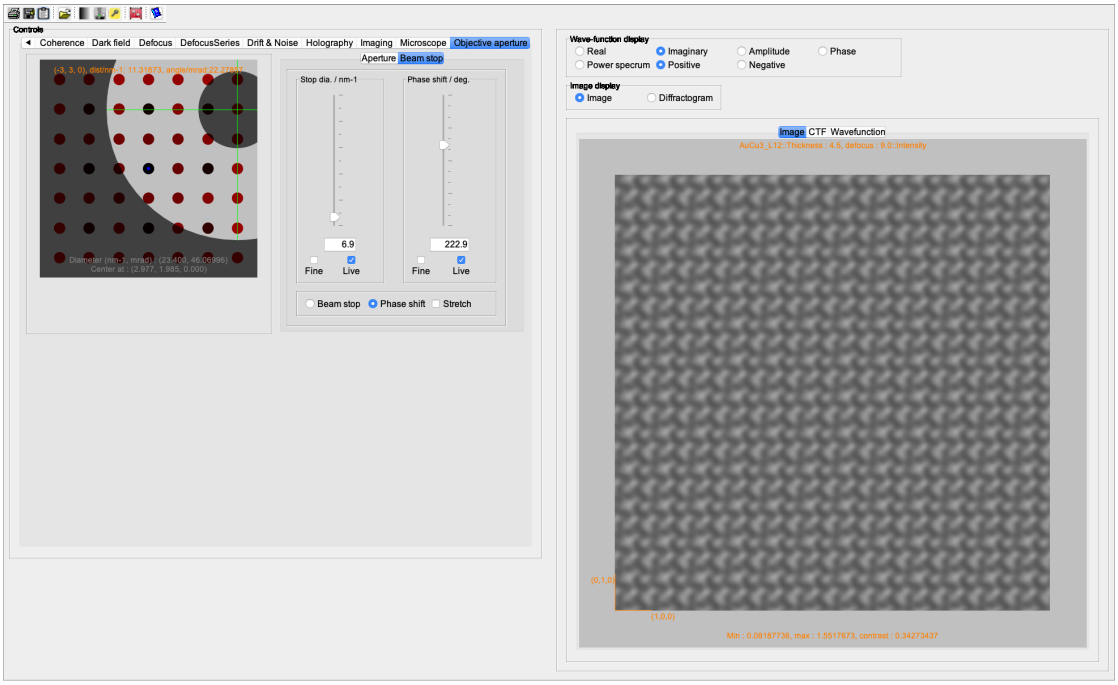
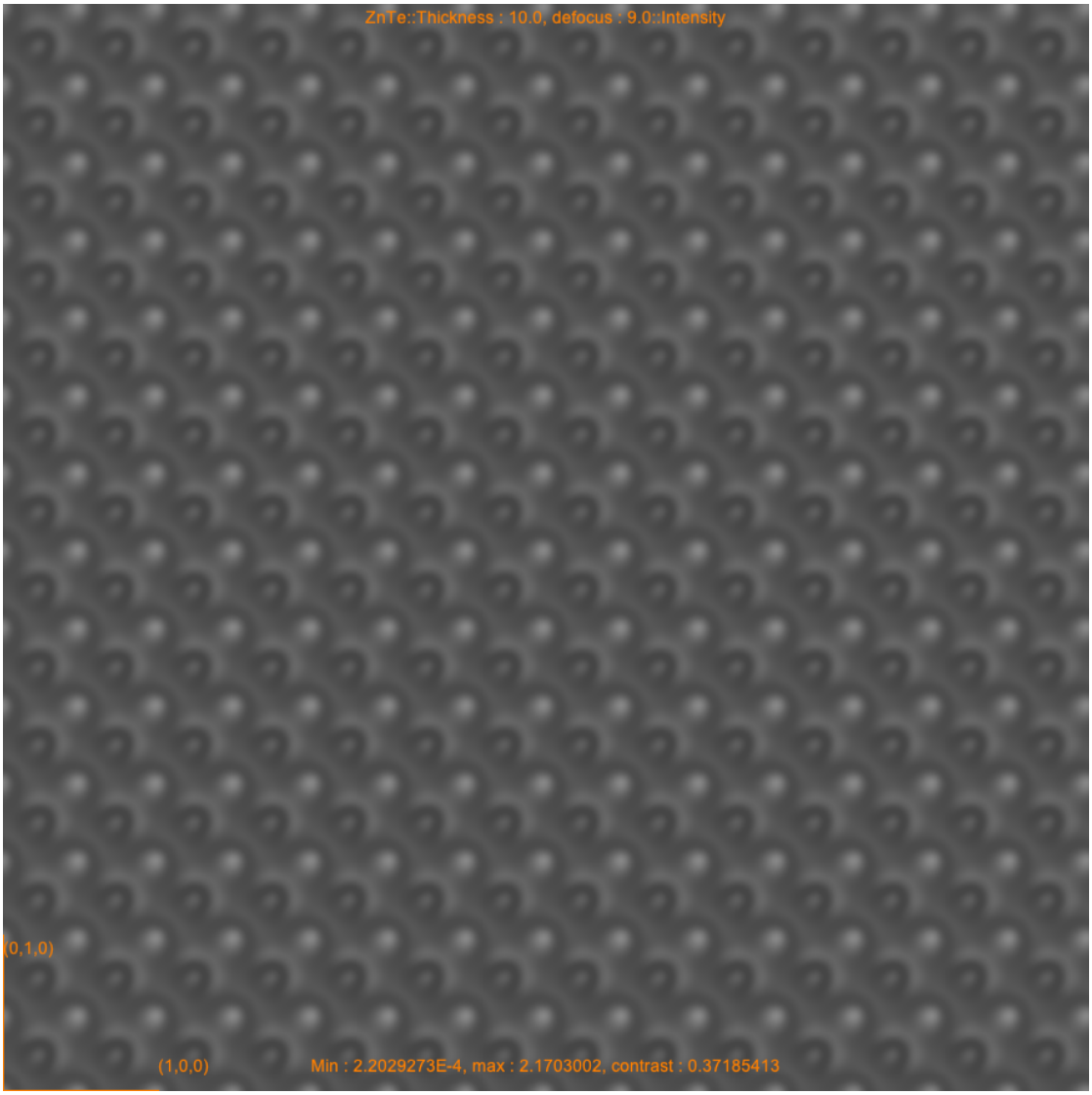


Figure 66: **Zernike phase contrast** with out of axis objective aperture and a beam stop that phase shifts the transmitted beam and {100} reflections.



(a) HRTEM imager allows to move, resize the objective aperture or the beam stop and shift the blocked reflection(s) interactively.

Figure 67: HRTEM imager, objective aperture settings.

9 HRSTEM imager

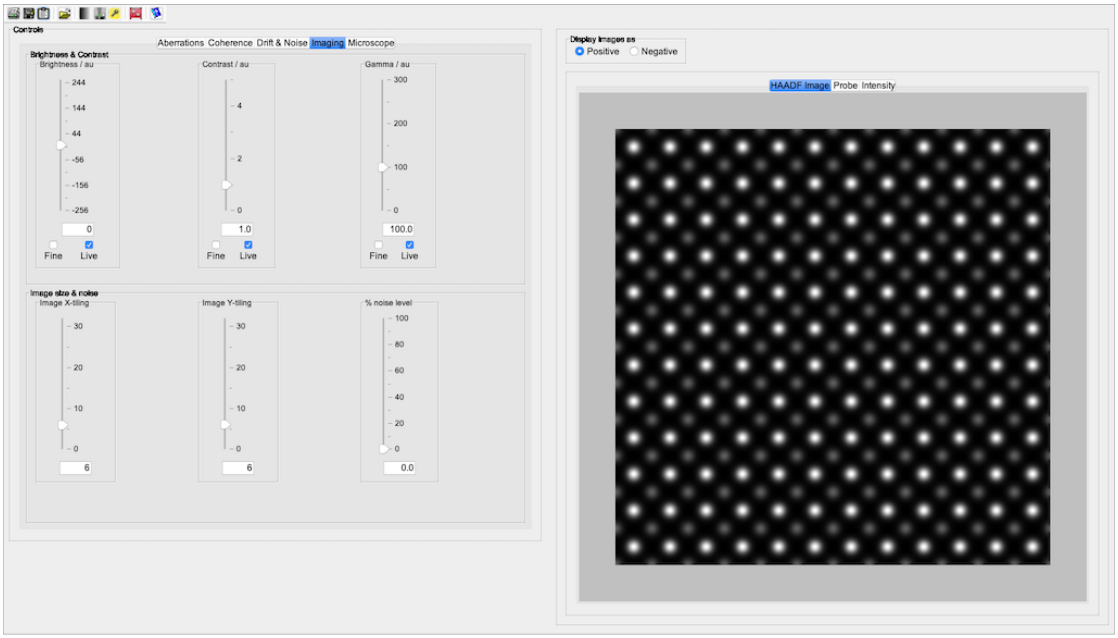


Figure 68: HRSTEM imager.

9.1 Tool buttons

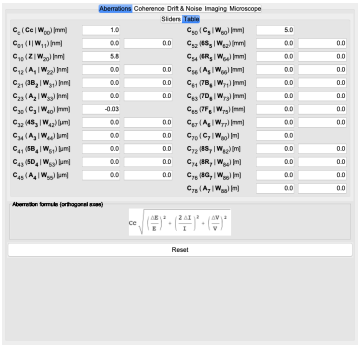
The tool buttons allow to:

- : print the HAADF image.
- : save the HAADF image.
- : transfer the dialogue to the clipboard.
- : open a saved multislice HAADF intensity image ($xxxSTEM\_nnnn.ems$).
- : set the default gray **LUT**.
- : open the **Microscope** dialogue (Fig. 108).
- : open the **Keeper** dialogue (Fig. 90).
- : reset the wave-front aberrations and imaging conditions.
- : display a help file.

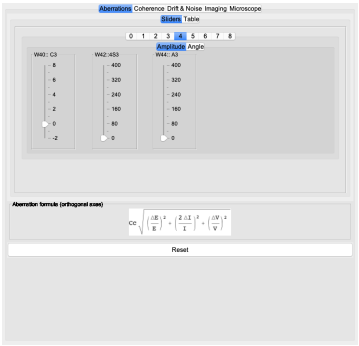
9.2 Controls and images tabs

The controls tabs allow to:

- **Aberrations** : change the aberrations of the probe intensity (Figs 69a, 69b).
- **Coherence** : change the coherence of the illumination (Fig. 69c).
- **Drift & Noise** : introduce probe drift or vibration & thermal magnetic noise (Fig. 69d).
- **Imaging** : duplicate the HAADF or object intensity image and modify their contrast (Fig. 69e)
- **Microscope** : modify the microscope parameters (Fig. 69f).

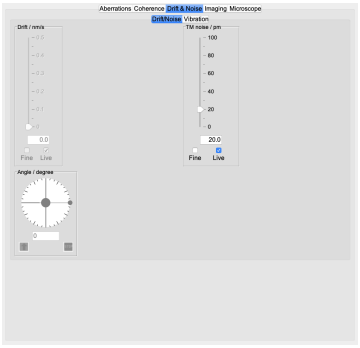


(a) Aberrations settings (table view).

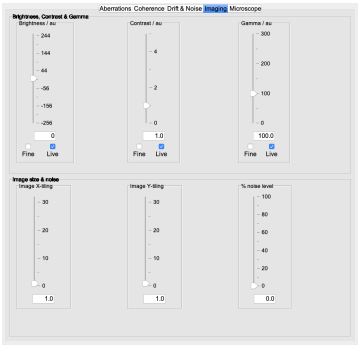


(b) Aberrations settings (slider controls).

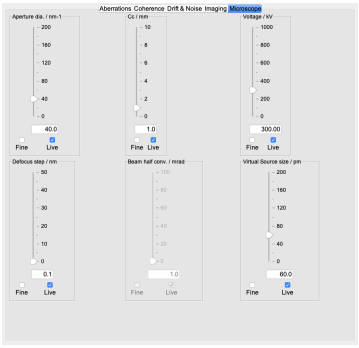
(c) Illumination coherence settings.



(d) Drift & Noise settings.



(e) Imaging settings.



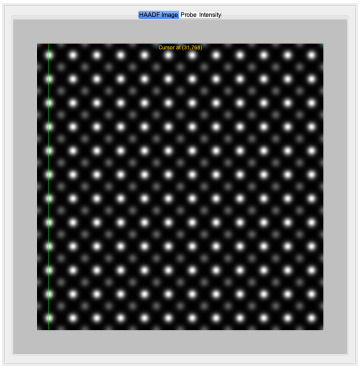
(f) Microscope settings.

Figure 69: HRSTEM imager controls.

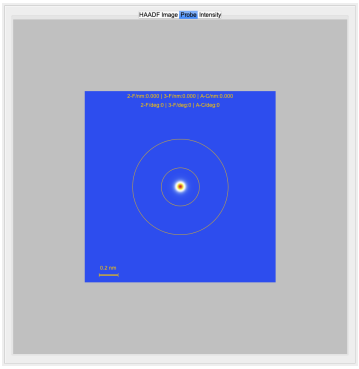
The images tabs allow to display:

- **HAADF image** : the HAADF image (Figs 70a).

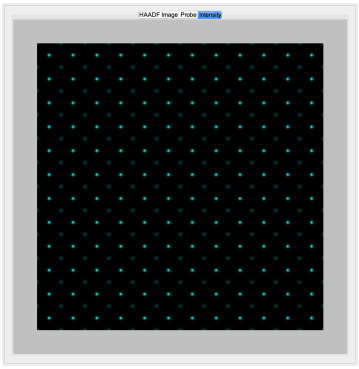
- **Probe** : the probe intensity (Fig. 70b).
- **Intensity** : the object intensity (Fig. 70c).



(a) HAADF image obtained by convolution of the probe intensity with the object intensity.



(b) Probe intensity.

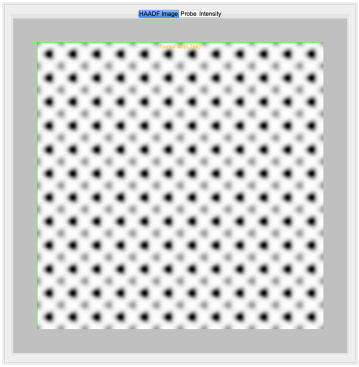


(c) Object intensity.

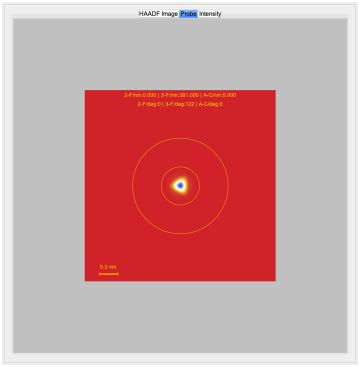
Figure 70: HRSTEM imager (**HAADF image**, **Probe** & **Intensity** tabs

Any aberration up to wave-front aberration order 8 (W_{80} to W_{88} is introduced interactively using the controls of the **Aberrations** tab, for example 3-fold astigmatism (Fig. 71).

(a) HAADF image obtained by convolution of the probe intensity with the object intensity.



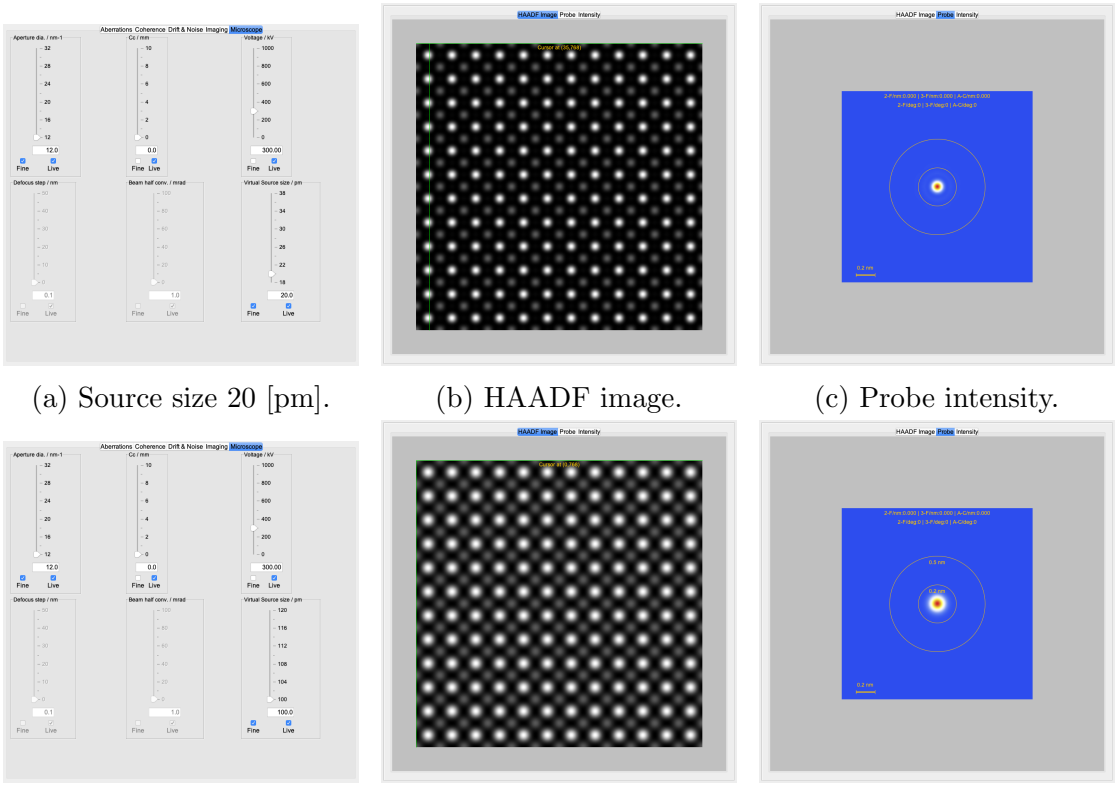
(b) HAADF image (inversed contrast).



(c) Probe intensity.

Figure 71: Introducing 3-fold astigmatism.

The coherence of the illumination is controlled using the **Coherence** tab and the **Microscope** tab allows to change the virtual source size (Fig. 72).

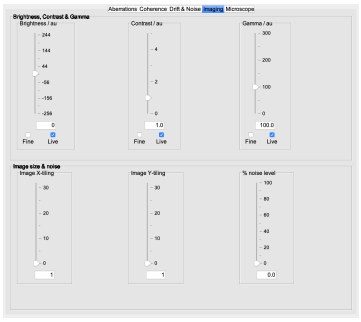


(a) Source size 20 [pm]. (b) HAADF image. (c) Probe intensity.

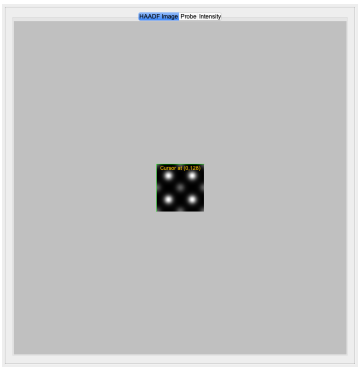
(d) Source size 100 [pm]. (e) HAADF image. (f) Probe intensity.

Figure 72: Effect of source size change.

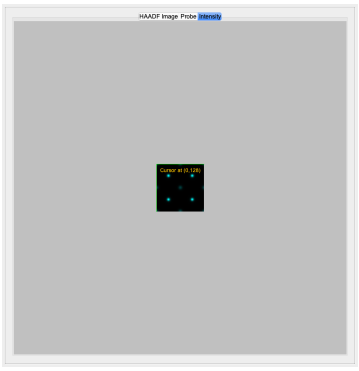
The **tiling** of the HAADF image and object intensity is controlled using the **Imaging** tab (Fig. **??**).



(a) Images tiling 1 x 1.

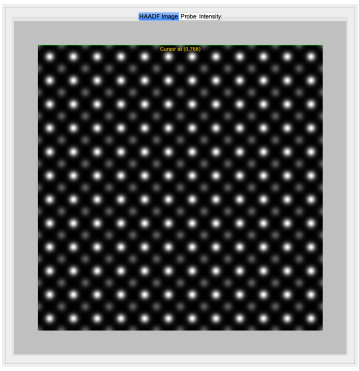


(b) HAADF image.

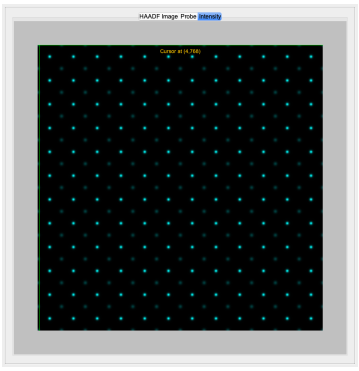


(c) Object intensity.

(d) Images tiling 6 x 6.



(e) HAADF image.



(f) Probe intensity.

Figure 73: Imaging **x** & **y** image-tiling.

10 Camera MTF

The measurement of the camera **M**odulation **T**ransfer **F**unction (MTF) requires to load several images of the camera noise pattern (Fig. 74). This procedure measures what is called the **N**oise **T**ransfer **F**unction. **Noise** images of the CCD camera are acquired, i.e. images obtained without a specimen and with an illumination as uniform as possible (typically 10 noise images) (Fig. 77a). The images are then subtracted one by one at a time in order to cancel the non-uniformity of the illumination. A diffractogram is calculated and rotationally averaged to obtain the NTF profile which is finally fitted using a mathematical expression (exponential, gaussian, lorentzian or a mixed formula). The NTF usually over evaluates the MTF.

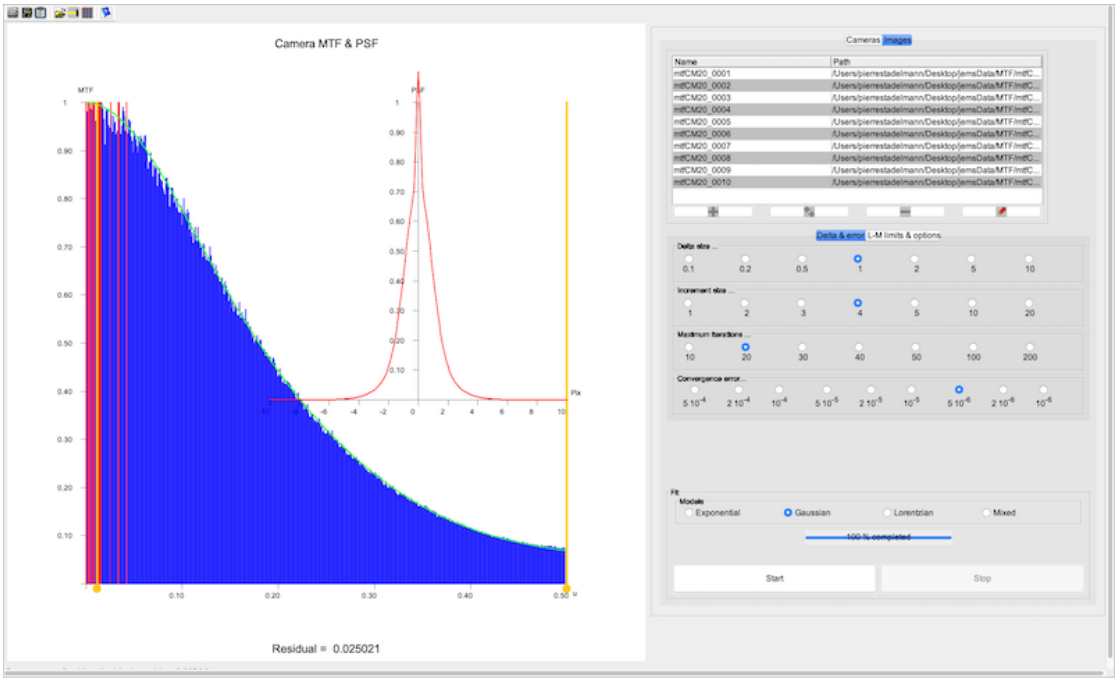


Figure 74: Camera MTF frame.

10.1 Tool buttons

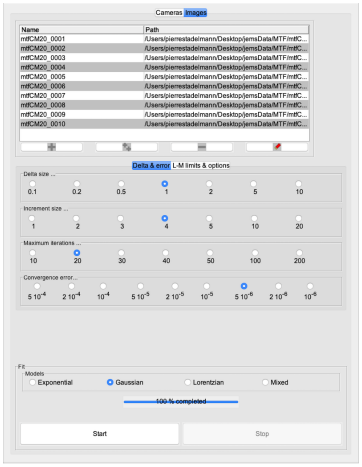
The crystal builder tool buttons allow to:

- : print the fitting drawing.
- : save the fitting drawing.

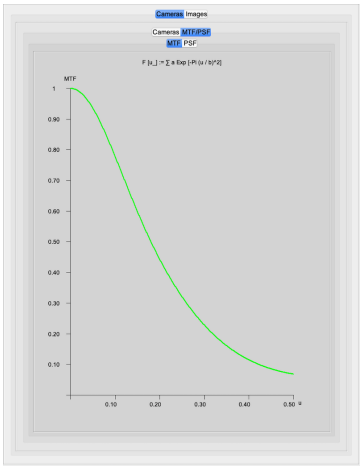
-  : transfer the frame to the clipboard.
-  : open a noise pattern image (Fig. 76a).
-  : start the fitting procedure (requires at least 2 images).
-  : display a table of the fitted function and the fitted parameters (Fig. 76b).
-  : display a help file.

10.2 Tabs

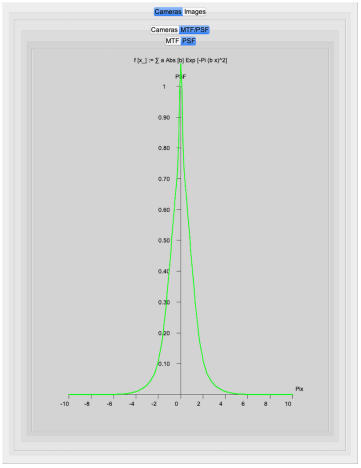
The camera MTF frame is separated in 2 panels, the left one is used to follow the MTF fitting and the right one shows the NTF images and the selection of the fitting MTF model (Fig. 75).



(a) Table of noise images, parameters of fitting procedure, MTF fitting model selection.



(b) Camera normalized MTF.

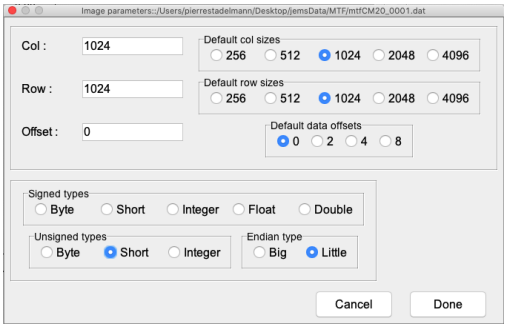


(c) Camera PSF.

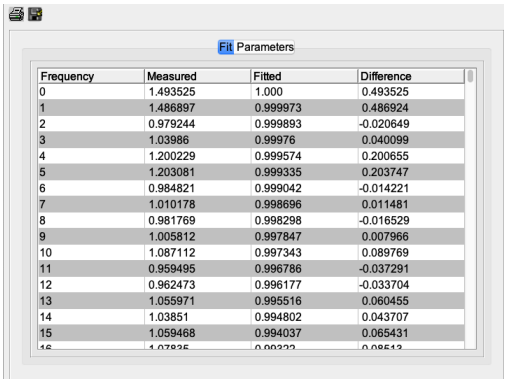
Figure 75: Crystal MTF → tabs.

The noise pattern images should ideally be acquired with a camera saturation $\sim 2/3$, typically 6'000 to 8'000 counts for the MSC Gatan CCD camera (24 μm, 1024×1024 pixels). The dialogue loading **Gatan data only** images requires to specify the dimension of the images, the data offset as well as the pixel type (Fig.

76a). Fig. 77a shows a noise image. Its diffractogram (Fig. 77b) and a few profiles taken across the diffractogram that show the non-uniformity of the illumination (Fig. 77c). The Dirac delta function observed at the center of the diffractogram is not taken into account during the MTF fitting, the domain of of fitting being limited by the movable yellow lines of Fig. 74.



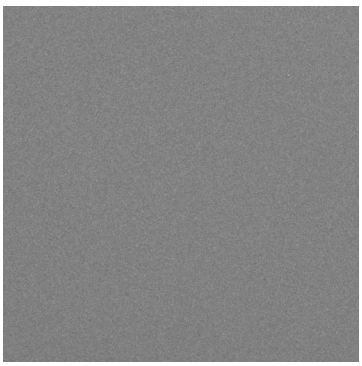
(a) Gatan data only images 1024×1024 unsigned short image format.



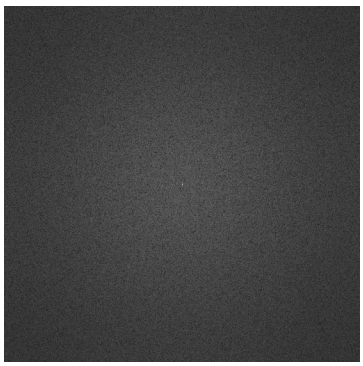
Frequency	Measured	Fitted	Difference
0	1.493525	1.000	0.493525
1	1.486897	0.999973	0.486924
2	0.979244	0.999893	-0.020649
3	1.03986	0.99976	0.040099
4	1.200229	0.999574	0.200655
5	1.203081	0.999335	0.203747
6	0.984821	0.999042	-0.014221
7	1.010178	0.998696	0.011481
8	0.981769	0.998298	-0.016529
9	1.005812	0.997847	0.007966
10	1.087112	0.997343	0.089769
11	0.959495	0.996786	-0.037291
12	0.962473	0.996177	-0.033704
13	1.055971	0.995516	0.060455
14	1.03851	0.994802	0.043707
15	1.059468	0.994037	0.065431

(b) Experimental MTF values & fitted function as a function of the image frequency.

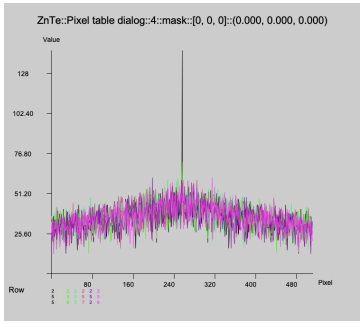
Figure 76: Data only load dialogue and fitted parameters table.



(a) CCD camera noise image.



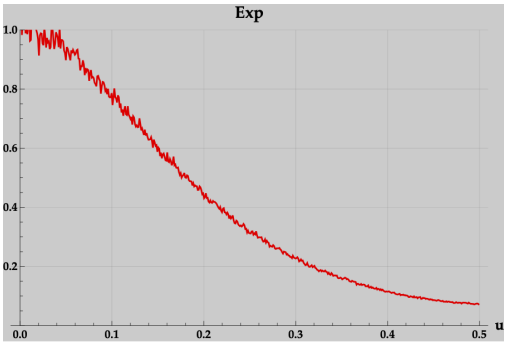
(b) Diffractogram of noise image.



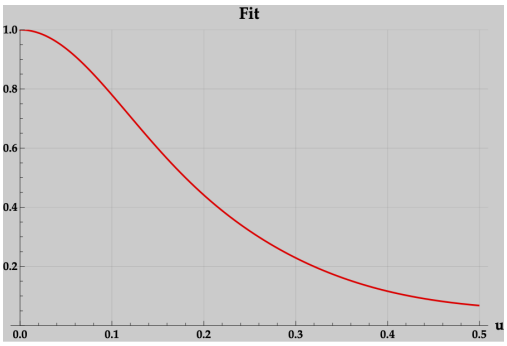
(c) Profiles across the center of diffractogram.

Figure 77: 1024×1024 Gatan CCD camera noise, diffractogram, profiles.

The experimental and fitted normalized NTF are plotted on Fig. 78. The maximum image frequency is the Nyquist frequency, 511 for 1024×1024 sized images.



(a) Mathematica plot of the measured NTF.



(b) Mathematica plot of the fitted NTF.

Figure 78: Mathematica normalized NTF plots.

11 Apertures dialogue

11.1 Tool buttons

The tool buttons allow to:

- : transfer the dialogue to the clipboard.
- : display a help file.

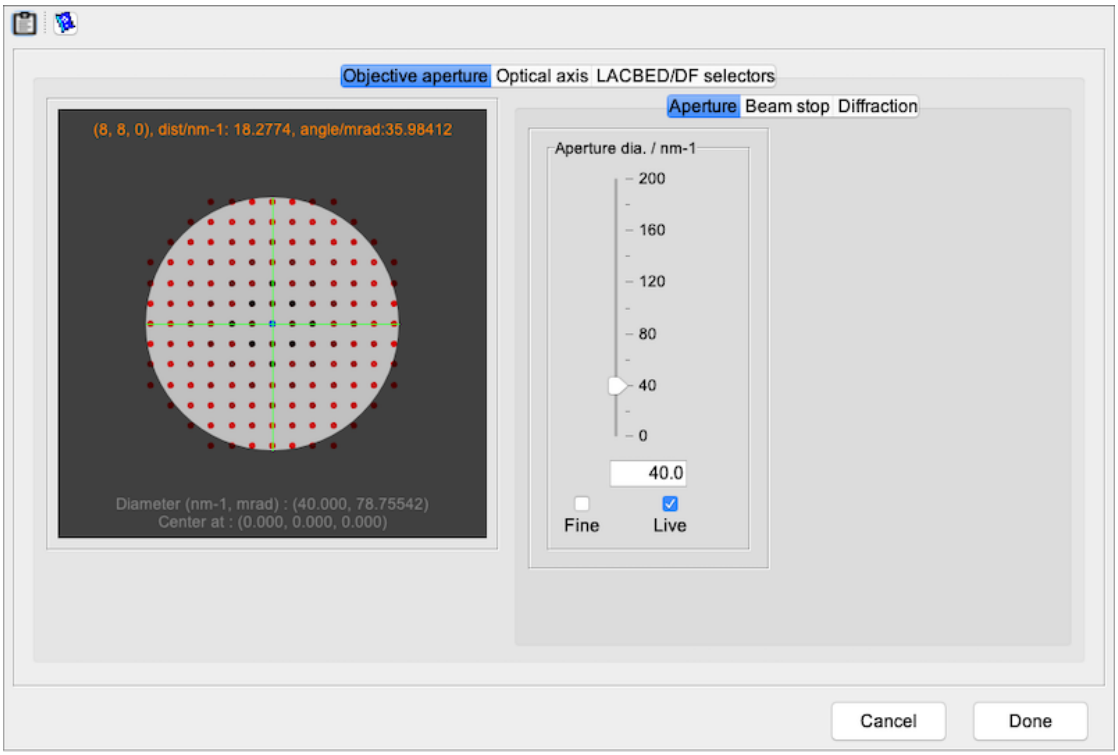
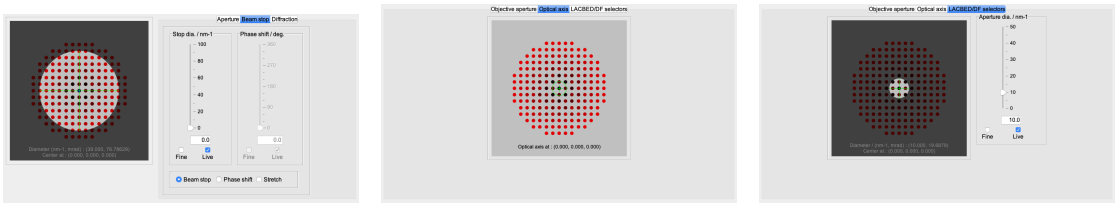


Figure 79: Apertures dialogue.

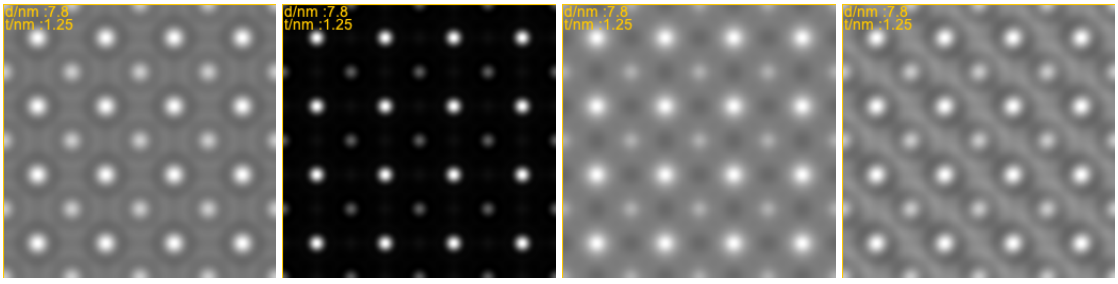


(a) Beam stop (Zernike phase contrast).

(b) Optical axis settings.

(c) **L**arge **A**ngle **C**onvergent **B**eam **D**iffraction (LACBED) or **D**ark **F**ield (DF) aperture.

Figure 80: Objective aperture dialogue tabs.

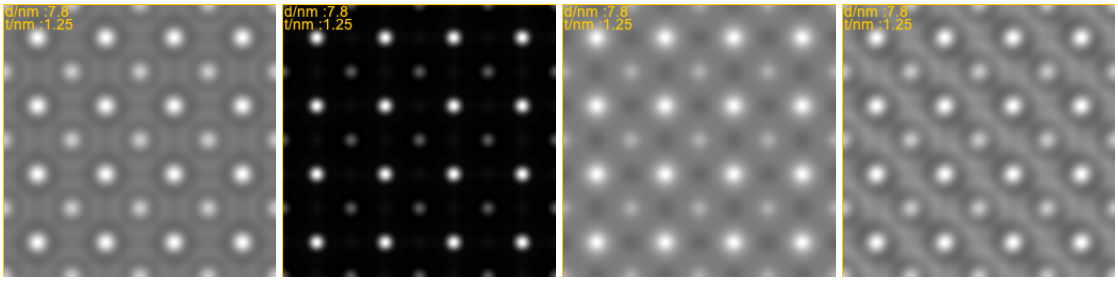


(a) Aperture at (000).

(b) Aperture at (000), (000) reflection blocked.

(c) Aperture at (000), (000) reflection phase shifted 90.0 [deg].

(d) Aperture at (220), (220) reflection phase shifted 90.0 [deg.].



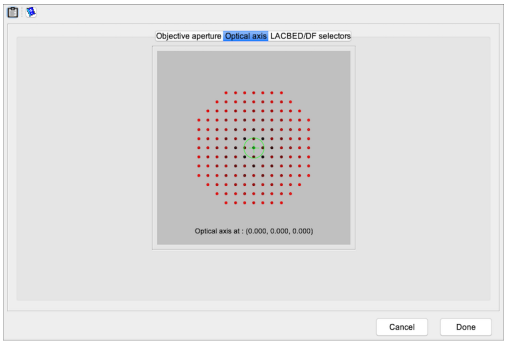
(e) Aperture at (000).

(f) Aperture at (000), (000) reflection blocked.

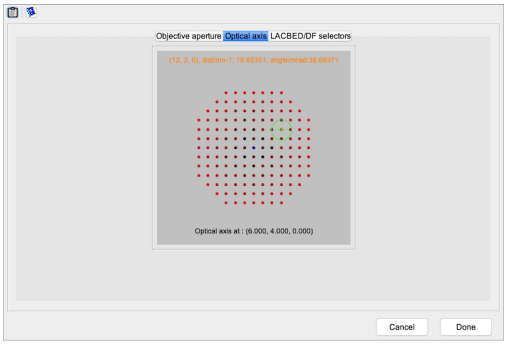
(g) Aperture at (000), (000) reflection phase shifted 90.0 [deg].

(h) Aperture at (220), (220) reflection phase shifted 90.0 [deg.].

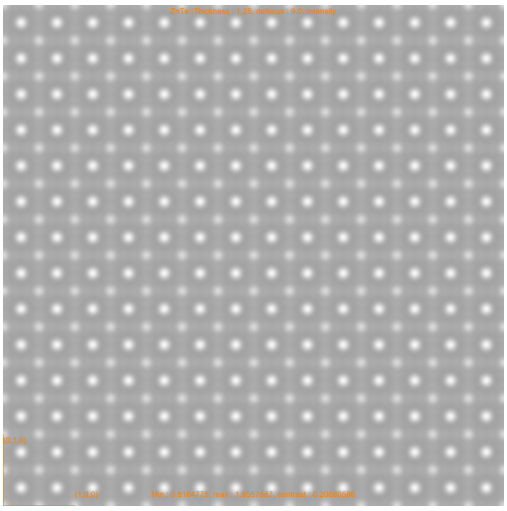
Figure 81: HRTEM images with different objective aperture settings.



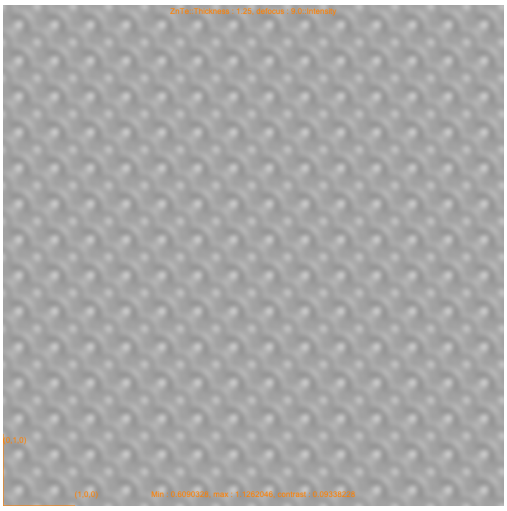
(a) Optical axis centered $(0, 0, 0)$.



(b) Optical axis shifted to $(6, 4, 0)$.

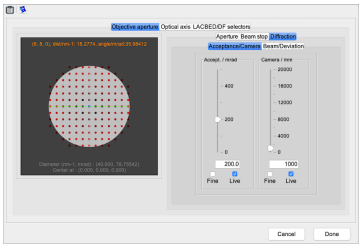


(c) Optical axis on axis (at (000)).

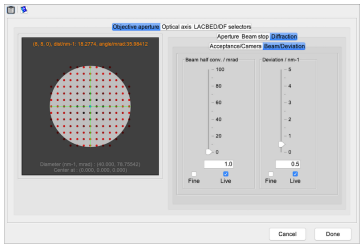


(d) Optical axis at (220).

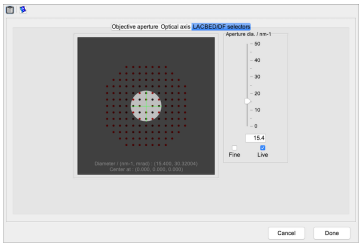
Figure 82: Effect of the optical axis shift (not to be confused with a crystal tilt).



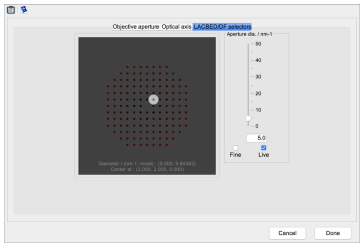
(a) Acceptance angle and camera length.



(b) Beam convergence and deviation.



(c) SAED or LACBED aperture on axis.



(d) SAED or LACBED aperture off axis.

Figure 83

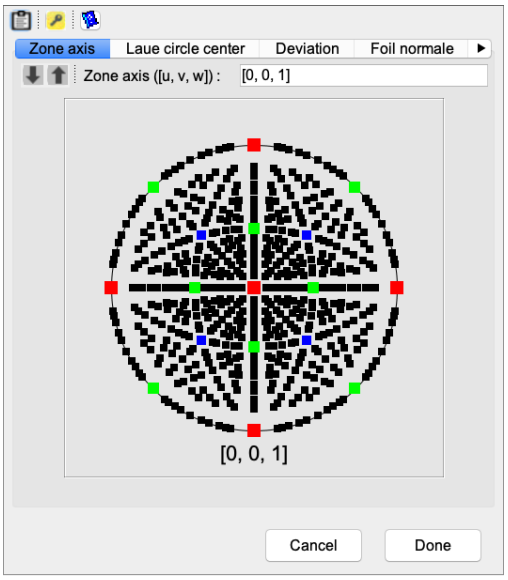
12 Specimen

The specimen dialogue sets parameters related to the orientation of the thin crystal slice with respect to the optical axis of the microscope ($[uvw]$ zone axis indices and (hkl) indices of the center of the Laue circle) as well as the number of Laue zones and the deviation, i.e. maximum distance of a (hkl) reciprocal node to the Ewald sphere.

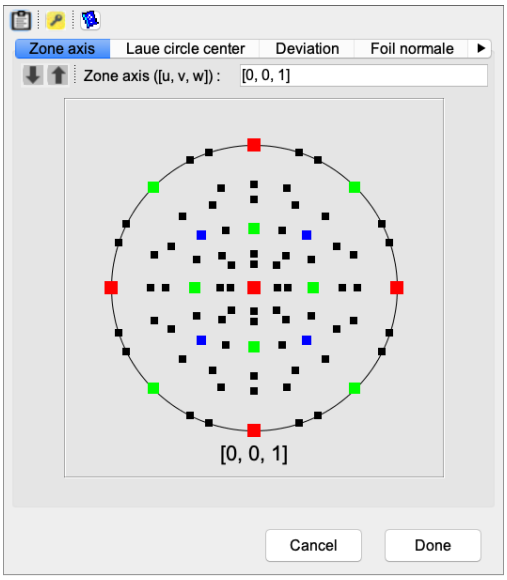
12.1 Tool buttons

The tool buttons allow to:

- : transfer the dialogue to the clipboard.
- : open the keeper dialogue (Fig. 90).
- : display a help file.

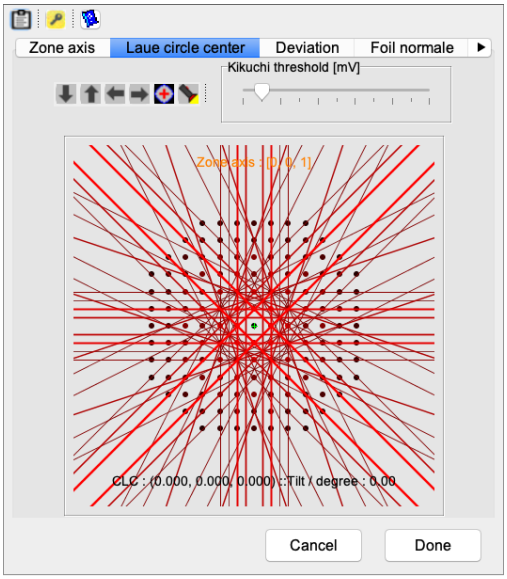


(a) Specimen dialogue, $[uvw]$ zone axis selection (default).

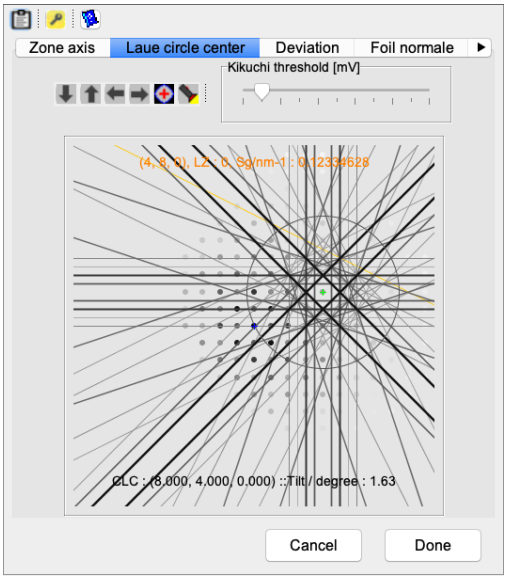


(b) $[uvw]$ zone axis selection with less choice.

Figure 84: Use the arrows tool buttons to decrease/increase the number of plotted zone axis. $[uvw]$ zone indices can be entered directly (keyboard return key to confirm).

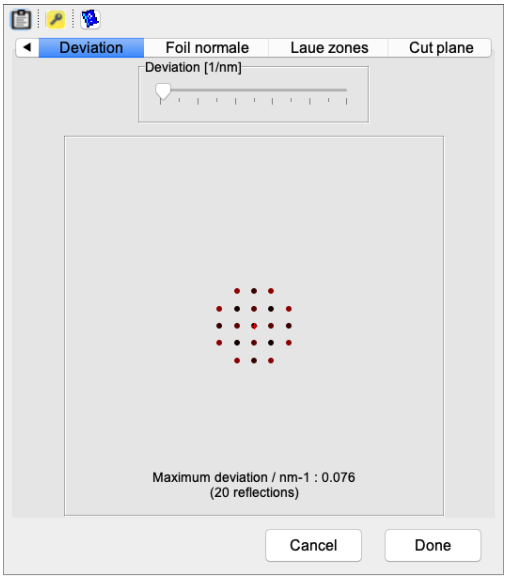


(a) Default CLC is setting (000).

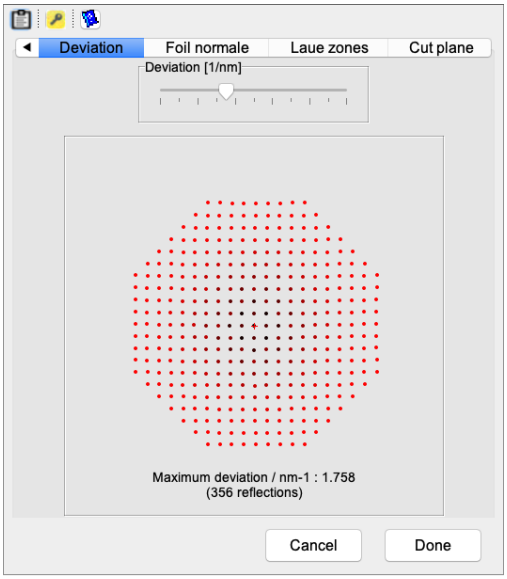


(b) CLC moved to $(8, 4, 0)$ *rightarrow* crystal tilt 1.63 $[deg]$

Figure 85: Use the arrows tool buttons to move the **C**enter of the **Laue C**ircle (CLC).

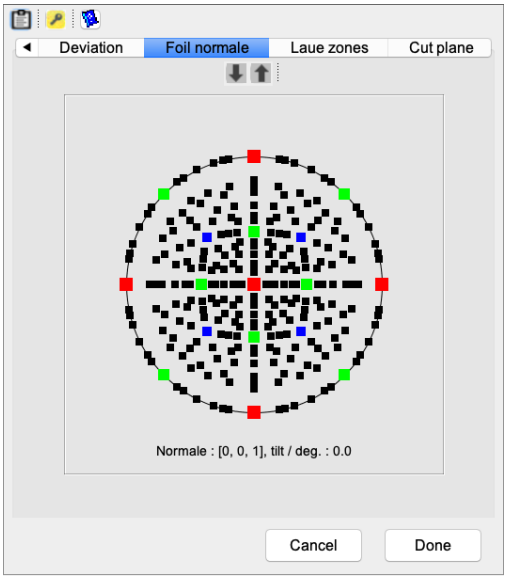


(a) Small deviation → small number of reflections.

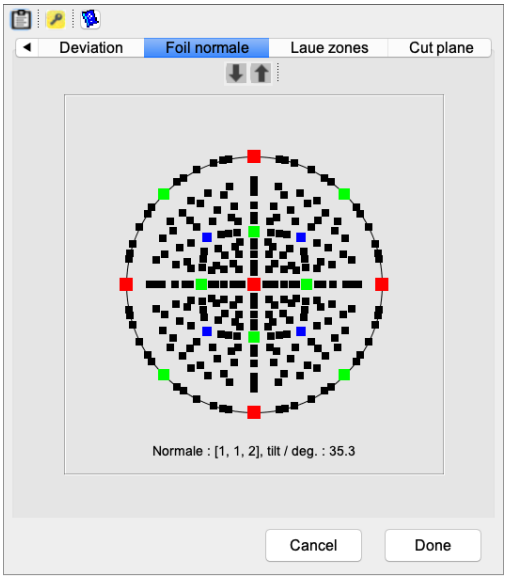


(b) Large deviation → large number of reflections.

Figure 86: The deviation slider defines the maximum distance of a reflection to the Ewald sphere.

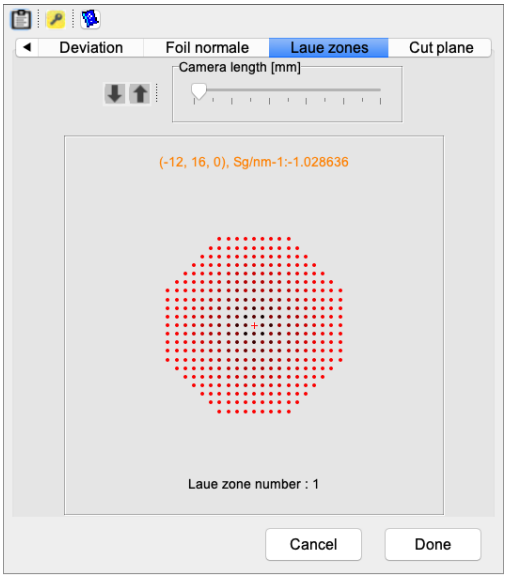


(a) Foil normale is parallel to the zone axis by default.

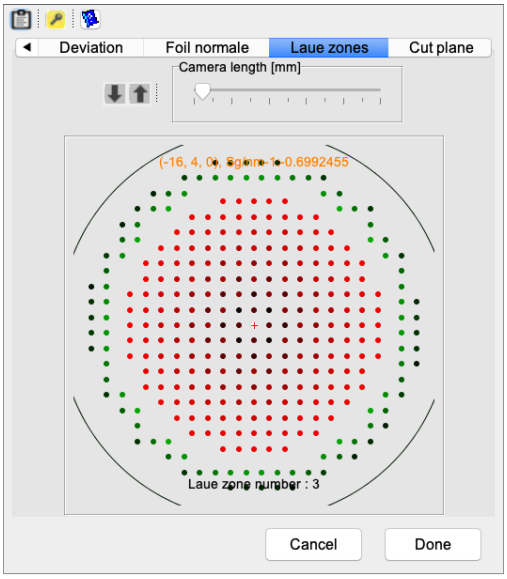


(b) Foil normale set to $[1, 1, 2] \rightarrow$ tilt 35.3 $[deg]$.

Figure 87: The foil normale sets the angle of the normale to the entrance surface of the tilted foil.

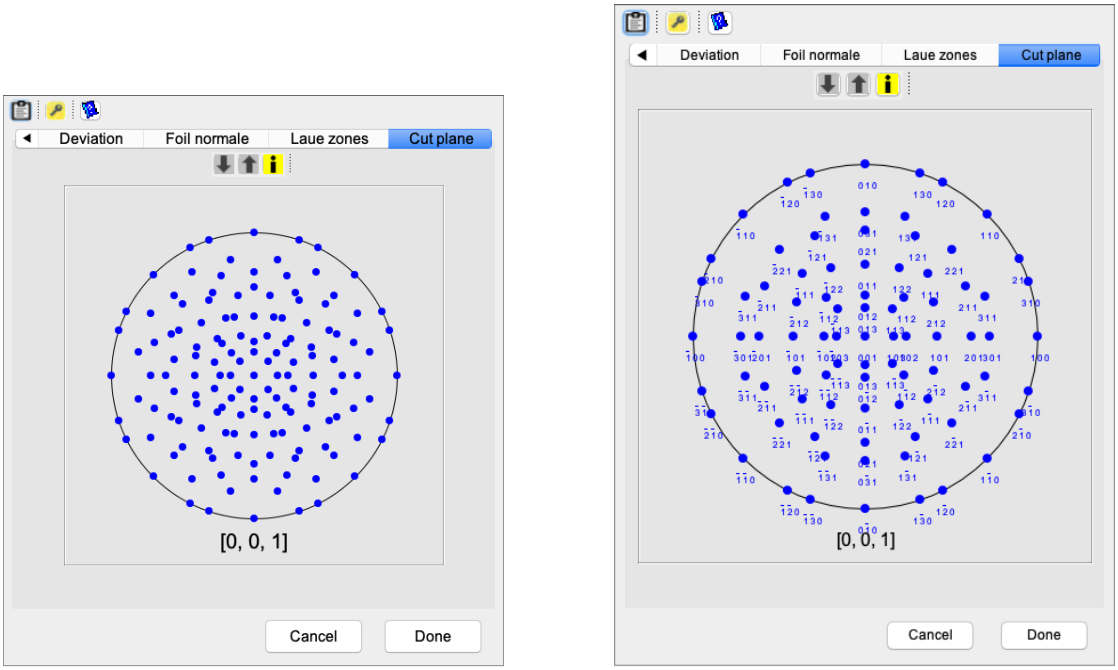


(a) Default is only **Z**eroth **O**rder **L**aue **Z**one.



(b) **F**irst **O**rder **L**aue **Z**one.

Figure 88: The arrow tool buttons increase/decrease the number of Laue zones.


Deviation
Foil normale
Laue zones
Cut plane
[0, 0, 1]
Cancel
Done
Deviation
Foil normale
Laue zones
Cut plane
[0, 0, 1]
Cancel
Done

(a) (b)

Figure 89

13 Keeper dialogue

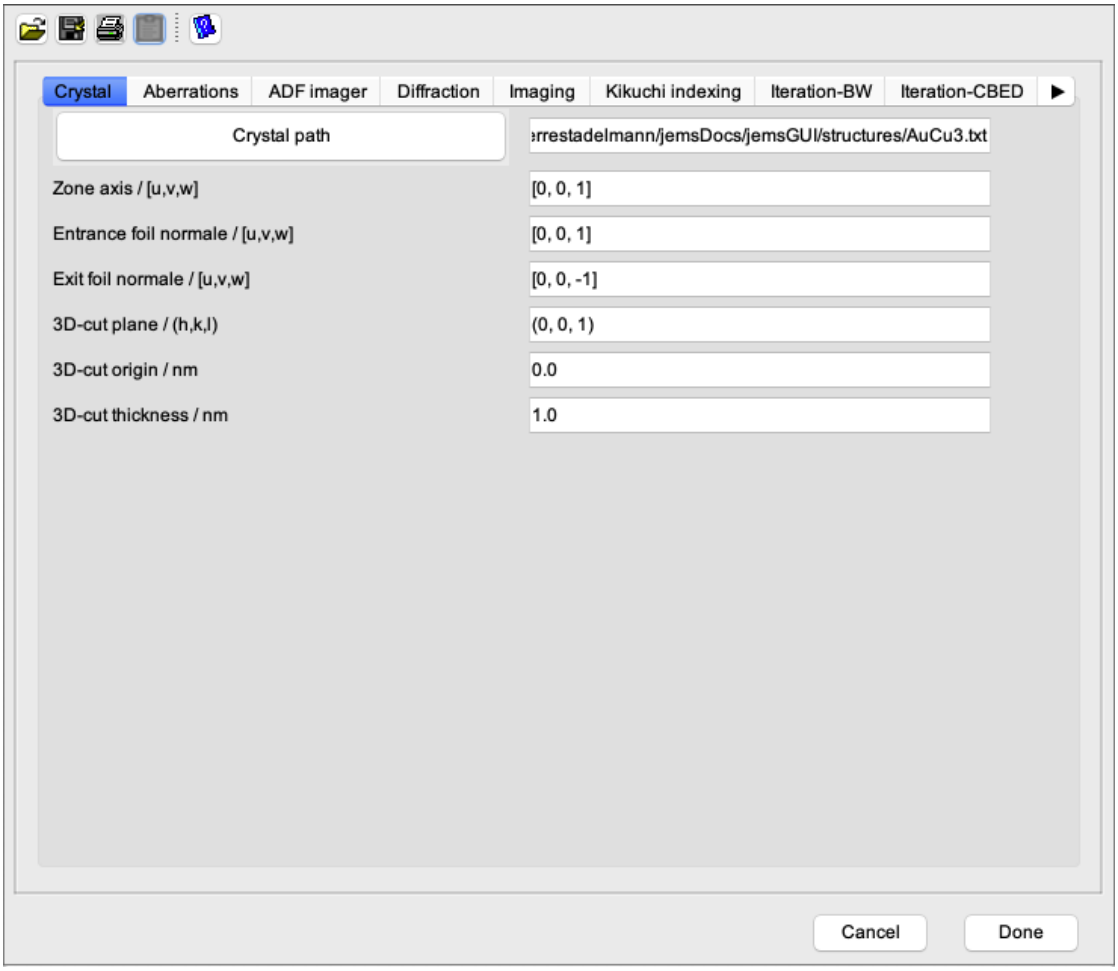


Figure 90: The **Keeper** dialogue keeps most jems parameters.

The **Keeper** dialogue allows to keep the set of parameters defined for the simulations. The **crystal path** is set using the Crystal path button.

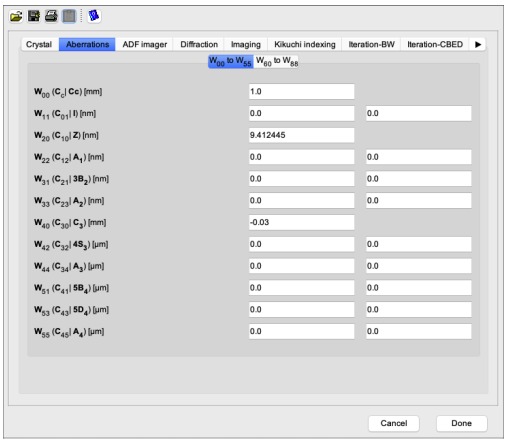
13.1 Tool buttons

The tool buttons allow to:

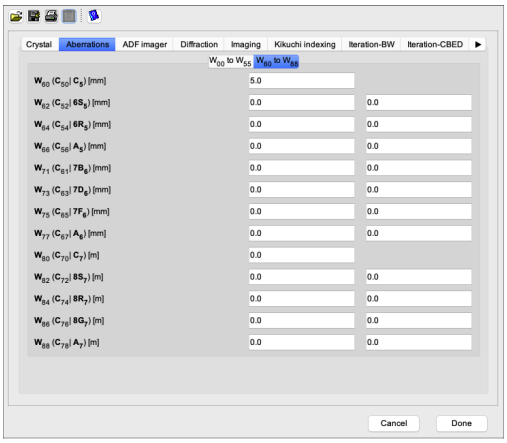
- : open a set of parameters stored in a *keeper* file.
- : save the current parameters in a *keeper* file.

-  : print the current parameters.
-  : transfer the dialogue to the clipboard.
-  : display a help file.

The **Aberrations** tabs keep the wave-front aberrations W_{ij}, where **i** denotes the power of radial aberration angle and **j**-fold azimutal angle. In this notation only even **i** or **j** indices are permitted. The labels are also given in the equivalent geometric aberrations notation as defined by Krivanek C_{ij} and Haider C_c, I, Z, A_1, ... (Fig. 91) [31].



(a) Wave-front aberrations $W_{00} \rightarrow W_{55}$.



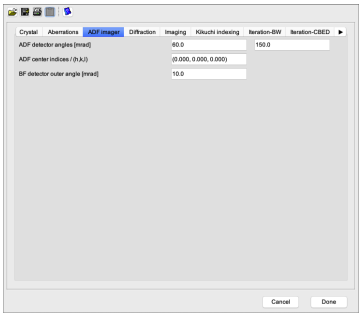
(b) Wave-front aberrations $W_{60} \rightarrow W_{88}$.

Figure 91: Wave-front aberrations defined to order 8.

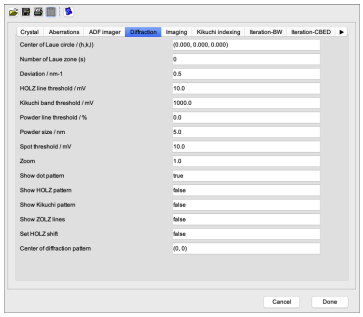
The 3 tabs of Fig. 92 keep parameters related to ADF, HRTEM and SAED diffraction [32].

[31] Wave-front aberration W_{00} is the chromatic aberration, i.e. the aberration that only dependent on the wavelength.

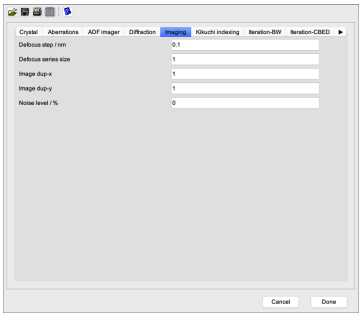
[32] The sign of the under-defocus is defined in the **Parameters** → **Preferences** → **Imaging** → **Others**.



(a) BF, annular dark field and HAADF detector diameters.



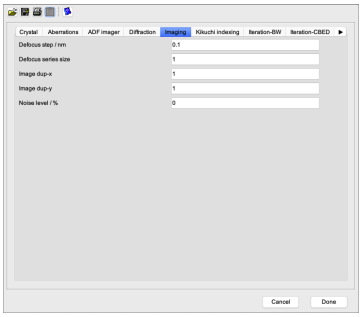
(b) Diffraction parameters.



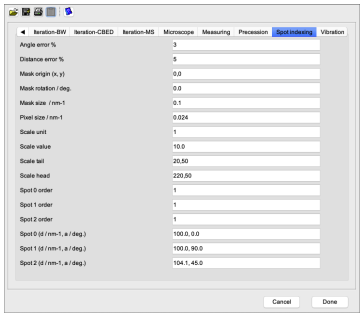
(c) Defocus step, size of defocus series, image duplication and Poisson noise.

Figure 92: ADF imager, Diffraction and Imaging tabs.

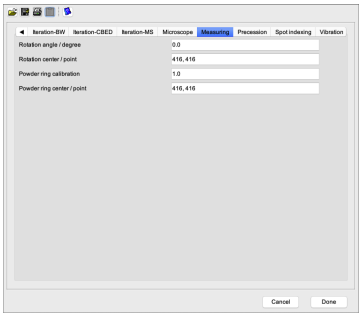
The 3 tabs keeping parameters related to diffraction patterns indexing are shown on Fig. 93, the 3 tabs keeping the Bloch-wave and multislice iterations parameters on 94 and the 3 tabs keeping the microscope, precession, vibration and drift parameters on Fig. 95.



(a) Kikuchi indexing parameters.

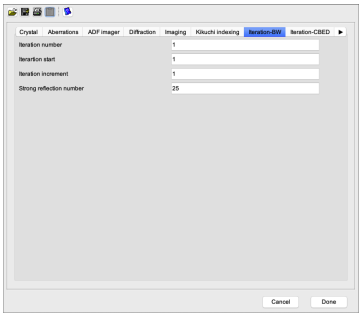


(b) Spot indexing parameters.

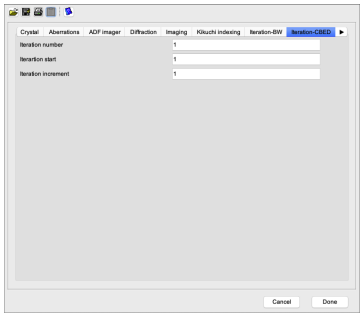


(c) Parameters related to rotation and powder ring pattern center.

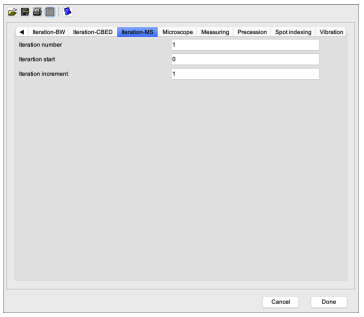
Figure 93: Kikuchi and SAED patterns indexing.



(a) Parameters of Bloch-wave calculations.

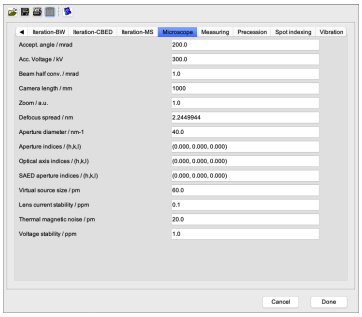


(b) Parameters of CBED calculations.

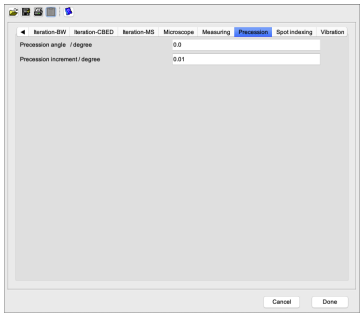


(c) Parameters of multislice calculations.

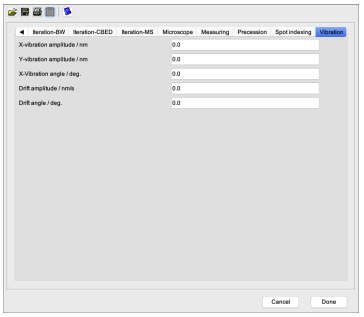
Figure 94: Parameters related to Bloch-wave and multislice calculations.



(a) Microscope parameters.



(b) Precession radial angle and azimutal increment.



(c) Vibration and drift imaging parameters.

Figure 95: Microscope, precession and vibration parameters.

14 Wave-front aberrations dialogue

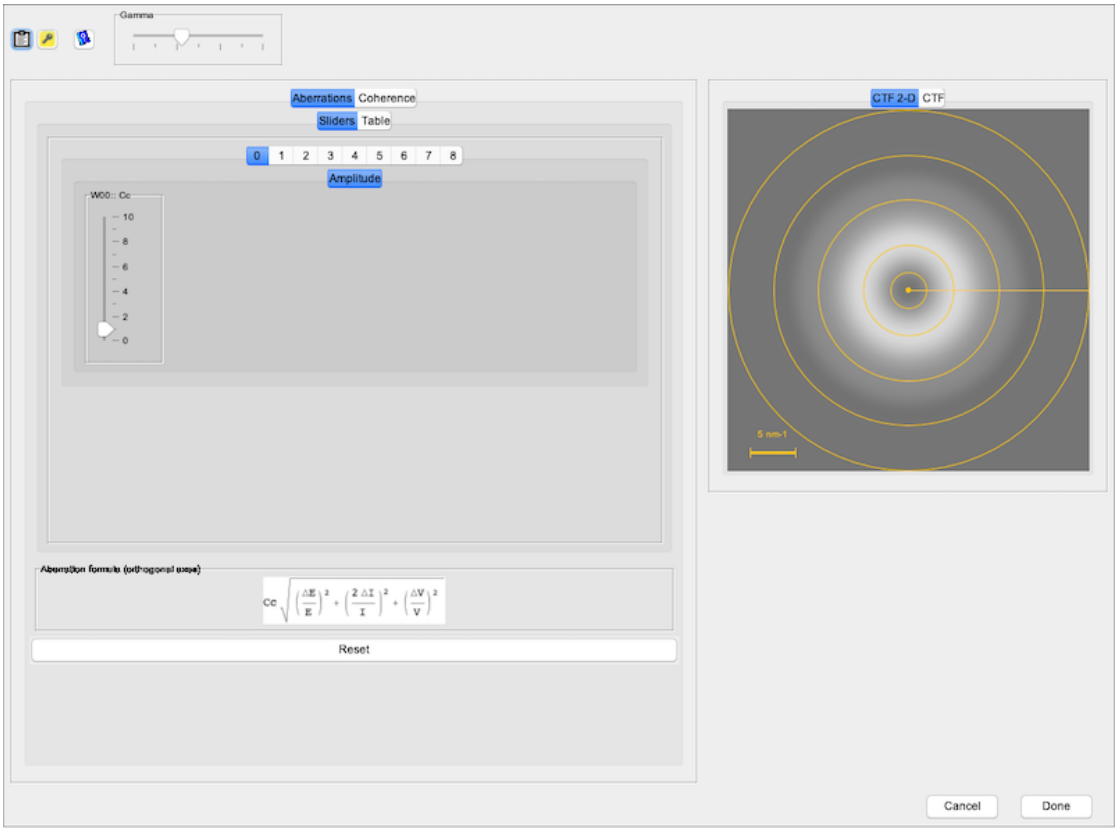


Figure 96: Wave-front aberration and **C**ontrast **T**ransfer **F**unction.

14.1 Tool buttons

The tool buttons allow to:

- : transfer the dialogue to the clipboard.
- : open the keeper dialogue (Fig. 90).
- : display a help file.

15 Transfer function

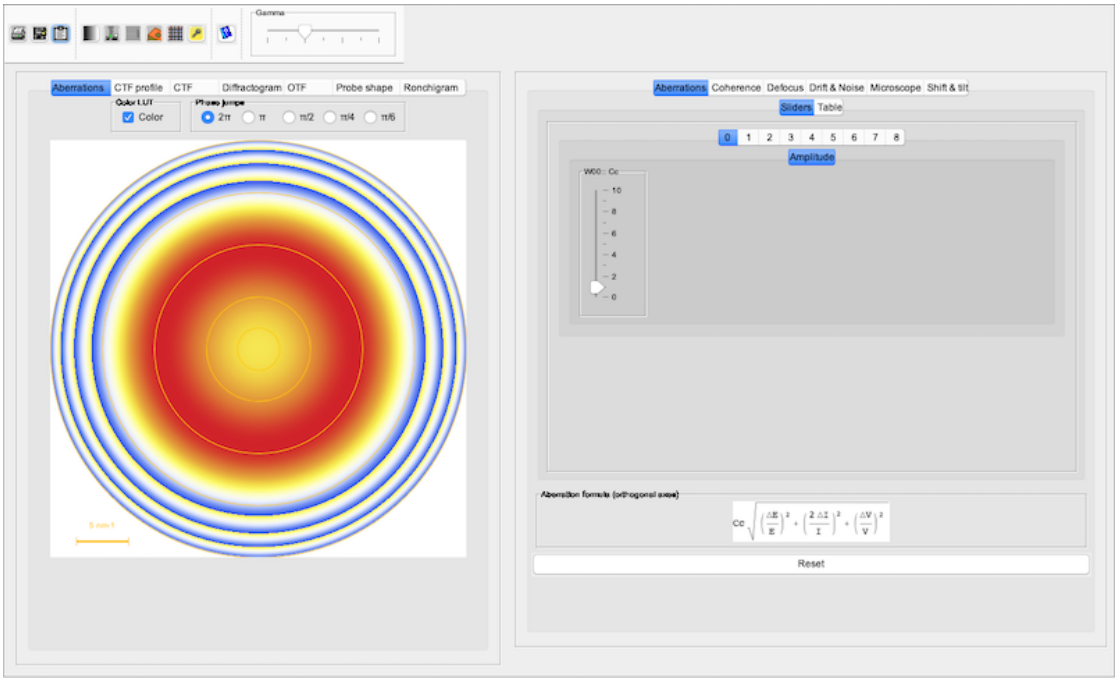


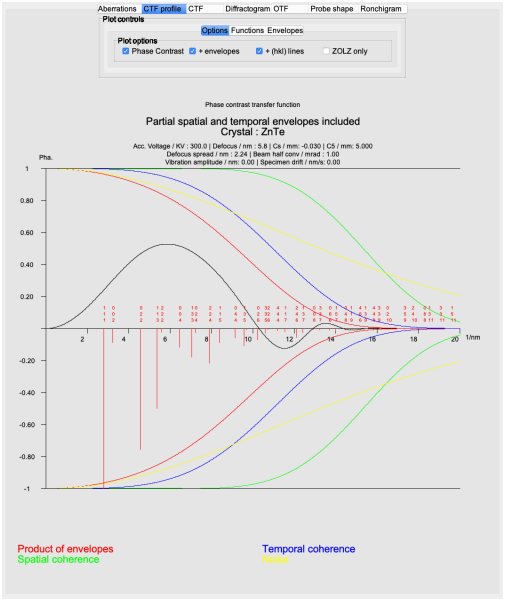
Figure 97: Wave-front aberrations.

15.1 Tool buttons

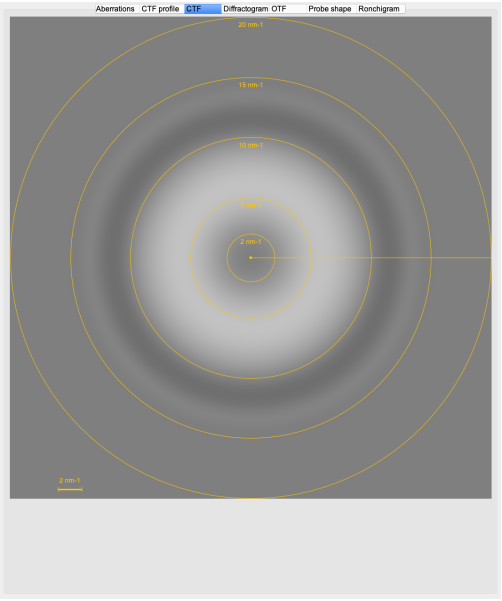
The tool buttons allow to:

- : print the image panel.
- : save the image panel.
- : transfer the frame to the clipboard.
- : reset the gray scale.
- : open the **Microscope** dialogue (Fig. 108).
- : make a tilt tableau (Fig. 105).
- : open the **Specimen** dialogue (Fig. 84a).
- : tabulate the image panel.
- : open the **Keeper** dialogue (Fig. 90).

-  : display a help file.

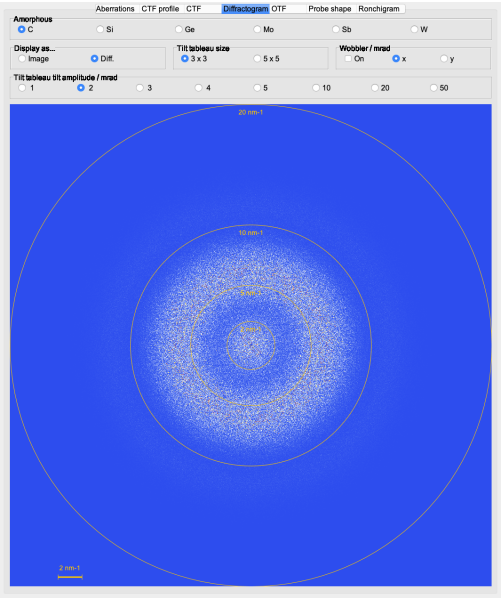


(a) CTF profile tab (with envelopes and ZnTe powder lines).

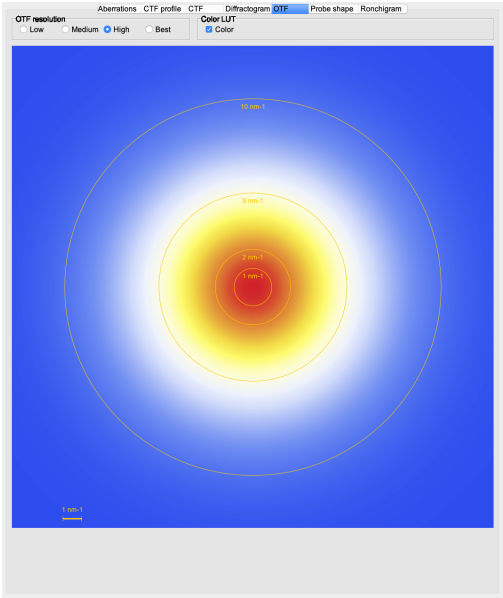


(b) CTF 2-D tab.

Figure 98: **C**ontrast **T**ransfer **F**unction (CTF).

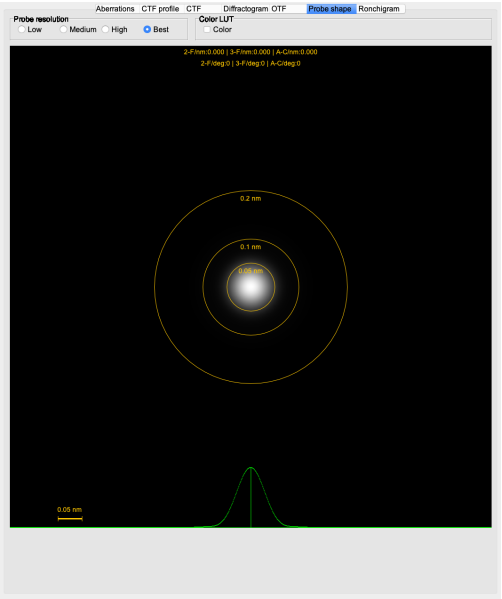


(a) Diffractogram tab (amorphous carbon thin film).

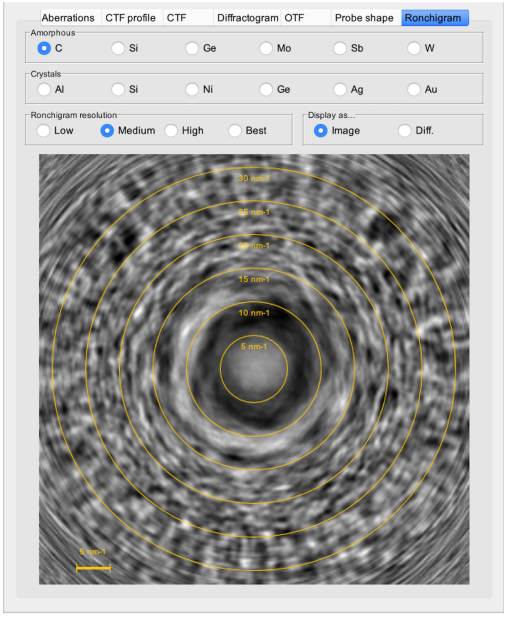


(b) OTF tab.

Figure 99: Diffractogram and **O**ptical **T**ransfer **F**unction.

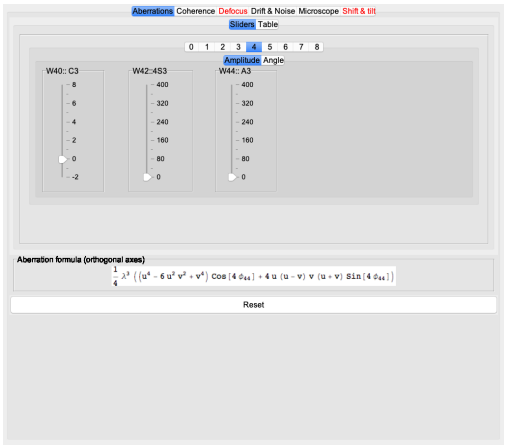


(a) Probe shape tab (intensity).



(b) Ronchigram tab.

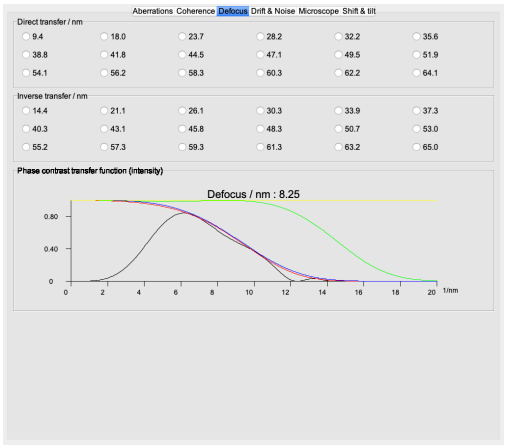
Figure 100: Probe shape and Ronchigram.



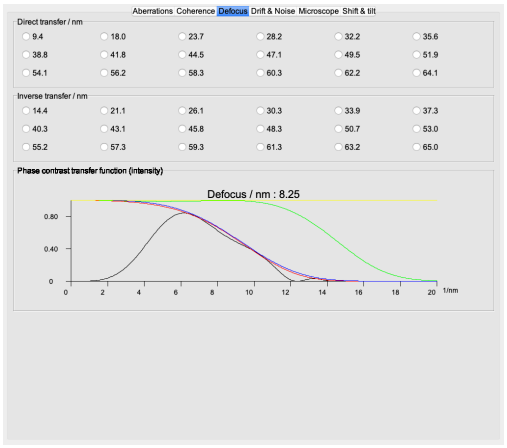
(a) Aberration settings tab.

(b) Coherence settings tab.

Figure 101: Aberrations and coherence settings.

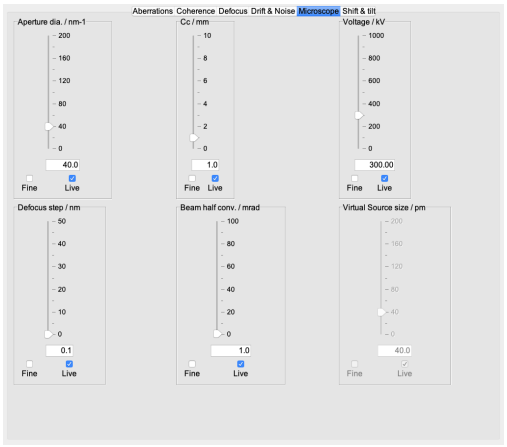


(a)

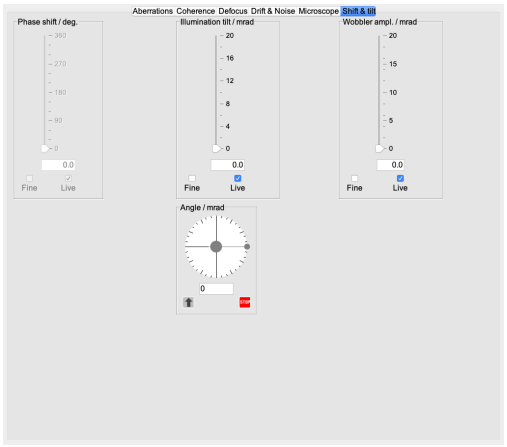


(b)

Figure 102: Defocus and drift or noise settings.

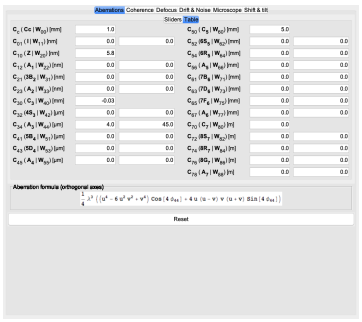


(a)

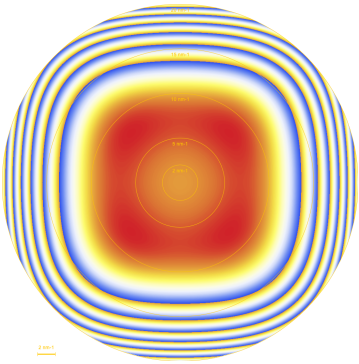


(b)

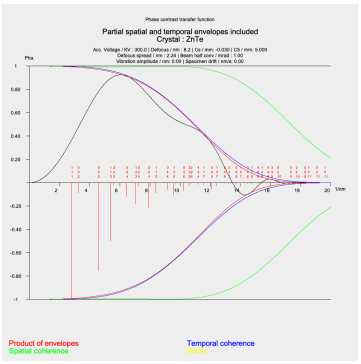
Figure 103: Microscope and shift or tilt settings.



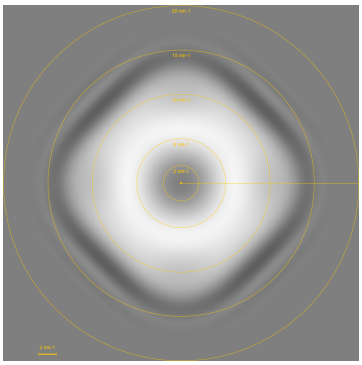
(a) Table of aberrations, w_{44} = 4 [μm].



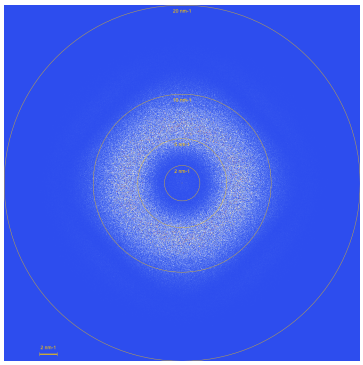
(b) Wave-front aberrations ($w_{44} = 4$ [μm]).



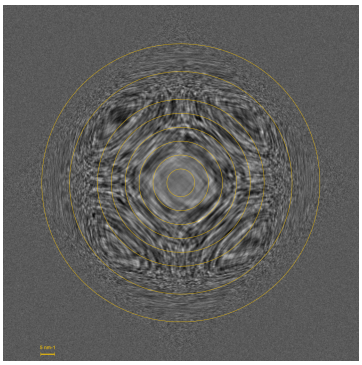
(c) Aberrated CTF profile ($w_{44} = 4$ [μm]).



(d) CTF 2-D ($w_{44} = 4$ [μm]).

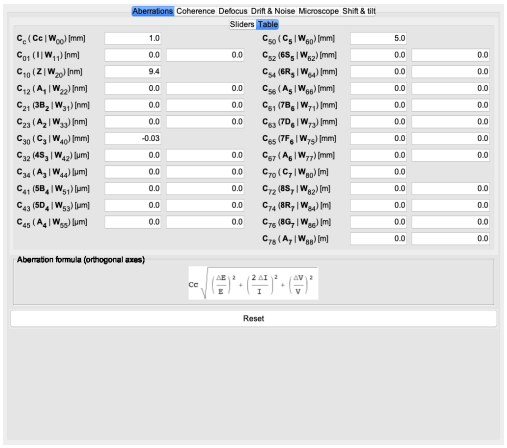


(e) Diffractogram ($w_{44} = 4$ [μm]).

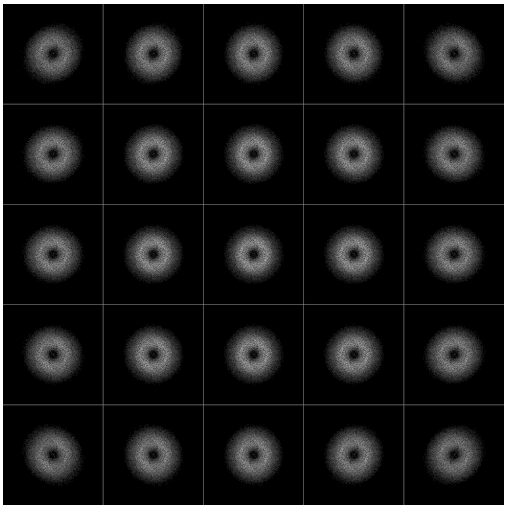


(f) Ronchigram ($w_{44} = 4$ [μm]).

Figure 104: Wave-front aberrations, CTF, diffractogram and Ronchigram with 4-fold astigmatism 4 [μm].

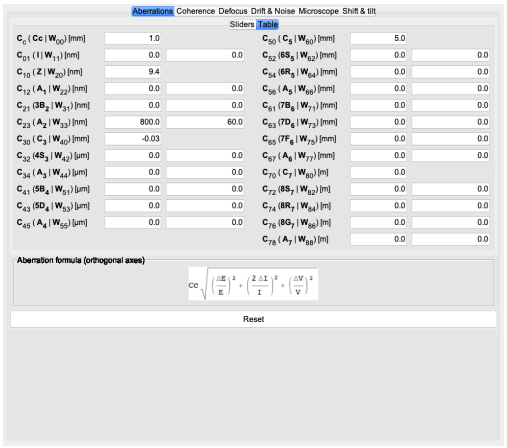


(a) Table of aberrations

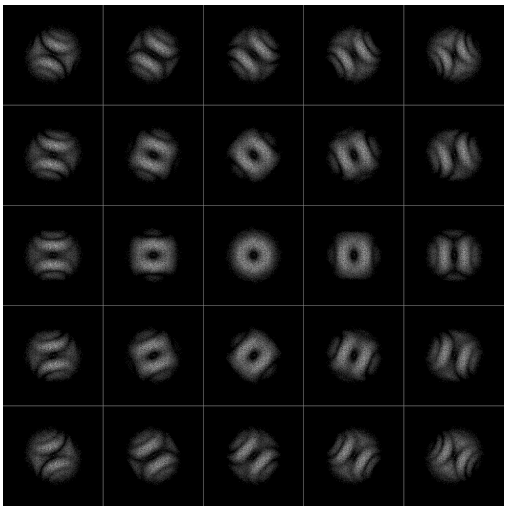


(b) Tilt tableau.

Figure 105: Tilt tableau no aberrations, tilt amplitude 2 [mrad].

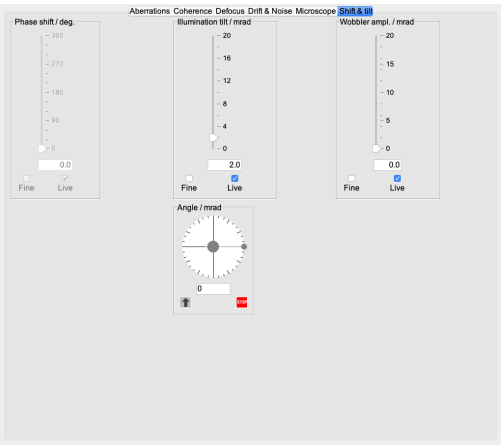


(a) Table of aberrations.

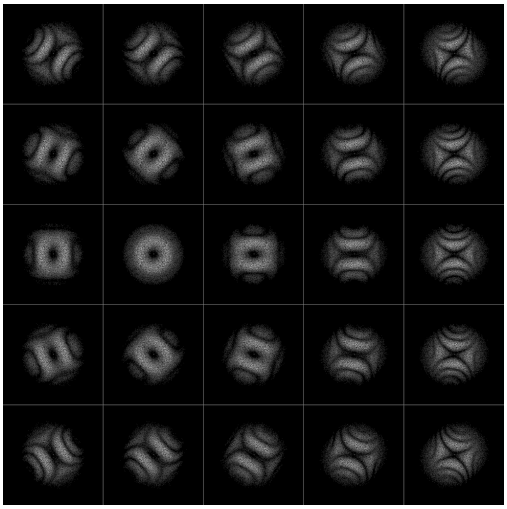


(b) Tilt tableau, 3-fold astigmatism 800 [nm], 60 [deg].

Figure 106: Tilt tableau 3-fold astigmatism, tilt amplitude 2 [mrad].



(a) Tilted illumination 2 [mrad].



(b) Tilt tableau, 3-fold astigmatism 800 [nm], 60 [deg], illumination tilt 2 [mrad].

Figure 107: Tilt tableau, 3-fold astigmatism and tilted illumination 2 [mrad].

16 Microscope dialogue

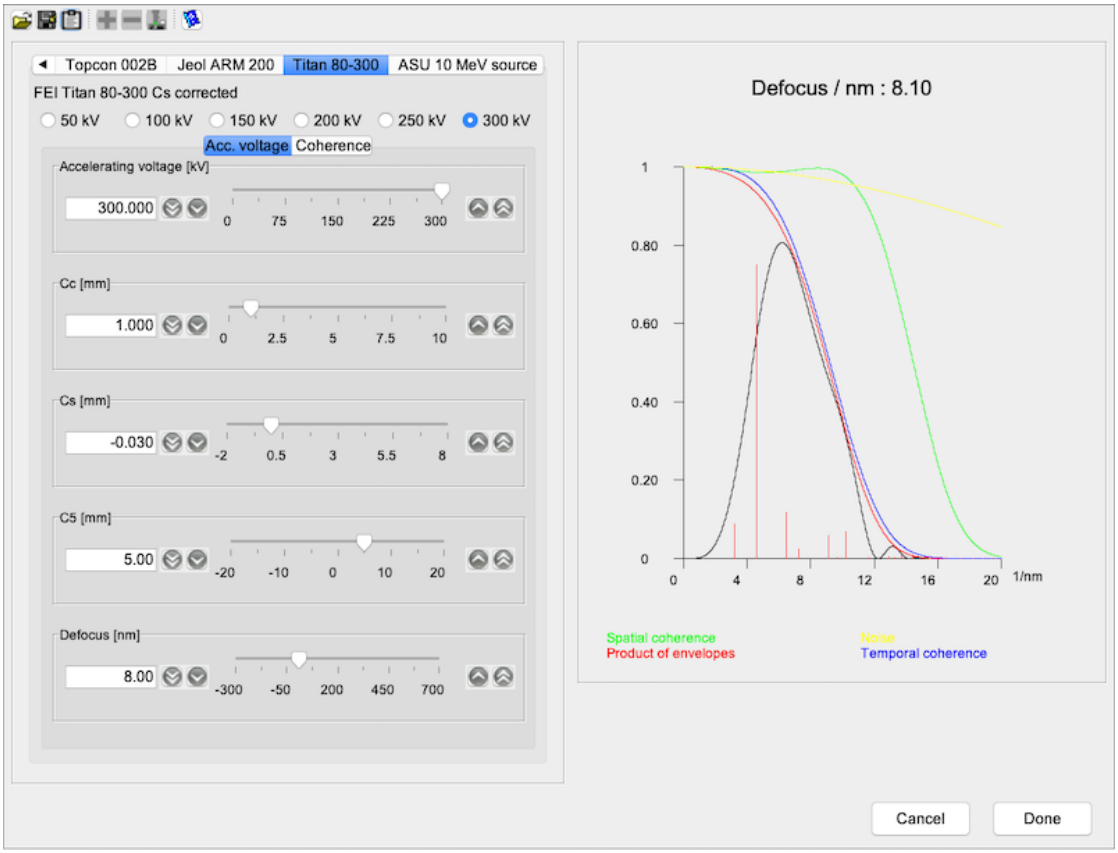


Figure 108: Microscope dialogue.

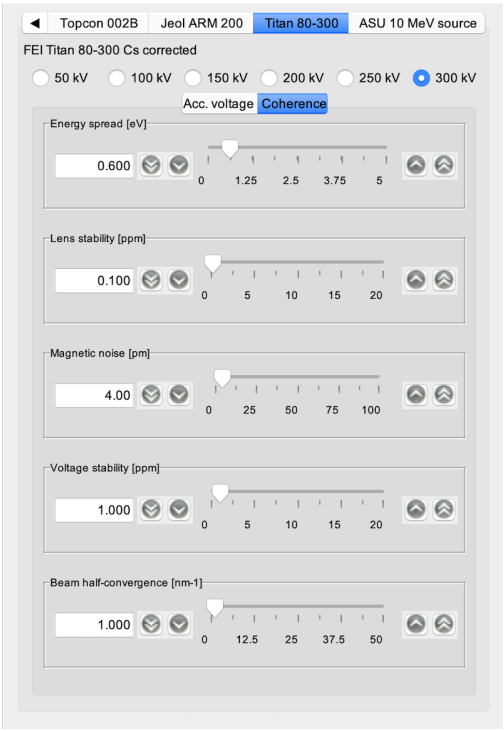
16.1 Tool buttons

The tool buttons allow to:

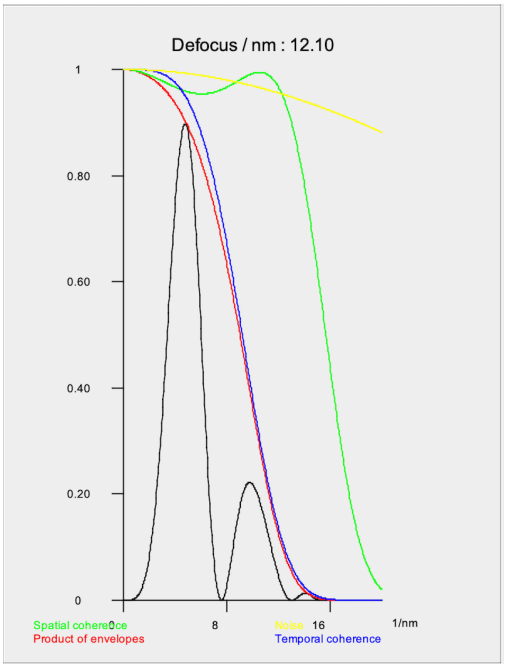
- : load a microscope table.
- : save the table of microscopes.
- : transfer the frame to the clipboard.
- : add a new microscope.
- : delete the selected microscope.
- : load the default microscope table.

-  : open the specimen dialogue (Fig. 84a).
-  : display a help file.

The plot of Fig. 109b shows the intensity of the **C**ontrast **T**ransfer **F**unction with positive sign for the underfocus. The **Parameters** → **Preferences** → **Imaging** → **Others** tab allows to use the opposite sign.
The yellow envelope introduces the effect of **T**hermal **M**agnetic **N**oise that can attenuate the CTF of aberrations corrected microscopes.



(a) Tab to control partial temporal and spatial coherence.



(b) CTF intensity plot.

Figure 109: CTF plot (positive underfocus).

17 Crystallographic calculator

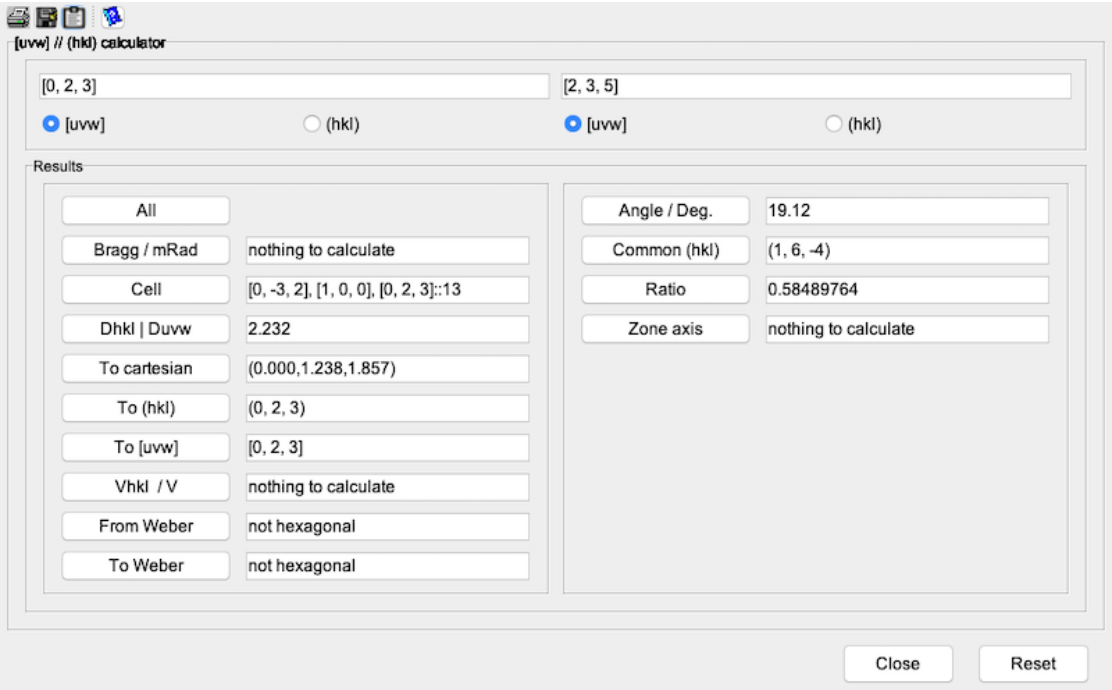


Figure 110: Crystallographic calculator.

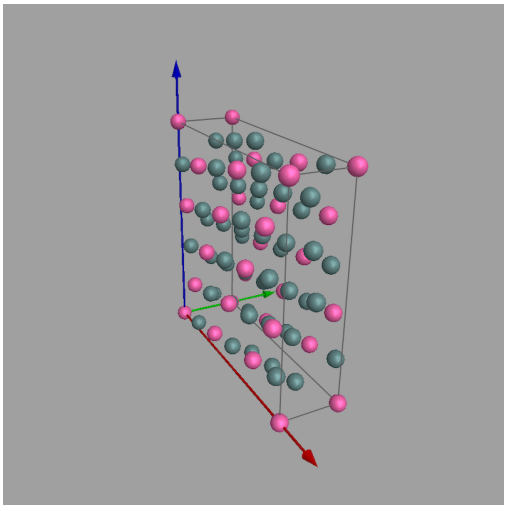
17.1 Tool buttons

The tool buttons allow to:

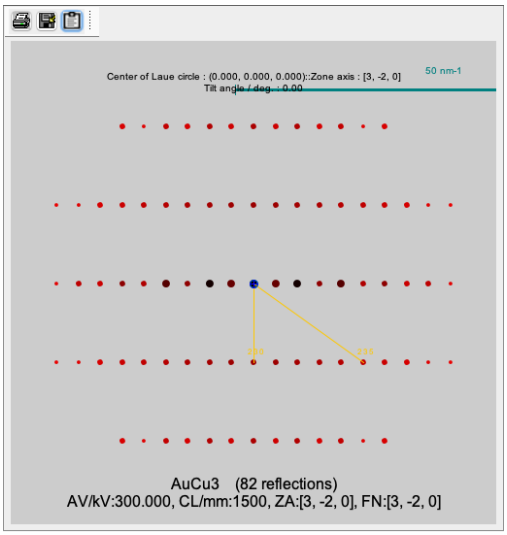
- : print the frame.
- : save the frame.
- : transfer the frame to the clipboard.
- : display a help file.

The crystallographic calculator performs several calculations related to direct or reciprocal space. Fig. 110 shows a typical calculation of the angle between 2 zone axis directions ($[2,3,0]$ & $[2,3,5]$). It also shows the orthogonal cell with $[0,0,1]$ parallel to $[2,3,0]$ (Fig. 111a). When the calculation is performed with 2 (h,k,l) reflections the SAED pattern defined by them is shown (Fig. 111b) [33].

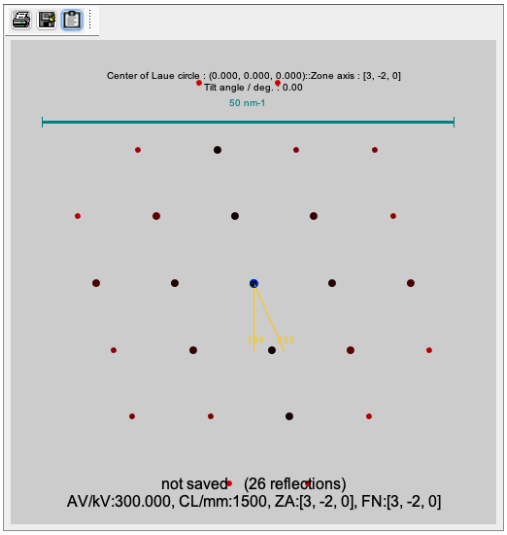
[33] When the calculations are first performed with $< uvw >$ directions, the following calculations with $\{hkl\}$ reflections use the new unit orthogonal unit cell. (Figs. 111c, 111d)



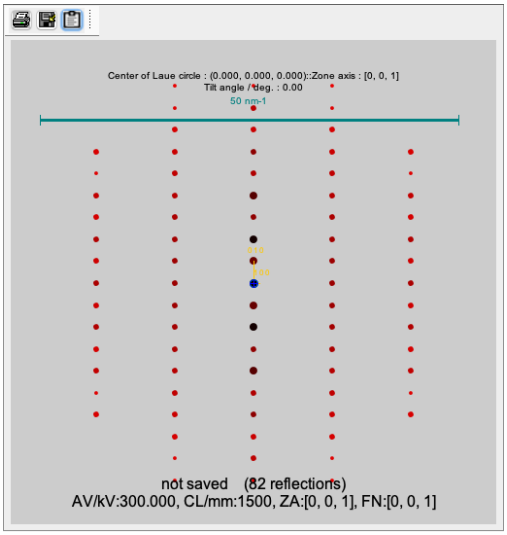
(a) Orthogonal cell with $[0, 0, 1]$ parallel to $[2, 3, 0]$.



(b) SAED pattern defined by $(2, 3, 0)$ and $(2, 3, 5)$ reflections.

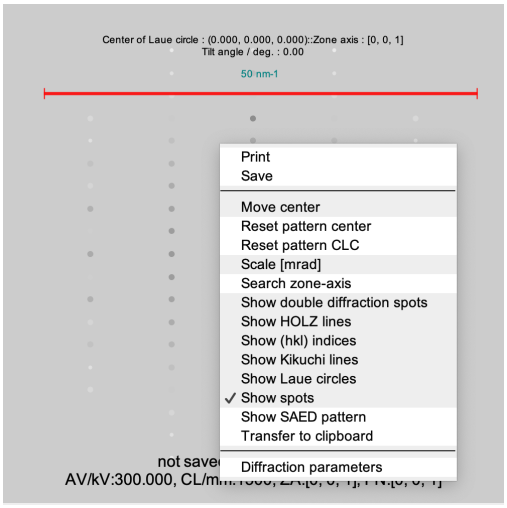


(c) SAED pattern defined by $(2, 3, 0)$ and $(2, 3, 5)$ reflections. The **not saved** label indicates that the 2 (hkl) reflections refer to the new orthogonal cell.

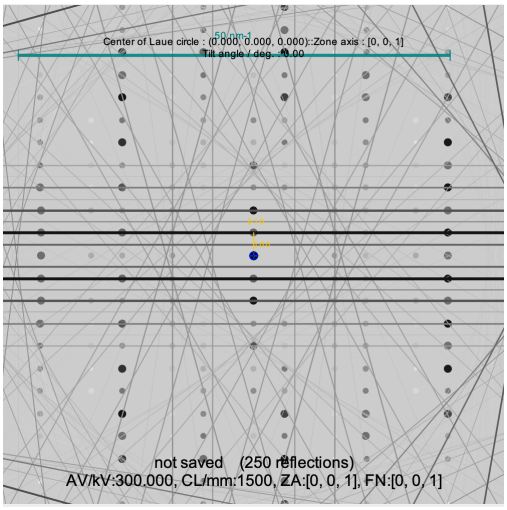


(d) SAED pattern defined by $(1, 0, 0)$ and $(0, 1, 0)$ reflections, i.e. the $[2, 3, 0]$ SAED pattern from $AuCu_3$ unit cell.

Figure 111: Crystallographic calculator SAED plots with the orthogonal cell.



(a) Popup menu attached to the SAED pattern.



(b) SAED pattern with Kikuchi lines.

Figure 112: Popup menu and Kikuchi lines.

18 Stereogram frame

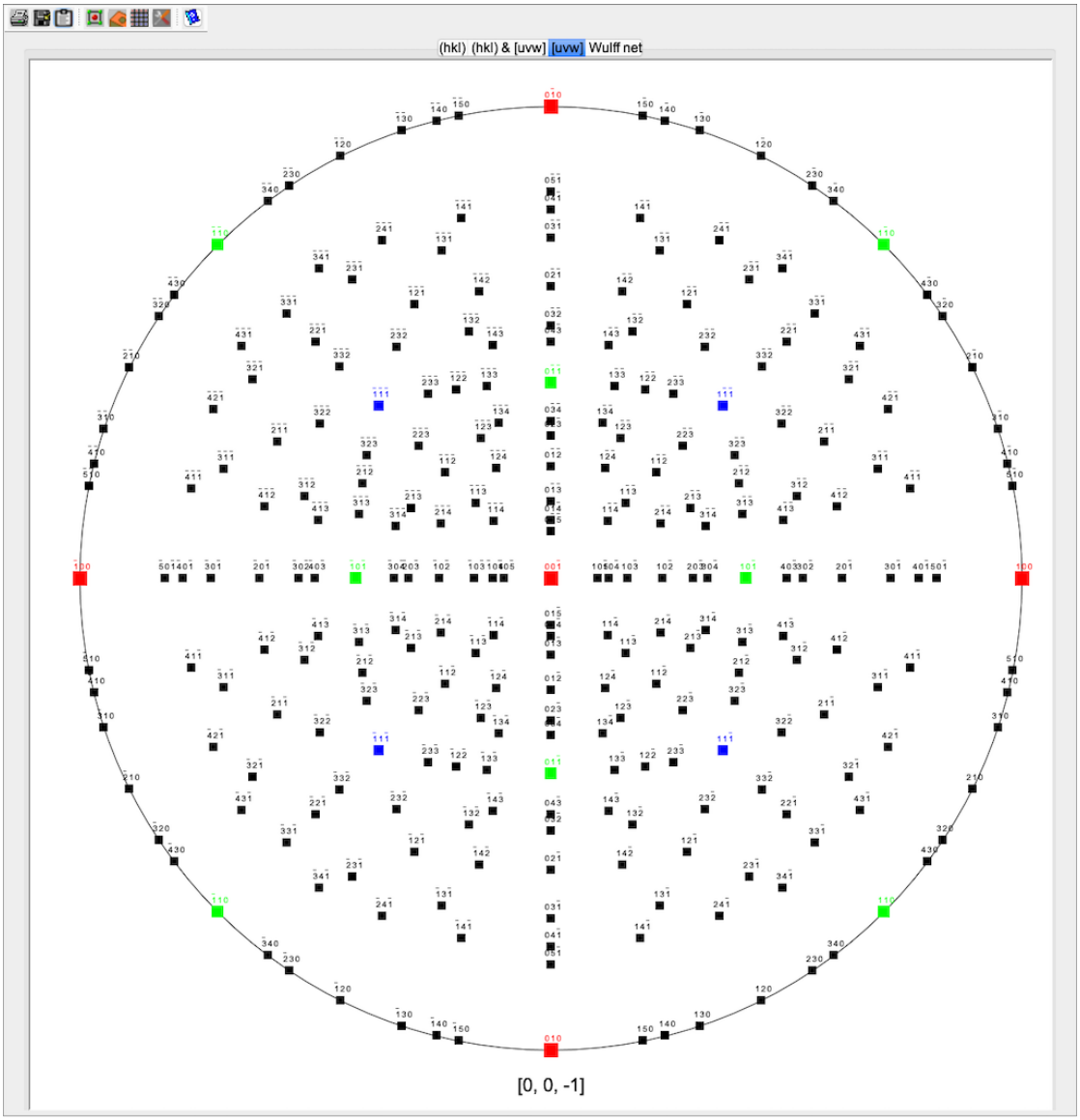


Figure 113: Stereogram frame.

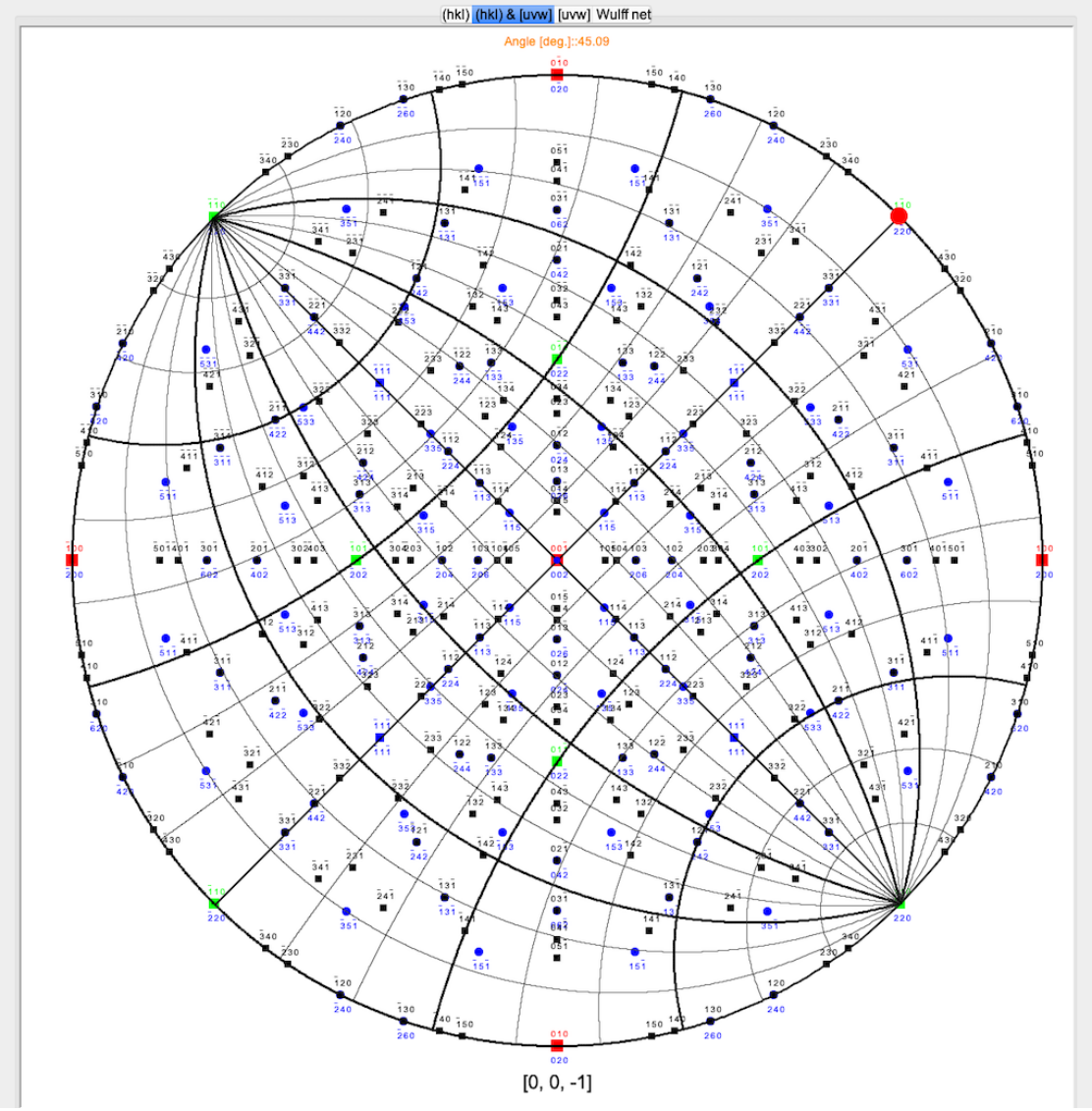


Figure 114: $< uvw >$ stereogram and Wulff net.

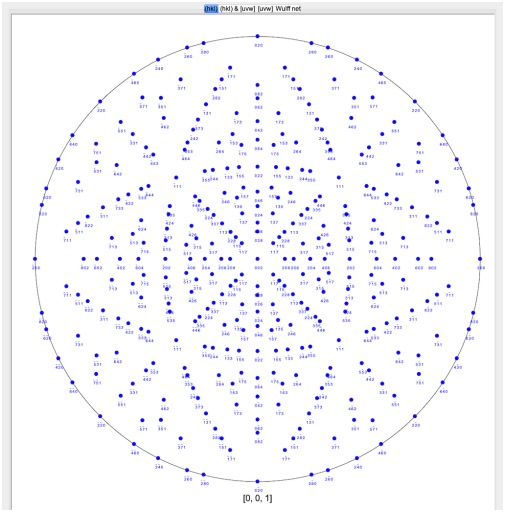
18.1 Tool buttons

The tool buttons allow to:

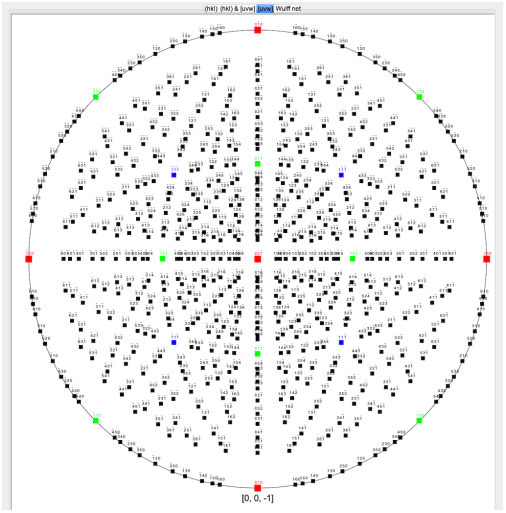
- : print the stereographic projection.
- : save the stereographic projection.
- : transfer the frame to the clipboard.

-  : overlay stereograms.
-  : make a table of zone axis.
-  : open the toolbox.
-  : display a help file.

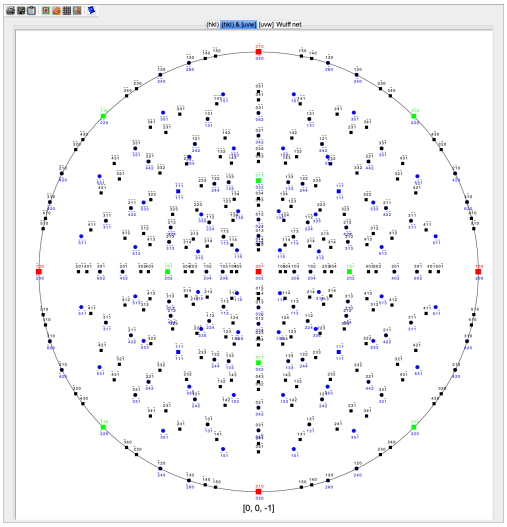
18.2 Tabs



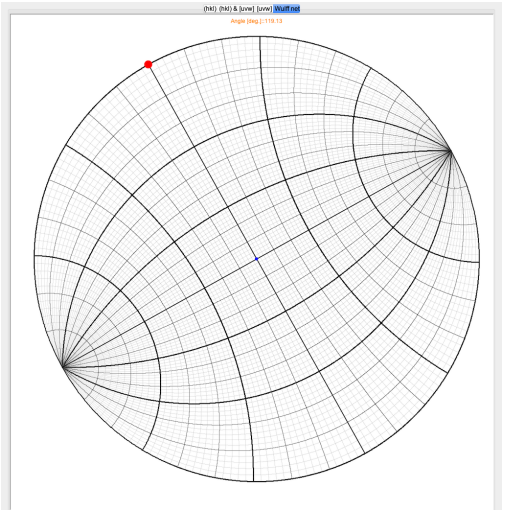
(a) Indexed $\{hkl\}$ stereogram.



(b) Indexed $< uvw >$ stereogram.



(c) Superposed $\{hkl\}$ and $< uvw >$ stereograms.



(d) Wulff net.

Figure 115: Stereogram tabs.

19 Powder pattern frame

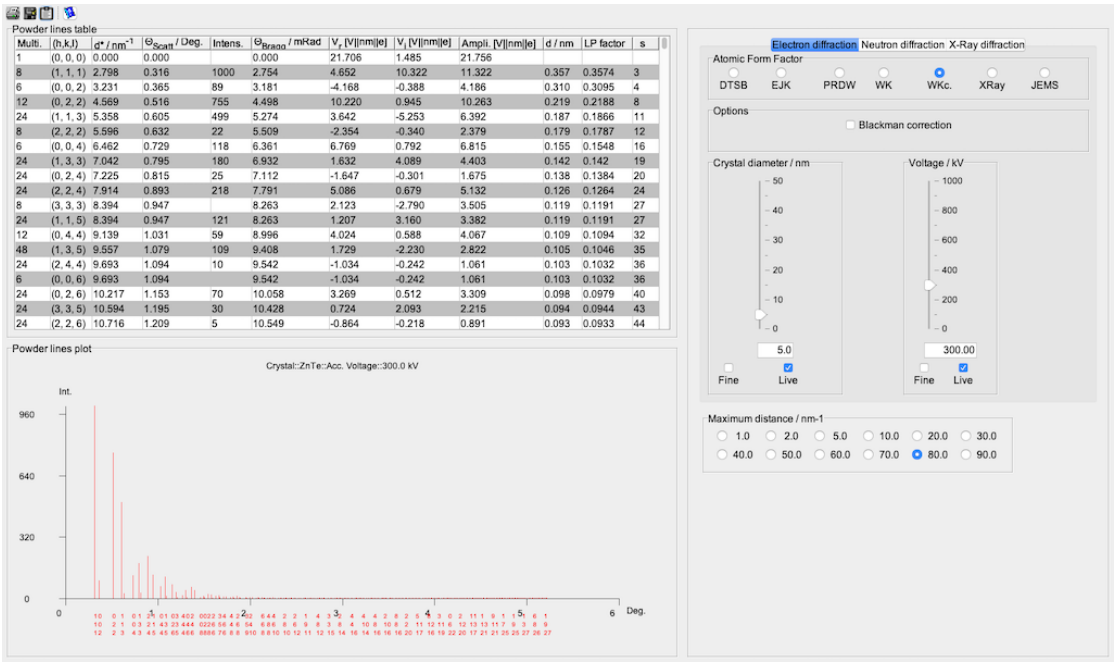


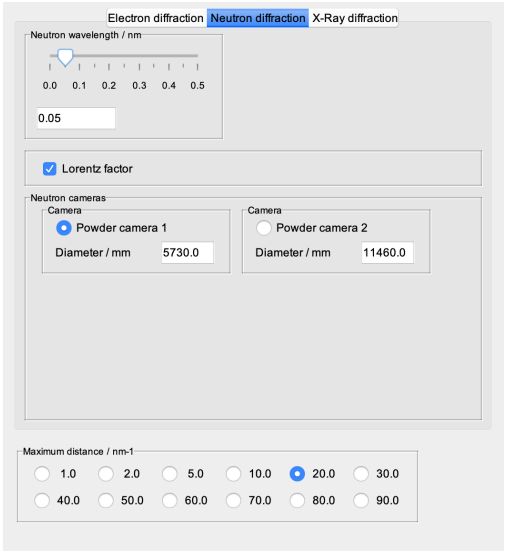
Figure 116: Powder pattern frame.

19.1 Tool buttons

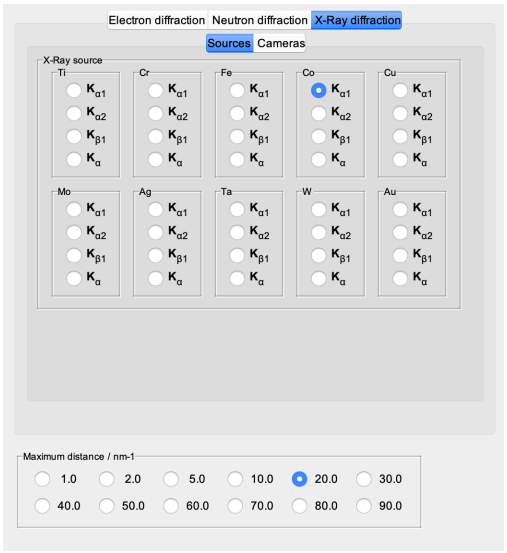
The tool buttons allow to:

- : print the stereogram.
- : save the stereogram image.
- : transfer the frame to the clipboard.
- : display a help file.

The powder pattern plots only show the lines position and intensity (Fig, 116). The parameters of the different radiations are gathered in the 3 tabs on the right panel. Controls to plot neutron and X-Ray powder patterns allows to change the wavelength of the radiation (Figs 117a, 117b). The horizontal axis unit can be either degree or nm^{-1} (Figs 118a, 118b).

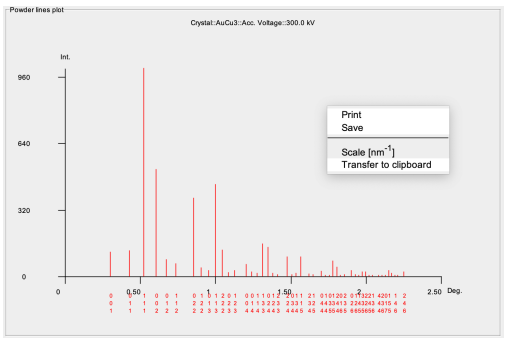


(a) Controls for neutron powder pattern plots.

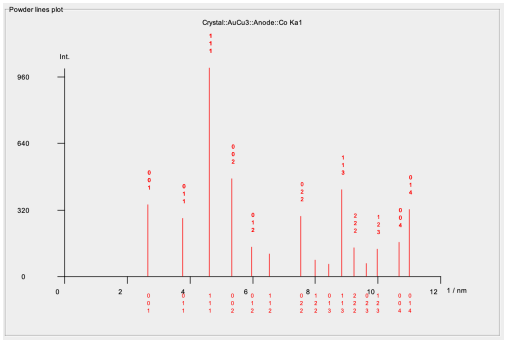


(b) Controls for X-Ray powder pattern plots.

Figure 117: Tabs of Neutron and X-Ray powder pattern controls.



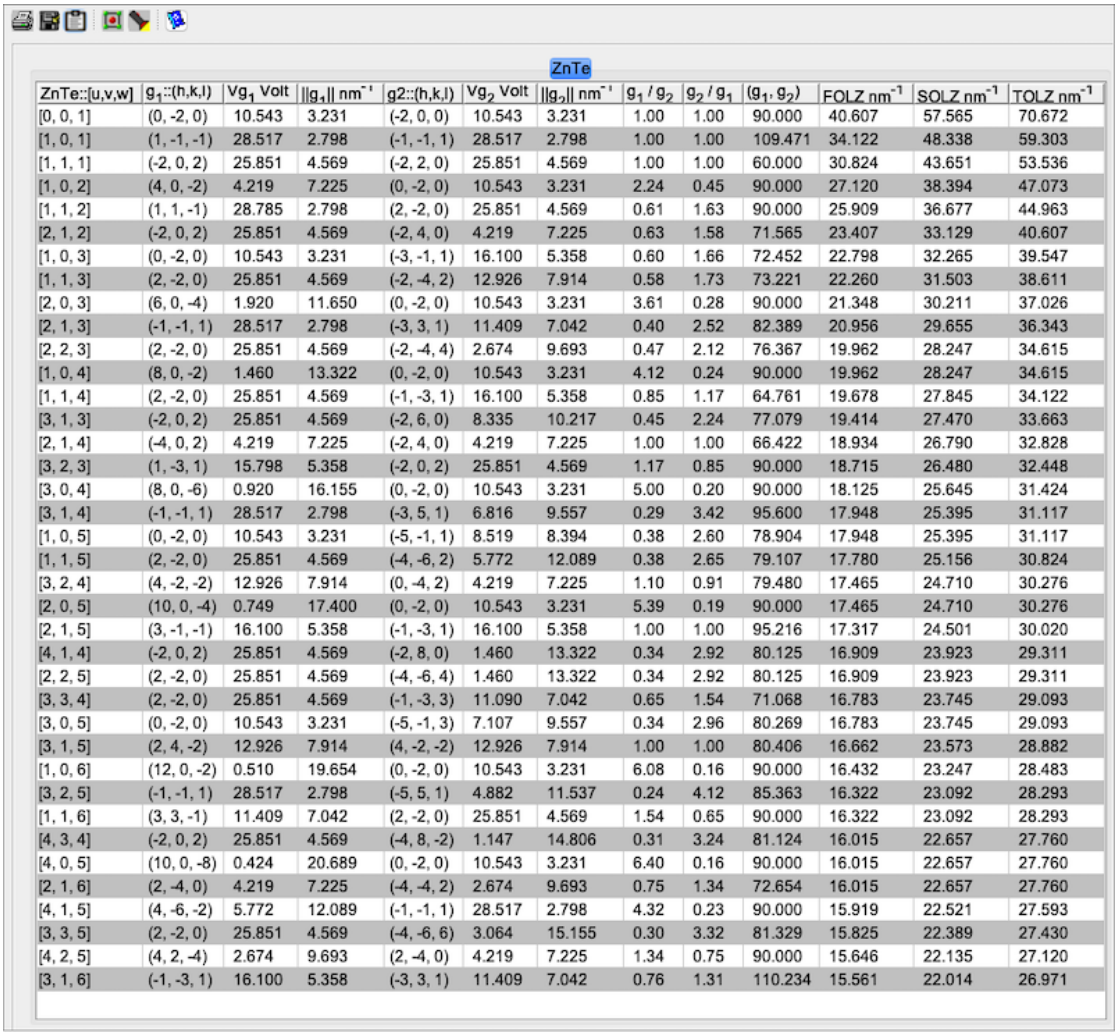
(a) Electron powder pattern and popup menu to switch horizontal axis unit from degree to nm^{-1}.



(b) X-Ray powder pattern with indexed reflections and nm^{-1} unit (Co $K_\alpha 1$ source).

Figure 118: Electron and X-Ray powder patterns.

20 Zone axis geometry frame



ZnTe

ZnTe::[u,v,w]	g_1::(h,k,l)	Vg_1 Volt	$\|\|g_1\|\|$ nm^{-1}	g2::(h,k,l)	Vg_2 Volt	$\|\|g_2\|\|$ nm^{-1}	g_1 / g_2	g_2 / g_1	(g_1, g_2)	FOLZ nm^{-1}	SOLZ nm^{-1}	TOLZ nm^{-1}
[0, 0, 1]	(0, -2, 0)	10.543	3.231	(-2, 0, 0)	10.543	3.231	1.00	1.00	90.000	40.607	57.565	70.672
[1, 0, 1]	(1, -1, -1)	28.517	2.798	(-1, -1, 1)	28.517	2.798	1.00	1.00	109.471	34.122	48.338	59.303
[1, 1, 1]	(-2, 0, 2)	25.851	4.569	(-2, 2, 0)	25.851	4.569	1.00	1.00	60.000	30.824	43.651	53.536
[1, 0, 2]	(4, 0, -2)	4.219	7.225	(0, -2, 0)	10.543	3.231	2.24	0.45	90.000	27.120	38.394	47.073
[1, 1, 2]	(1, 1, -1)	28.785	2.798	(2, -2, 0)	25.851	4.569	0.61	1.63	90.000	25.909	36.677	44.963
[2, 1, 2]	(-2, 0, 2)	25.851	4.569	(-2, 4, 0)	4.219	7.225	0.63	1.58	71.565	23.407	33.129	40.607
[1, 0, 3]	(0, -2, 0)	10.543	3.231	(-3, -1, 1)	16.100	5.358	0.60	1.66	72.452	22.798	32.265	39.547
[1, 1, 3]	(2, -2, 0)	25.851	4.569	(-2, -4, 2)	12.926	7.914	0.58	1.73	73.221	22.260	31.503	38.611
[2, 0, 3]	(6, 0, -4)	1.920	11.650	(0, -2, 0)	10.543	3.231	3.61	0.28	90.000	21.348	30.211	37.026
[2, 1, 3]	(-1, -1, 1)	28.517	2.798	(-3, 3, 1)	11.409	7.042	0.40	2.52	82.389	20.956	29.655	36.343
[2, 2, 3]	(2, -2, 0)	25.851	4.569	(-2, -4, 4)	2.674	9.693	0.47	2.12	76.367	19.962	28.247	34.615
[1, 0, 4]	(8, 0, -2)	1.460	13.322	(0, -2, 0)	10.543	3.231	4.12	0.24	90.000	19.962	28.247	34.615
[1, 1, 4]	(2, -2, 0)	25.851	4.569	(-1, -3, 1)	16.100	5.358	0.85	1.17	64.761	19.678	27.845	34.122
[3, 1, 3]	(-2, 0, 2)	25.851	4.569	(-2, 6, 0)	8.335	10.217	0.45	2.24	77.079	19.414	27.470	33.663
[2, 1, 4]	(-4, 0, 2)	4.219	7.225	(-2, 4, 0)	4.219	7.225	1.00	1.00	66.422	18.934	26.790	32.828
[3, 2, 3]	(1, -3, 1)	15.798	5.358	(-2, 0, 2)	25.851	4.569	1.17	0.85	90.000	18.715	26.480	32.448
[3, 0, 4]	(8, 0, -6)	0.920	16.155	(0, -2, 0)	10.543	3.231	5.00	0.20	90.000	18.125	25.645	31.424
[3, 1, 4]	(-1, -1, 1)	28.517	2.798	(-3, 5, 1)	6.816	9.557	0.29	3.42	95.600	17.948	25.395	31.117
[1, 0, 5]	(0, -2, 0)	10.543	3.231	(-5, -1, 1)	8.519	8.394	0.38	2.60	78.904	17.948	25.395	31.117
[1, 1, 5]	(2, -2, 0)	25.851	4.569	(-4, -6, 2)	5.772	12.089	0.38	2.65	79.107	17.780	25.156	30.824
[3, 2, 4]	(4, -2, -2)	12.926	7.914	(0, -4, 2)	4.219	7.225	1.10	0.91	79.480	17.465	24.710	30.276
[2, 0, 5]	(10, 0, -4)	0.749	17.400	(0, -2, 0)	10.543	3.231	5.39	0.19	90.000	17.465	24.710	30.276
[2, 1, 5]	(3, -1, -1)	16.100	5.358	(-1, -3, 1)	16.100	5.358	1.00	1.00	95.216	17.317	24.501	30.020
[4, 1, 4]	(-2, 0, 2)	25.851	4.569	(-2, 8, 0)	1.460	13.322	0.34	2.92	80.125	16.909	23.923	29.311
[2, 2, 5]	(2, -2, 0)	25.851	4.569	(-4, -6, 4)	1.460	13.322	0.34	2.92	80.125	16.909	23.923	29.311
[3, 3, 4]	(2, -2, 0)	25.851	4.569	(-1, -3, 3)	11.090	7.042	0.65	1.54	71.068	16.783	23.745	29.093
[3, 0, 5]	(0, -2, 0)	10.543	3.231	(-5, -1, 3)	7.107	9.557	0.34	2.96	80.269	16.783	23.745	29.093
[3, 1, 5]	(2, 4, -2)	12.926	7.914	(4, -2, -2)	12.926	7.914	1.00	1.00	80.406	16.662	23.573	28.882
[1, 0, 6]	(12, 0, -2)	0.510	19.654	(0, -2, 0)	10.543	3.231	6.08	0.16	90.000	16.432	23.247	28.483
[3, 2, 5]	(-1, -1, 1)	28.517	2.798	(-5, 5, 1)	4.882	11.537	0.24	4.12	85.363	16.322	23.092	28.293
[1, 1, 6]	(3, 3, -1)	11.409	7.042	(2, -2, 0)	25.851	4.569	1.54	0.65	90.000	16.322	23.092	28.293
[4, 3, 4]	(-2, 0, 2)	25.851	4.569	(-4, 8, -2)	1.147	14.806	0.31	3.24	81.124	16.015	22.657	27.760
[4, 0, 5]	(10, 0, -8)	0.424	20.689	(0, -2, 0)	10.543	3.231	6.40	0.16	90.000	16.015	22.657	27.760
[2, 1, 6]	(2, -4, 0)	4.219	7.225	(-4, -4, 2)	2.674	9.693	0.75	1.34	72.654	16.015	22.657	27.760
[4, 1, 5]	(4, -6, -2)	5.772	12.089	(-1, -1, 1)	28.517	2.798	4.32	0.23	90.000	15.919	22.521	27.593
[3, 3, 5]	(2, -2, 0)	25.851	4.569	(-4, -6, 6)	3.064	15.155	0.30	3.32	81.329	15.825	22.389	27.430
[4, 2, 5]	(4, 2, -4)	2.674	9.693	(2, -4, 0)	4.219	7.225	1.34	0.75	90.000	15.646	22.135	27.120
[3, 1, 6]	(-1, -3, 1)	16.100	5.358	(-3, 3, 1)	11.409	7.042	0.76	1.31	110.234	15.561	22.014	26.971

Figure 119: Table of zone axis geometry for indexing SAED patterns.

20.1 Tool buttons

The tool buttons allow to:

- : print the zone axis table.
- : save the zone axis table.
- : transfer the frame to the clipboard.

-  : open another crystal and create and add a zone axis table.
-  : index a SAED pattern using the table(s).
-  : display a help file.

21 Transform unit cell dialogue

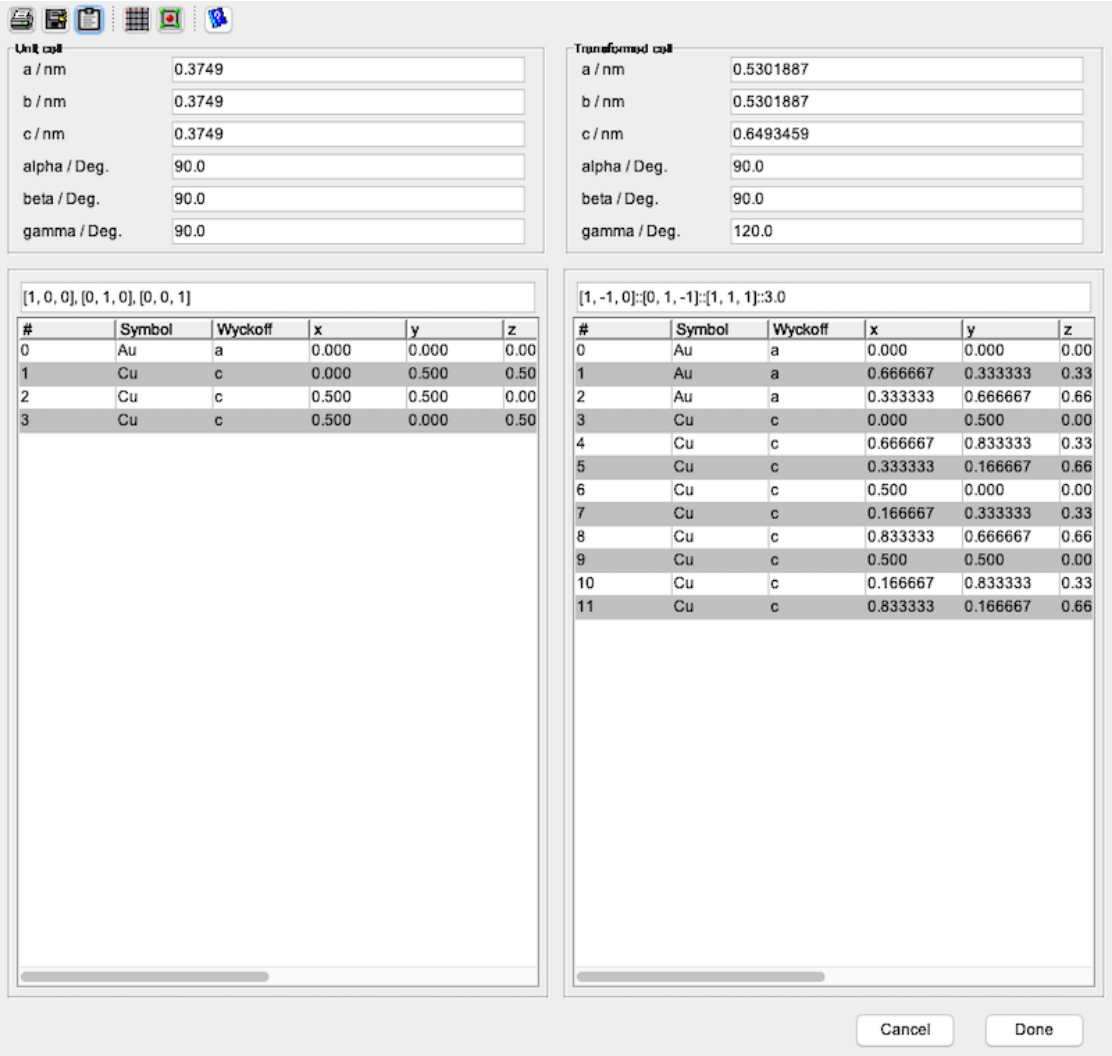


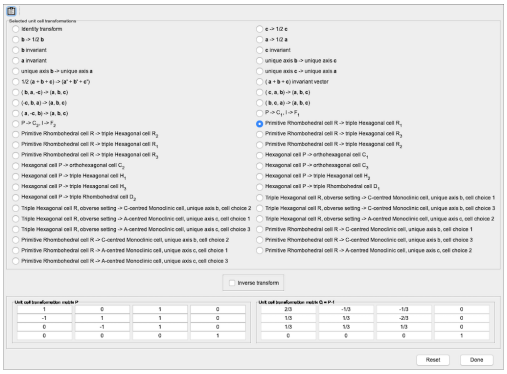
Figure 120: Transform unit cell dialogue.

21.1 Tool buttons

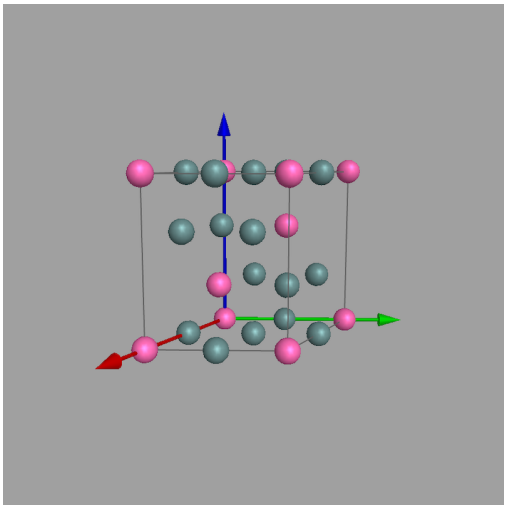
The tool buttons allow to:

- : print the dialogue.
- : save the dialogue image.
- : transfer the dialogue to the clipboard.

-  : select a unit cell transformation (Fig. 121a).
-  : show the transform unit cell (Fig. 121b).
-  : display a help file.



(a) Table of unit cell transforms.



(b) 3-D view of transformed unit cell.

Figure 121: $AuCu_3$ transformed unit cell.

22 Make orthogonal dialogue

The left table shows the unit cell parameters and atoms position of the original cell. The orthogonal cell parameters and atoms position are shown on the right table. The orthogonal cell $[0, 0, 1]$ direction is parallel to ZnTe $[1, 2, 1]$ direction, its $[1, 0, 0]$ and $[0, 1, 0]$ directions are parallel to the ZnTe $[1, -1, 1]$ and $[1, 0, -1]$ directions. Its volume is 6 times the volume of the ZnTe unit cell. The orthogonal cell can be pretty large depending on the *uvw* direction (Fig. 124) [34].

22.1 Tool buttons

The tool buttons allow to:

-  : print the frame.
-  : save the frame.
-  : transfer the frame to the clipboard.
-  : open the specimen dialogue (Fig. 84a).
-  : show the orthogonal unit cell (Fig. 123).
-  : display a help file.

[34] The lattice angles are still 90^o though they can be slightly lower depending on the original unit cell.

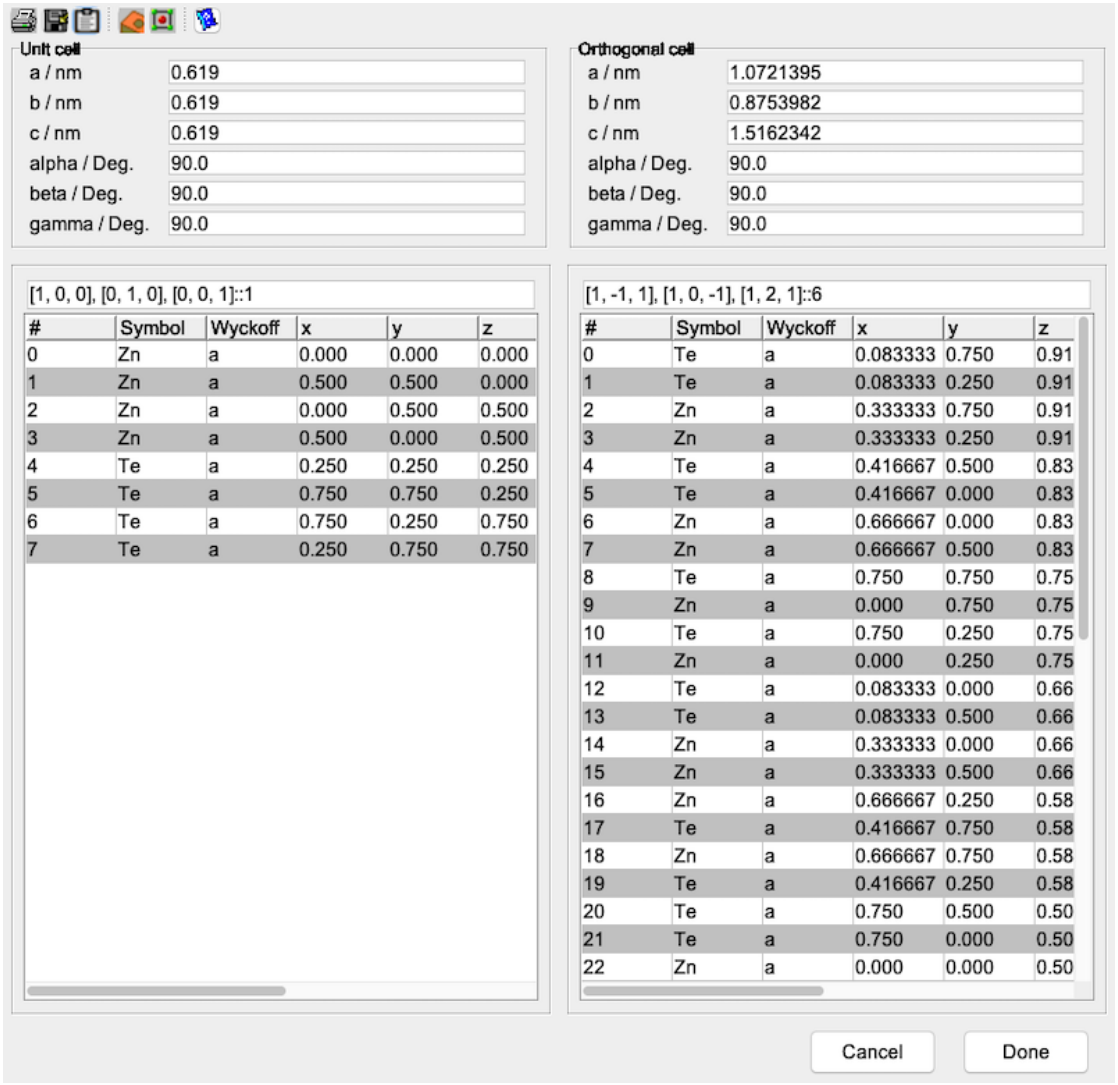


Figure 122: Dialogue to create orthogonal cells.

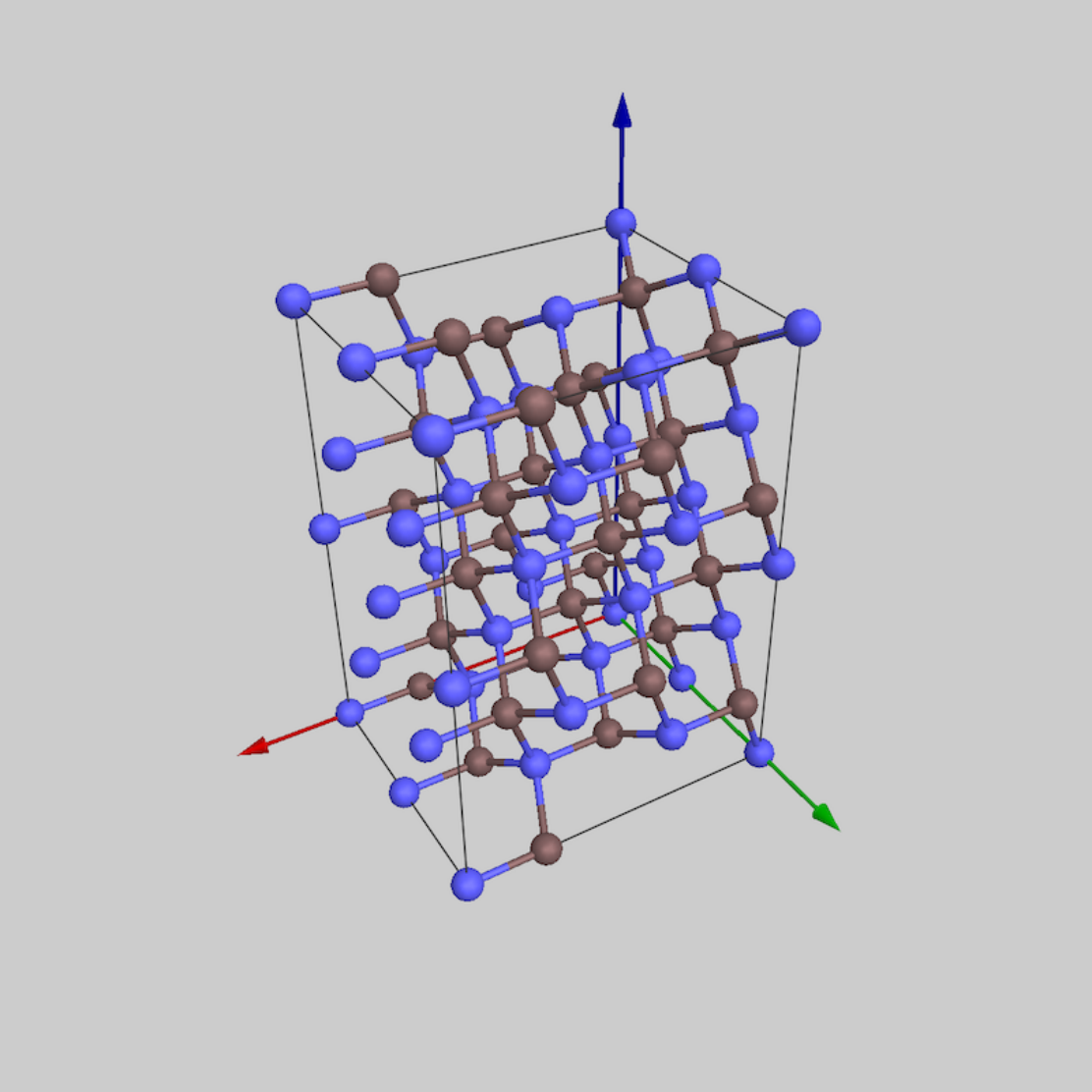


Figure 123: Orthogonal cell with $[0, 0, 1]$ parallel to ZnTe $[1, 2, 1]$ direction.

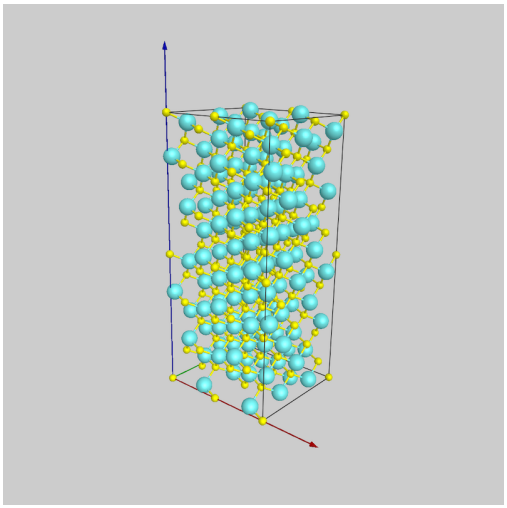
Orthogonal cell

a / nm	1.5162342
b / nm	1.3841261
c / nm	3.3904028
alpha / Deg.	90.0
beta / Deg.	90.0
gamma / Deg.	90.0

[2, -1, 1], [1, 0, -2], [2, 5, 1]::30

#	Symbol	Wyckoff	x	y	z
0	Te	a	0.666667	0.450	0.98
1	Te	a	0.166667	0.450	0.98
2	Zn	a	0.916667	0.700	0.98
3	Zn	a	0.416667	0.700	0.98
4	Te	a	0.083333	0.150	0.96
5	Te	a	0.583333	0.150	0.96
6	Zn	a	0.333333	0.400	0.96
7	Zn	a	0.833333	0.400	0.96
8	Te	a	0.500	0.850	0.95
9	Te	a	0.000	0.850	0.95
10	Zn	a	0.750	0.100	0.95
11	Zn	a	0.250	0.100	0.95
12	Te	a	0.416667	0.550	0.93
13	Te	a	0.916667	0.550	0.93
14	Zn	a	0.166667	0.800	0.93
15	Zn	a	0.666667	0.800	0.93
16	Zn	a	0.083333	0.500	0.91
17	Zn	a	0.583333	0.500	0.91
18	Te	a	0.333333	0.250	0.91
19	Te	a	0.833333	0.250	0.91
20	Te	a	0.250	0.950	0.90
21	Zn	a	0.000	0.200	0.90
22	Zn	a	0.500	0.200	0.90

(a) Orthogonal cell parameters and atoms position with $[0, 0, 1]$ parallel to ZnTe $[2, 5, 1]$ direction.



(b) Orthogonal cell 3-D view with $[0, 0, 1]$ parallel to ZnTe $[1, 2, 1]$ direction.

Figure 124: ZnTe $[2, 5, 1]$ orthogonal cell contains 240 atoms (8×30).

23 Image processing frame

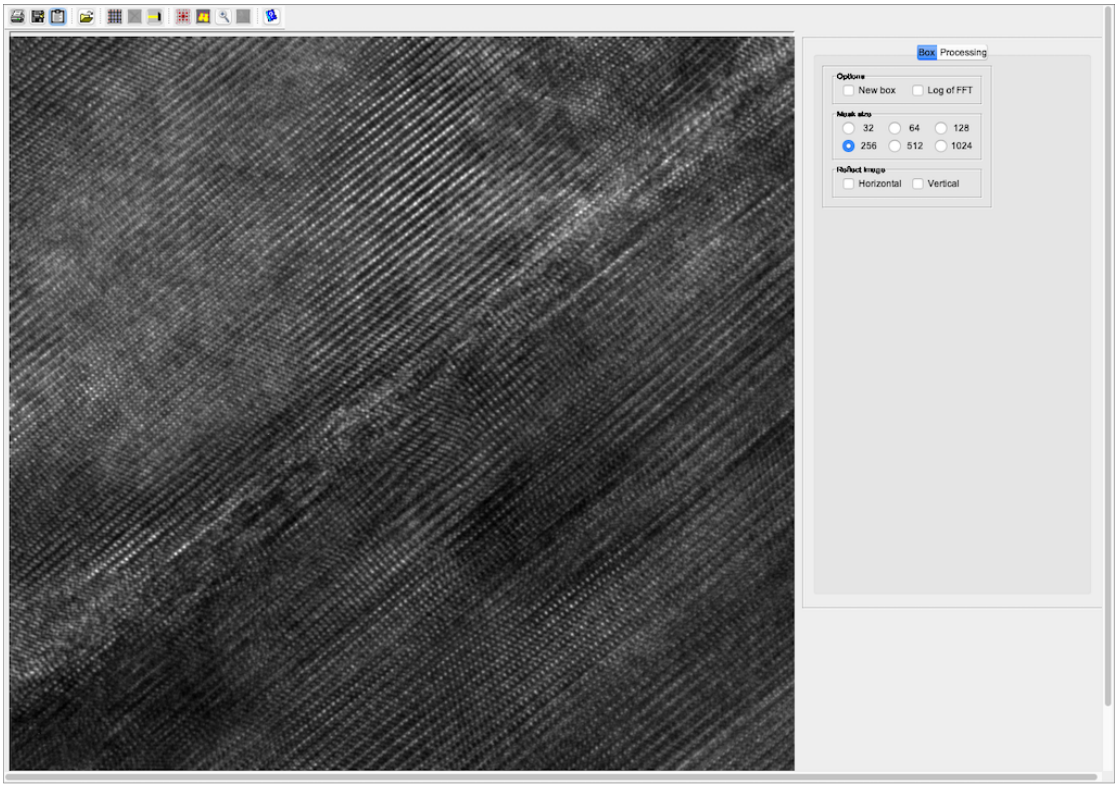


Figure 125: Image processing frame with experimental GaN HRTEM image loaded.

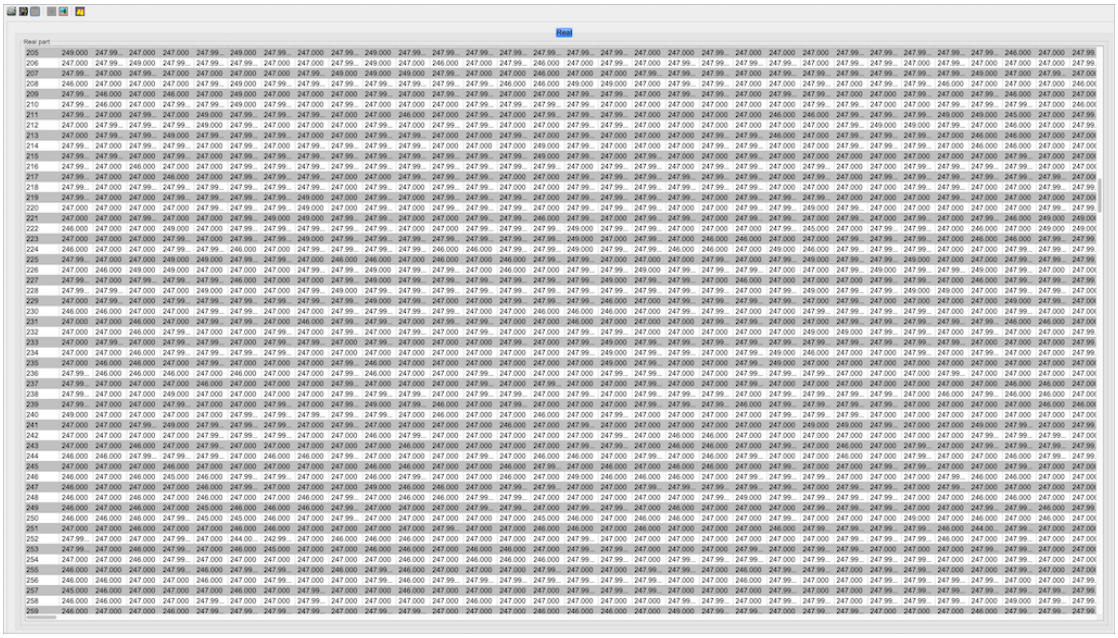
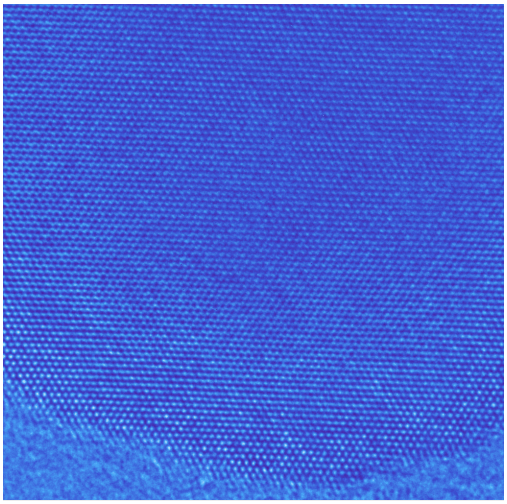


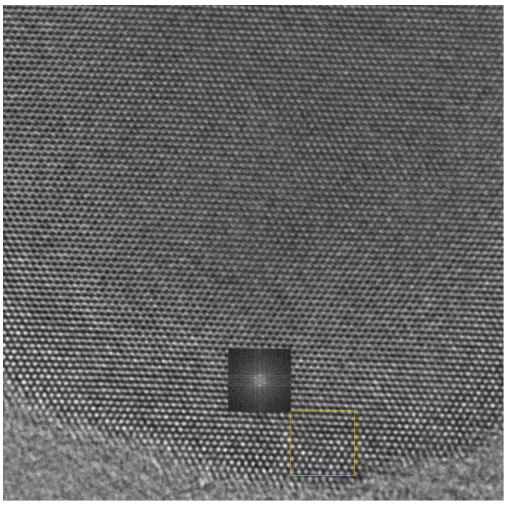
Figure 126: Table of image pixels.

Fig. 127 show a few examples of processing an experimental HRTEM image.

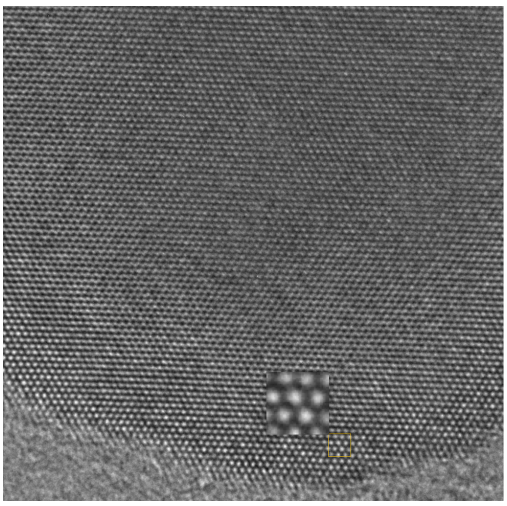


(a) Image processing frame after action **Colorize** .

(b) Image processing frame after action **Inverse** .



(c) Image processing local Fourier transform ( ).



(d) Image processing local magnifier (.)

Figure 127: Image processing of Si [100] HRTEM image (FEI CM-300).

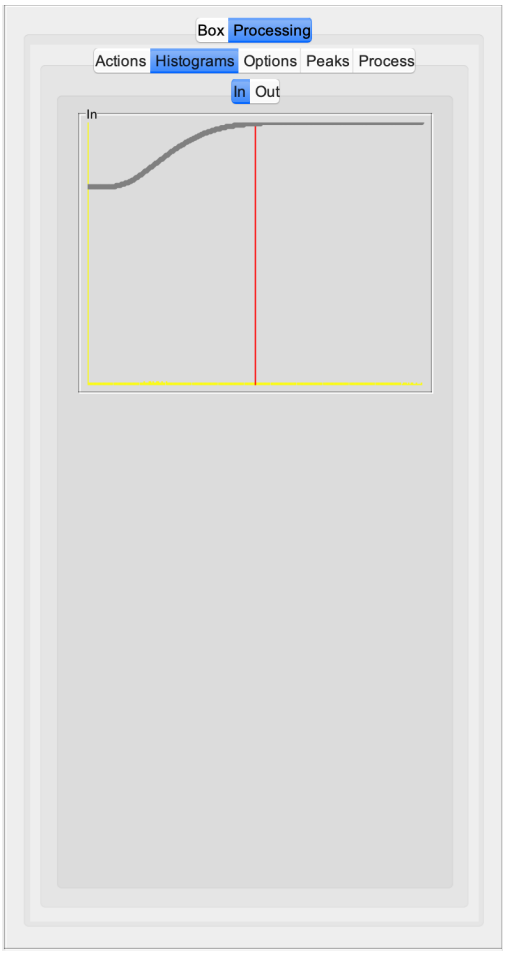
23.1 Tool buttons

The tool buttons allow to:

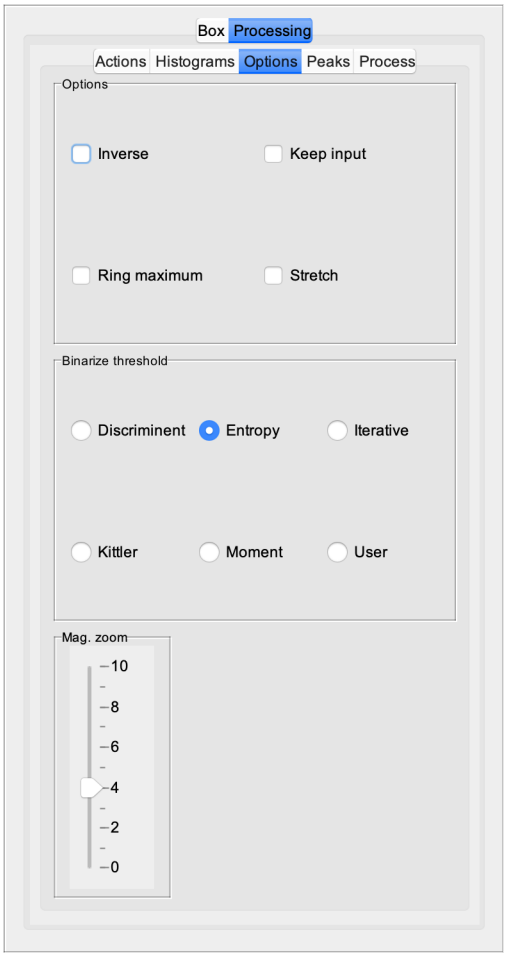
- : print the image.
- : save the image.

-  : transfer the frame to the clipboard.
-  : open an image.
-  : tabulate the image (Fig. 126).
-  : select and cut part of image.
-  : apply selected process (Fig. 129b).
-  : Fourier transform part of image.
-  : show 3-D view.
-  : magnify part of image.
-  : open the toolbox.
-  : display a help file.

23.2 Tabs

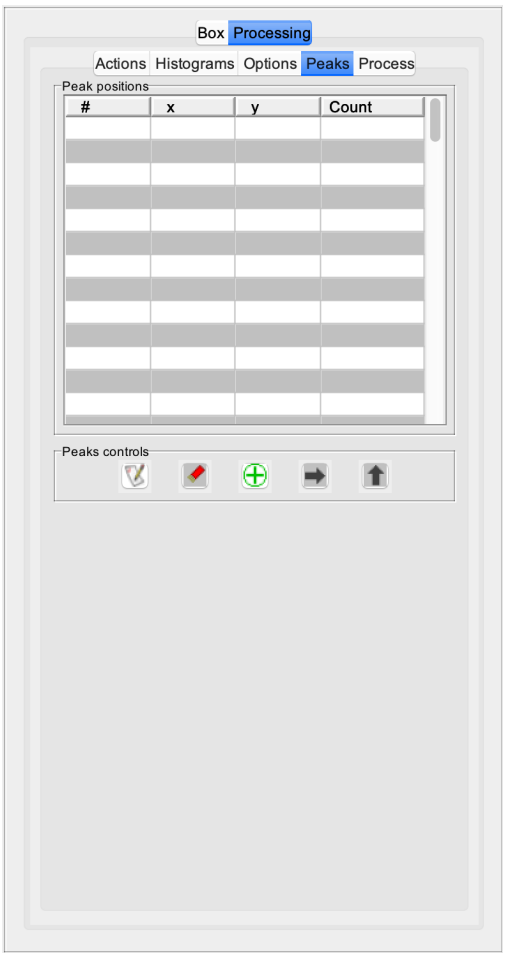


(a) Histograms tab that displays the image histogram before and after processing.

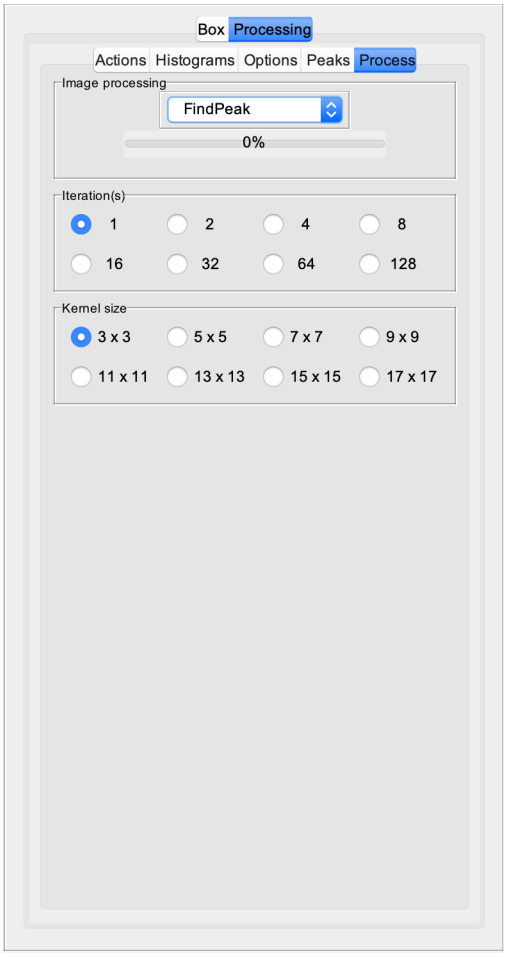


(b) Options tab that controls image contrast options and magnifier zoom.

Figure 128: Image processing tabs.



(a) Tab with image peaks position and label table.

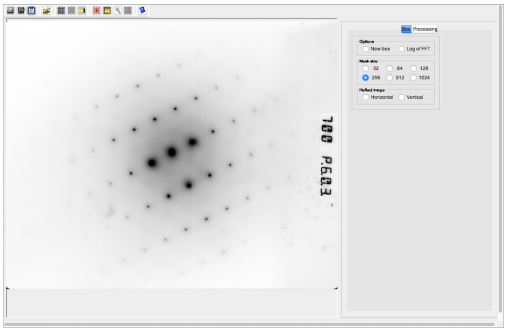


(b) Processing tab with a selection of processing kernel, number of iterations and kernel size.

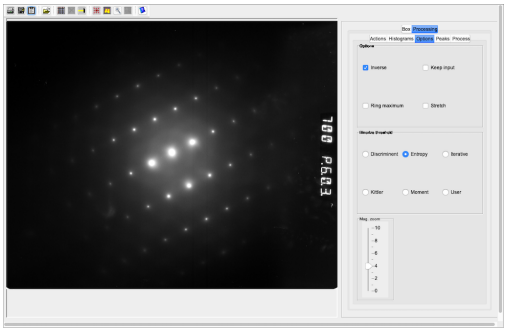
Figure 129: Image processing tabs.

23.3 Example

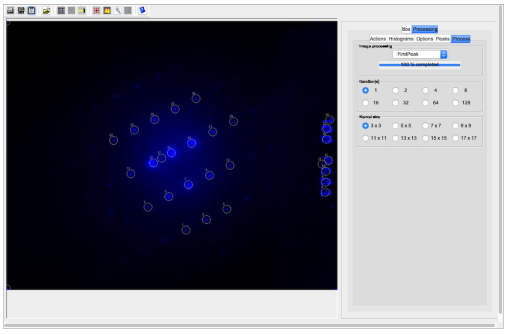
The image processing tab is available in several jems frame. It can be used to automatically identify the center of spots on diffraction patterns (Fig. 130).



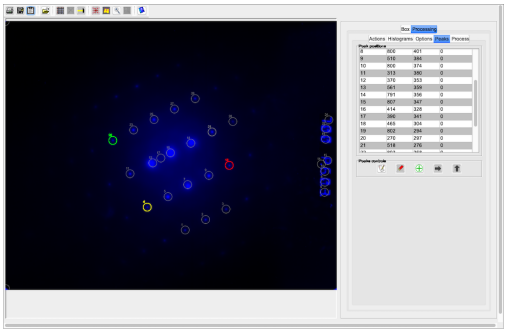
(a) GaN experimental siffraction pattern.



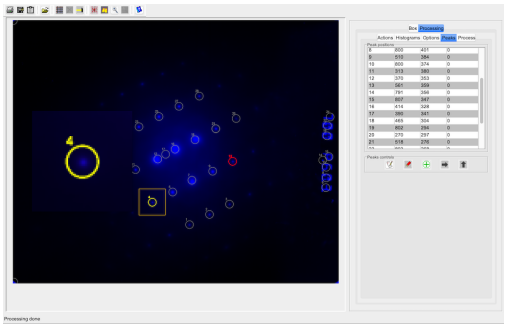
(b) Image contrast is inverted.



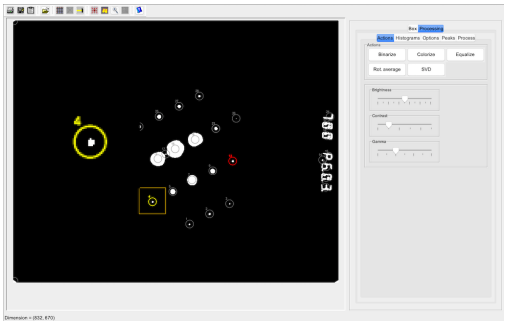
(c) Peaks are listed in the peaks table.



(d) Peaks are identified.



(e) The circle are centred on SAED spots (.)



(f) Binarizing the experimental image can help figure out where the spots are located.

Figure 130: Image processing to identify and list the diffraction spots.

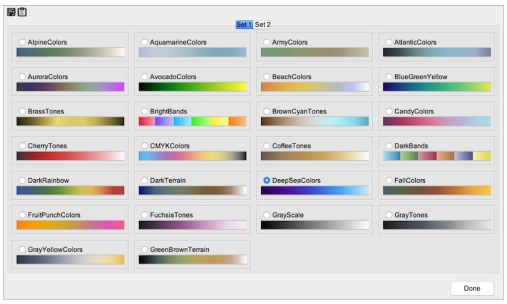
24 Colourise dialogue

The colourise dialogue offers 2 sets of color **L**ook**U**p **T**able (Fig. 131). The table contains 56 different LUTs including **TemperatureMap** and **ThermometerColors** (Figs. 131a, 131b).

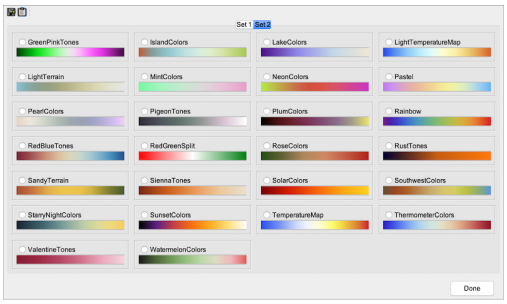
24.1 Tool buttons

The tool buttons allow to:

- : save the selected LUT set as an image.
- : transfer the dialogue to the clipboard.



(a) Color LUTs set 1.



(b) Color LUTs set 2.

Figure 131: Colourise dialogue.

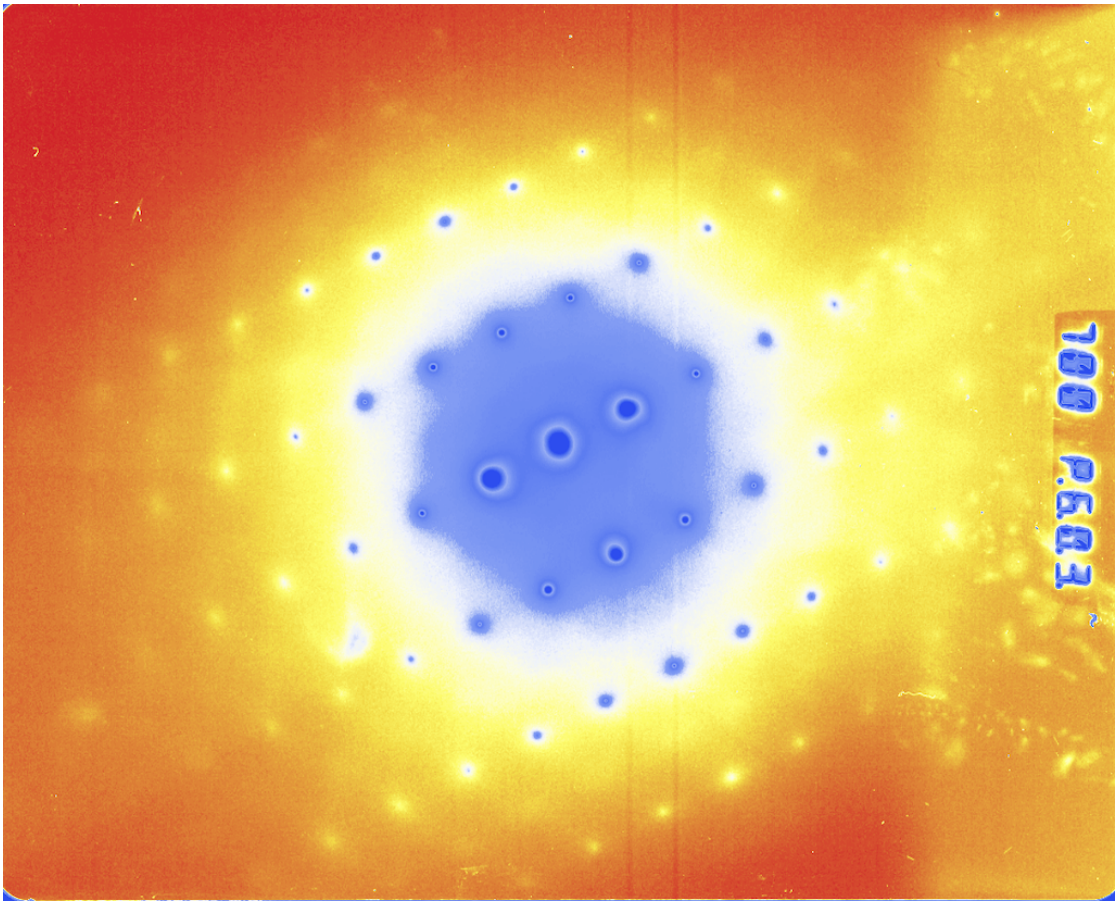


Figure 132: GaN SAED pattern with **TemperatureMap** LUT.

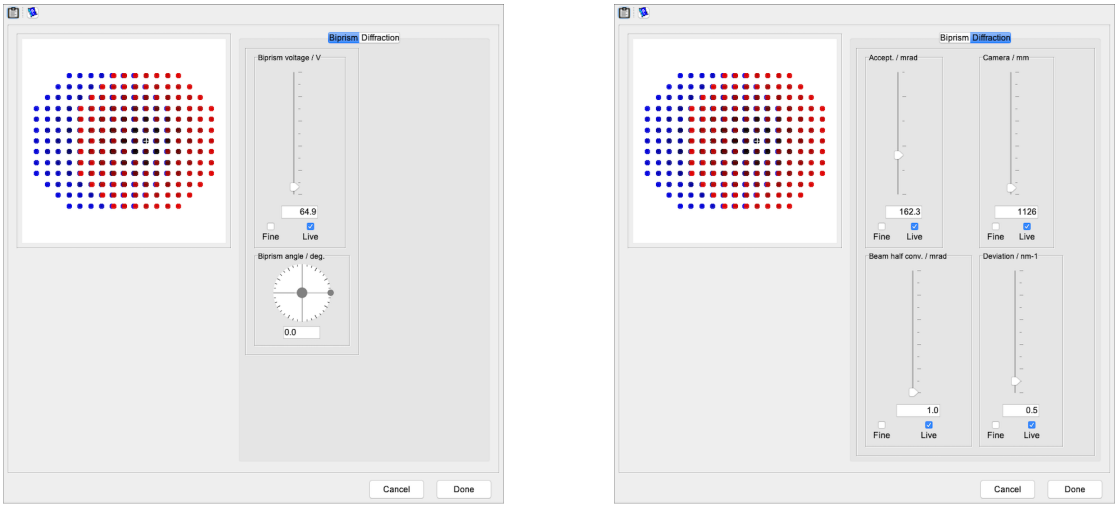
25 Holography dialogue

The holography dialogue allows to introduce in HRTEM image simulations the effect of a biprism (Fig. 133a).

25.1 Tool buttons

The tool buttons allow to:

- : transfer the dialogue to the clipboard.
- : open associated help file.

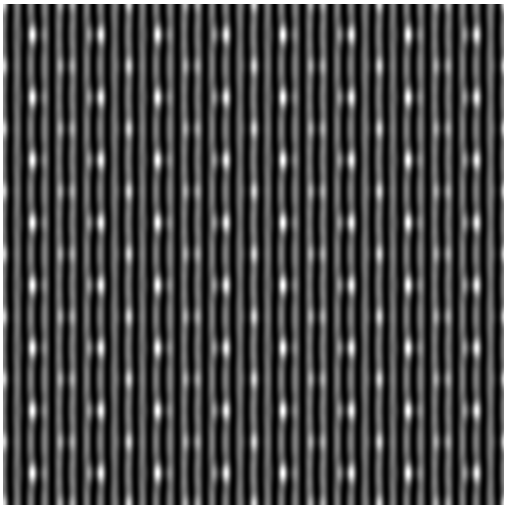


(a) Biprism settings.

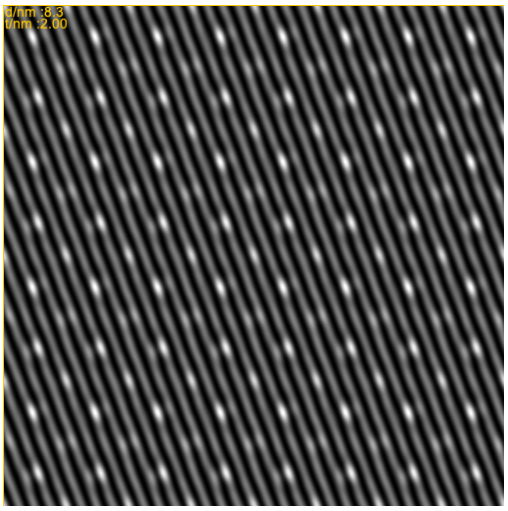
(b) Diffraction settings.

Figure 133: Holography dialogue allowing to change the biprism and diffraction settings.

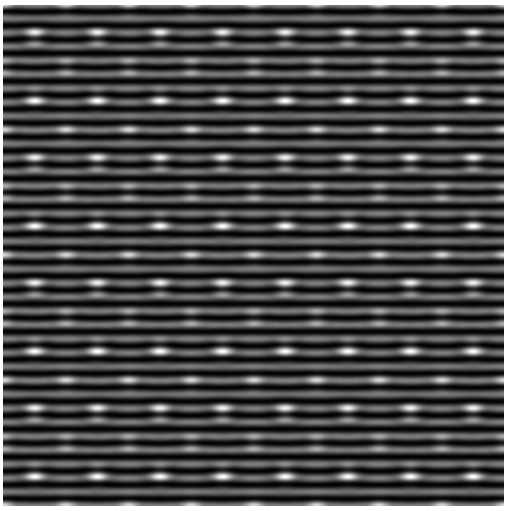
(a) ZnTe [001], no biprism.



(b) Biprism horizontal and voltage sets to some arbitrary value.



(c) Biprism rotated.



(d) Biprism rotated 90^o.

Figure 134: ZnTe HRTEM image simulations without and with some arbitrary biprism settings.

26 Electron powder pattern

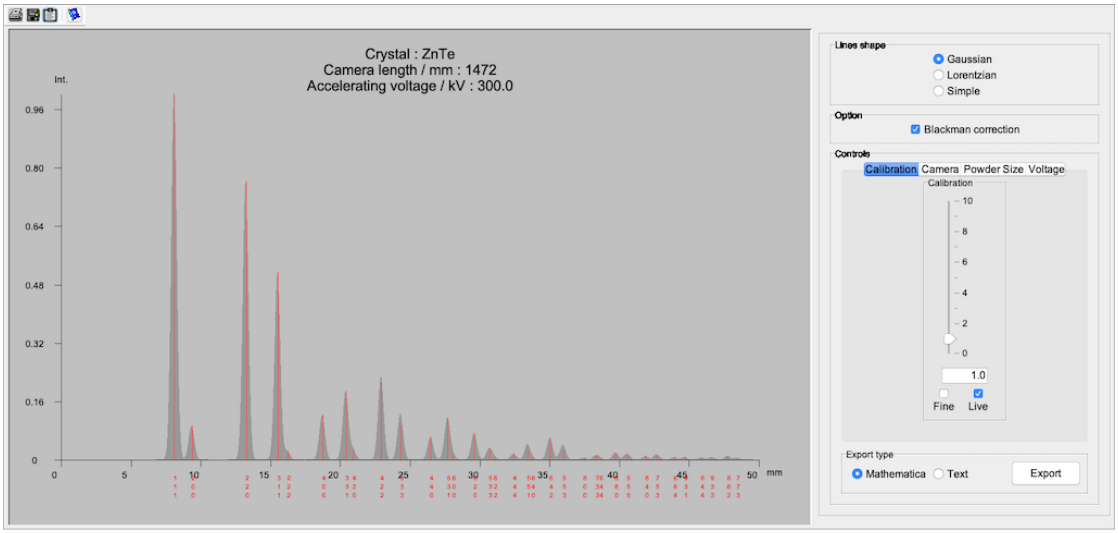


Figure 135: Table of ZnTe structure factors.

26.1 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the dialogue to the clipboard.
- : display a help file.

27 Rings pattern

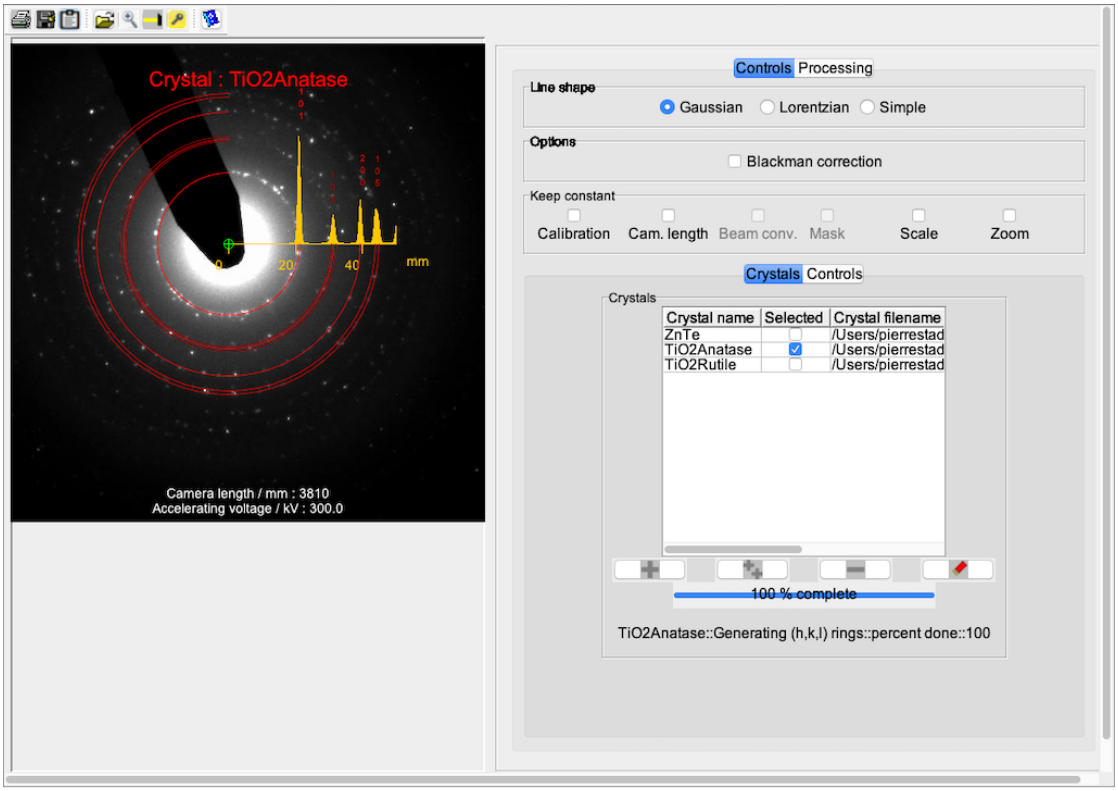


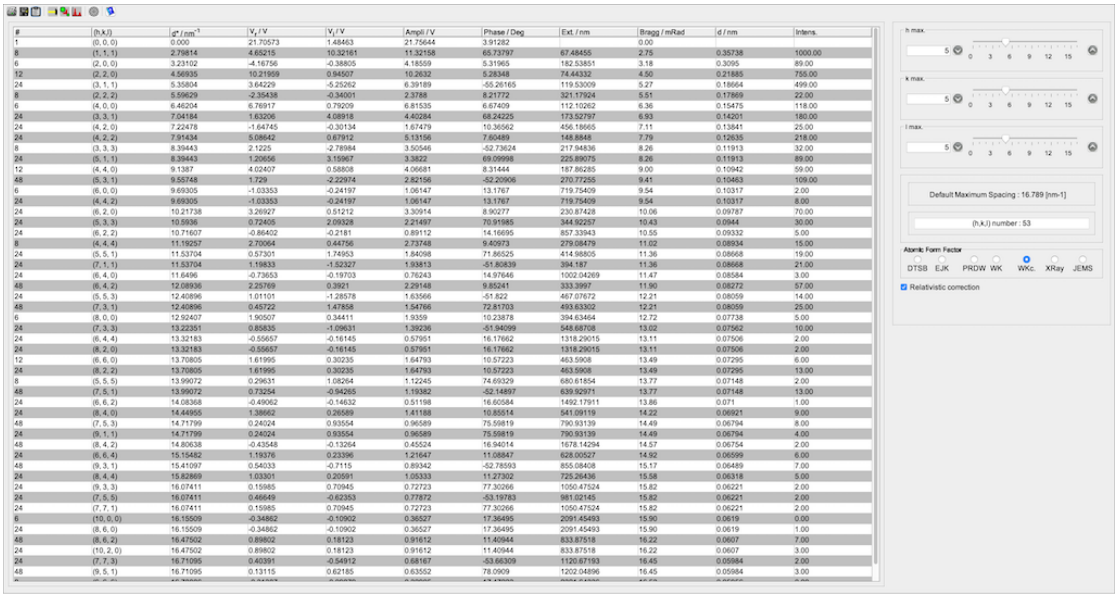
Figure 136: Table of ZnTe structure factors.

27.1 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the frame to the clipboard.
- : make a table with different maximum (hkl) indices.
- : reduce the table (Fig. 159).
- : display a powder pattern (Fig. 116).
- : display a ring pattern (Fig. 136).

-  : display a help file.



#	(h,k,l)	d^* / nm^{-1}	V_r / V	V_i / V	Ampli / V	Phase / Deg	Ext. / nm	Bragg / mRad	d / nm	Intens.
1	(0, 0, 0)	0.000	21.70573	1.48463	21.75644	3.91282		0.00		
8	(1, 1, 1)	2.79814	4.65215	10.32161	11.32158	65.73797	67.48455	2.75	0.35738	1000.00
6	(2, 0, 0)	3.23102	-4.16756	-0.38805	4.18559	5.31965	182.53851	3.18	0.3095	89.00
12	(2, 2, 0)	4.56935	10.21909	0.94507	10.2632	5.28348	74.44332	4.50	0.21885	755.00
24	(3, 1, 1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	499.00
8	(2, 2, 2)	5.59629	-2.35438	-0.34001	2.3788	8.21772	321.17924	5.51	0.17869	22.00
6	(4, 0, 0)	6.46204	6.76917	0.79209	6.81535	6.67409	112.10262	6.36	0.15475	118.00
24	(3, 3, 1)	7.04184	1.63206	4.08918	4.40284	68.24225	173.52797	6.93	0.14201	180.00
24	(4, 2, 0)	7.22478	-1.64745	-0.30134	1.67479	10.36562	456.18665	7.11	0.13841	25.00
24	(4, 2, 2)	7.91434	5.08642	0.67912	5.13156	7.60489	148.8848	7.79	0.12635	218.00
8	(3, 3, 3)	8.39443	2.1225	-2.78984	3.50546	-52.73624	217.94836	8.26	0.11913	32.00
24	(5, 1, 1)	8.39443	1.20656	3.11967	3.3822	69.09998	225.89075	8.26	0.11913	89.00
12	(4, 4, 0)	9.1387	4.02407	0.58808	4.06681	8.31444	187.86285	9.00	0.10942	59.00
48	(5, 3, 1)	9.55748	1.729	-2.22974	2.82156	-52.20906	270.77255	9.41	0.10463	109.00
6	(6, 0, 0)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	2.00
24	(4, 4, 2)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	8.00
24	(6, 2, 0)	10.21738	3.26927	0.51212	3.30914	8.90277	230.87428	10.06	0.09787	70.00
24	(5, 3, 3)	10.5936	0.72405	2.09328	2.21497	70.91985	344.92257	10.43	0.0944	30.00
24	(6, 2, 2)	10.71607	-0.86402	-0.2181	0.89112	14.16695	857.33943	10.55	0.09332	5.00
8	(4, 4, 4)	11.19257	2.70064	0.44756	2.73748	9.40973	279.08479	11.02	0.08934	15.00
24	(5, 5, 1)	11.53704	0.57301	1.74953	1.84098	71.86525	414.98805	11.36	0.08668	19.00
24	(7, 1, 1)	11.53704	1.19833	-1.52327	1.93813	-51.80839	394.187	11.36	0.08668	21.00
24	(6, 4, 0)	11.6496	-0.73653	-0.19703	0.76243	14.97646	1002.04269	11.47	0.08584	3.00
48	(6, 4, 2)	12.08936	2.25769	0.3921	2.29148	9.86241	333.3997	11.90	0.08272	57.00
24	(5, 5, 3)	12.40896	1.01101	-1.28578	1.63566	-51.822	467.07672	12.21	0.08059	14.00
48	(7, 3, 1)	12.40896	0.45722	1.47858	1.54766	72.81703	493.63302	12.21	0.08059	25.00
6	(8, 0, 0)	12.92407	1.90507	0.34411	1.9359	10.23878	394.63464	12.72	0.07738	5.00
24	(7, 3, 3)	13.22391	0.85835	-1.09631	1.39236	-51.94099	548.68708	13.02	0.07562	10.00
24	(6, 4, 4)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00
24	(8, 2, 0)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00
12	(6, 6, 0)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	6.00
24	(8, 2, 2)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	13.00
8	(5, 5, 5)	13.99072	0.29631	1.08264	1.12245	74.69329	680.61854	13.77	0.07148	2.00
48	(7, 5, 1)	13.99072	0.73254	-0.94265	1.19382	-52.14897	639.92971	13.77	0.07148	13.00
24	(6, 6, 2)	14.08368	-0.49062	-0.14632	0.51198	16.60584	1492.17911	13.86	0.071	1.00
24	(8, 4, 0)	14.44955	1.38662	0.26589	1.41188	10.85514	541.09119	14.22	0.06921	9.00
48	(7, 5, 3)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	8.00
24	(9, 1, 1)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	4.00
48	(8, 4, 2)	14.80638	-0.43548	-0.13264	0.45524	16.94014	1678.14294	14.57	0.06754	2.00
24	(6, 6, 4)	15.15482	1.19376	0.23396	1.21647	11.08847	628.00527	14.92	0.06599	6.00
48	(9, 3, 1)	15.41097	0.54033	-0.7115	0.89342	-52.78593	855.08408	15.17	0.06489	7.00
24	(8, 4, 4)	15.82869	1.03301	0.20591	1.05333	11.27302	725.26436	15.58	0.06318	5.00
24	(9, 3, 3)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00
24	(7, 5, 5)	16.07411	0.46649	-0.62353	0.77872	-53.19783	981.02145	15.82	0.06221	2.00
24	(7, 7, 1)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00
6	(10, 0, 0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	0.00
24	(8, 6, 0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	1.00
48	(8, 6, 2)	16.47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	7.00
24	(10, 2, 0)	16.47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	3.00
24	(7, 7, 3)	16.71095	0.40391	-0.54912	0.68167	-53.66309	1120.67193	16.45	0.05984	2.00
48	(9, 5, 1)	16.71095	0.13115	0.62185	0.63552	78.0909	1202.04896	16.45	0.05984	3.00

Figure 137: Table of non-equivalent ZnTe structure factors and their multiplicity.

28 Atomic Form Factor

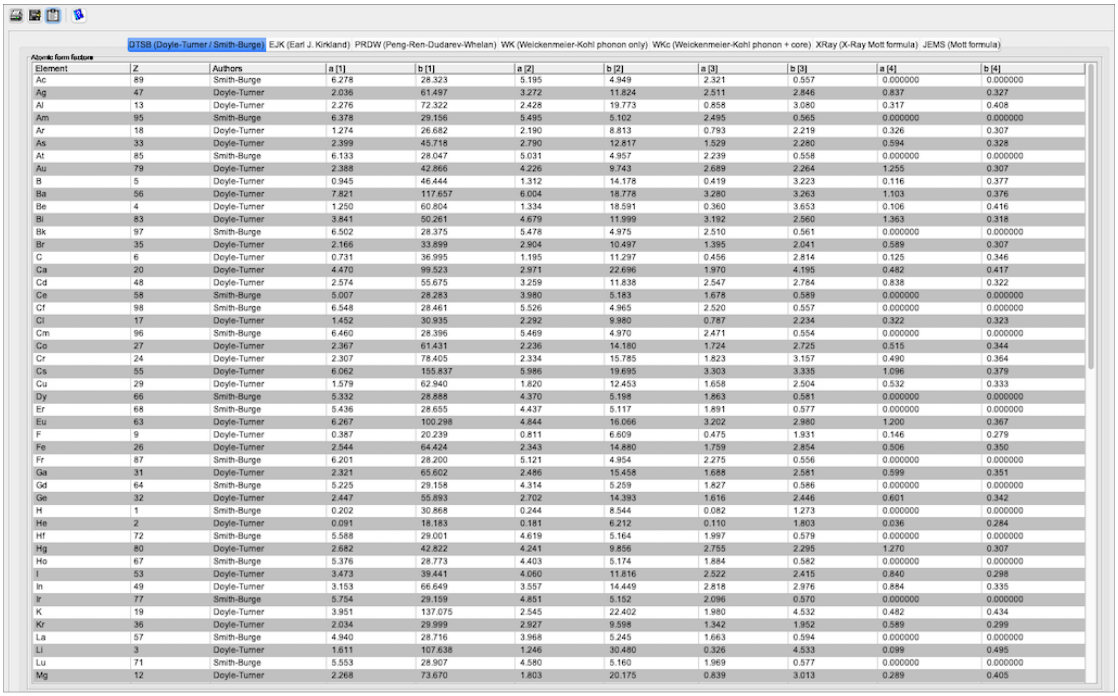
The **A**tomic **F**orm **F**actors (or electron scattering factors) are collected in tables referred by the authors of the tabulation (Fig. **??**). The AFF tabulations use different approximations. For simple qualitative calculations the Doyle-Turner/Smith-Burge tabulation is good and pretty equivalent to the others up to element atomic number 40-42. The best tabulations have been provided by Weickenmeier-Kohl since the absorption potential includes the calculation of **T**hermal **D**iffuse **S**cattering within the Einstein approximation (un-correlated atoms vibration).

The source of the AFF's are provided by the following references:

- **DTSB** : P. A. Doyle and P. S. Turner, Acta Cryst. **A**24 (1968) 390-397 (**DT**) or G. H. Smith and R. E. Burge, Acta Cryst. 15 (1962) 182-186 (**SB**).
- **EJK** : Earl J. Kirkland, Advanced Computing in Electron Microscopy, Springer, 2013.
- **PRDW** : L.-M. Peng, G. Ren, S. L. Dudarev and M. J. Whelan, Acta Cryst. **A**52 (1996) 257-276.
- **WK** : A. Weickenmeier and H. Kohl, Acta Cryst. Acta Cryst. **A**47 (1991) 590-597.
- **WKc** : A. Weickenmeier and H. Kohl, Acta Cryst. Acta Cryst. **A**54 (1998) 283-289.
- **XRay** : D. T. Cromer and J. T. Waber, Acta Cryst.18 (1) (1965) 104-109.
- **JEMS** : from D. T. Cromer and J. T. Waber, Acta Cryst. 18 (1) (1965) 104-109 (user modifiable).

Acurrate AFFs are necessary to compute the **A**tomic **S**cattering **A**mplitude as a function of the reduced scattering angle ($\frac{\sin\theta}{\lambda}$). A detailed comparison as well as a new parametrisation of the electron scattering factors has been provided recently by I. Lobato and D. Van Dyck[35]. These authors conclude that their new tabulation is an order of magnitude better than the previous ones. This tabulation is not yet introduced in jems.

[35] I. Lobato and D. Van Dyck, Acta Cryst. **A**70 (2014) 636-649.



Element	Z	Authors	a [1]	b [1]	a [2]	b [2]	a [3]	b [3]	a [4]	b [4]
Ac	89	Smith-Bunge	6.278	28.323	5.195	4.949	2.321	0.557	0.000000	0.000000
Ag	47	Doyle-Turner	2.036	61.497	3.272	11.824	2.511	2.846	0.837	0.327
Al	13	Doyle-Turner	2.276	72.322	2.428	19.773	0.858	3.080	0.317	0.408
Am	95	Smith-Bunge	6.378	29.156	5.495	5.102	2.495	0.565	0.000000	0.000000
Ar	18	Doyle-Turner	1.274	26.682	2.190	8.813	0.793	2.219	0.326	0.307
As	33	Doyle-Turner	2.399	45.718	2.790	12.817	1.529	2.260	0.594	0.328
At	85	Smith-Bunge	6.133	28.047	5.031	4.957	2.239	0.558	0.000000	0.000000
Au	79	Doyle-Turner	2.388	42.866	4.226	9.743	2.689	2.264	1.255	0.307
B	5	Doyle-Turner	0.945	46.444	1.312	14.178	0.419	3.223	0.116	0.377
Ba	56	Doyle-Turner	7.821	117.657	6.004	18.778	3.280	3.263	1.103	0.376
Be	4	Doyle-Turner	1.250	60.804	1.334	18.591	0.360	3.653	0.106	0.416
Bi	83	Doyle-Turner	3.841	50.261	4.679	11.999	3.192	2.560	1.363	0.318
Bk	97	Smith-Bunge	6.502	28.375	5.478	4.975	2.510	0.561	0.000000	0.000000
Br	35	Doyle-Turner	2.166	33.899	2.904	10.497	1.395	2.041	0.589	0.307
C	6	Doyle-Turner	0.731	36.995	1.195	11.297	0.456	2.814	0.125	0.346
Ca	20	Doyle-Turner	4.470	99.523	2.971	22.696	1.970	4.195	0.482	0.417
Cd	48	Doyle-Turner	2.574	55.675	3.259	11.838	2.547	2.784	0.838	0.322
Ce	58	Smith-Bunge	5.007	28.283	3.980	5.183	1.678	0.589	0.000000	0.000000
Cf	98	Smith-Bunge	6.548	28.461	5.526	4.965	2.520	0.557	0.000000	0.000000
Cl	17	Doyle-Turner	1.452	30.935	2.292	9.980	0.787	2.234	0.322	0.323
Cm	96	Smith-Bunge	6.460	28.396	5.469	4.970	2.471	0.554	0.000000	0.000000
Co	27	Doyle-Turner	2.367	61.431	2.236	14.180	1.724	2.725	0.515	0.344
Cr	24	Doyle-Turner	2.307	78.405	2.334	15.785	1.823	3.157	0.490	0.364
Cs	55	Doyle-Turner	6.062	155.837	5.986	19.695	3.303	3.335	1.096	0.379
Cu	29	Doyle-Turner	1.579	62.940	1.820	12.453	1.658	2.504	0.532	0.333
Dy	66	Smith-Bunge	5.332	28.888	4.370	5.198	1.863	0.581	0.000000	0.000000
Er	68	Smith-Bunge	5.436	28.655	4.437	5.117	1.891	0.577	0.000000	0.000000
Eu	63	Doyle-Turner	6.267	100.298	4.844	16.066	3.202	2.980	1.200	0.367
F	9	Doyle-Turner	0.387	20.239	0.811	6.609	0.475	1.931	0.146	0.279
Fe	26	Doyle-Turner	2.544	64.424	2.343	14.880	1.759	2.854	0.506	0.350
Fr	87	Smith-Bunge	6.201	28.200	5.121	4.954	2.275	0.556	0.000000	0.000000
Ga	31	Doyle-Turner	2.321	65.602	2.486	15.458	1.688	2.581	0.599	0.351
Gd	64	Smith-Bunge	5.225	29.158	4.314	5.259	1.827	0.586	0.000000	0.000000
Ge	32	Doyle-Turner	2.447	55.893	2.702	14.393	1.616	2.446	0.601	0.342
H	1	Smith-Bunge	0.202	30.868	0.244	8.544	0.082	1.273	0.000000	0.000000
He	2	Doyle-Turner	0.091	18.183	0.181	6.212	0.110	1.803	0.036	0.284
Hf	72	Smith-Bunge	5.588	29.001	4.619	5.164	1.997	0.579	0.000000	0.000000
Hg	80	Doyle-Turner	2.682	42.822	4.241	9.856	2.755	2.295	1.270	0.307
Ho	67	Smith-Bunge	5.376	28.773	4.403	5.174	1.884	0.582	0.000000	0.000000
I	53	Doyle-Turner	3.473	39.441	4.060	11.816	2.522	2.415	0.840	0.298
In	49	Doyle-Turner	3.153	66.649	3.557	14.449	2.818	2.976	0.884	0.335
Ir	77	Smith-Bunge	5.754	29.159	4.851	5.152	2.096	0.570	0.000000	0.000000
K	19	Doyle-Turner	3.951	137.075	2.545	22.402	1.980	4.532	0.482	0.434
Kr	36	Doyle-Turner	2.034	29.999	2.927	9.598	1.342	1.952	0.589	0.299
La	57	Smith-Bunge	4.940	28.716	3.968	5.245	1.663	0.594	0.000000	0.000000
Li	3	Doyle-Turner	1.611	107.638	1.246	30.480	0.326	4.533	0.099	0.495
Lu	71	Smith-Bunge	5.553	28.907	4.580	5.160	1.969	0.577	0.000000	0.000000
Mg	12	Doyle-Turner	2.268	73.670	1.803	20.175	0.839	3.013	0.289	0.405

Figure 138: Table of atomic form factors.

28.1 Tool buttons

The tool buttons allow to:

-  : print the table.
-  : save the table.
-  : transfer the dialogue to the clipboard.
-  : display a help file.

28.2 Popup menu

A **A**tomic **S**cattering **A**mplitude (ASA or **E**lectron **S**cattering **A**mplitude) plot shows the amplitude of the electron scattering as a function of the reduced scattering angle $\frac{\sin\theta}{\lambda}$ (independent of the electron wavelength). The ASA plot is created when any entry of the tables is selected (mouse click).

The popup menu attached to the ASA plots allows to:

- **Print** : print the AFF plot.
- **Save** : save the AFF plot.
- **Compare ASA's as Notebook** : create a Mathematica notebook that compares the AFF's of the different sources.
- **Log scale** : plot the AFF using a log scale.
- **Save ASA plot as Notebook** : save the ASA plot as a Mathematica notebook.
- **Save ASA table as Notebook** : save the ASA table as a Mathematica notebook at $\frac{\sin\theta}{\lambda} = 0$ (Fig. 140).
- **Scale x n** : set the ordinate scale of the plot.
- **Transfer to clipboard** : transfer the plot to the clipboard.

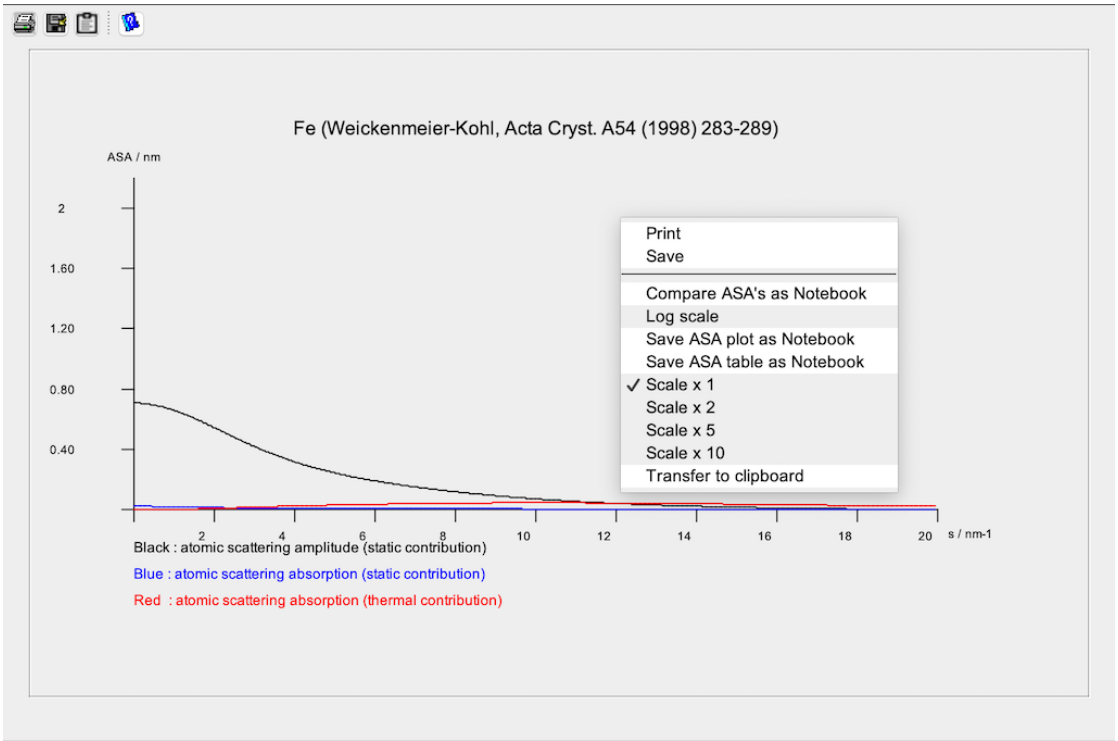
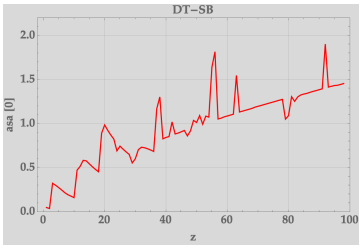
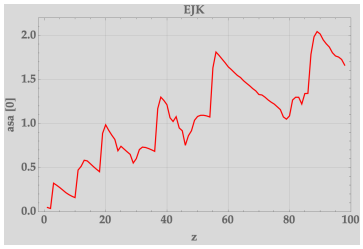


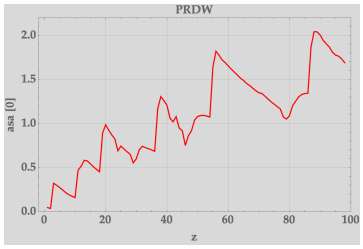
Figure 139: Fe atomic form factor (WKc) as a function of $\frac{\sin\theta}{\lambda} = 0$.



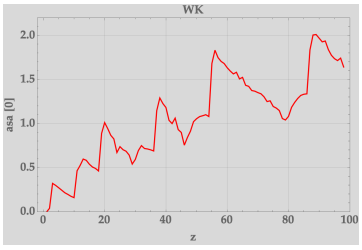
(a) Doyle-Turner and Smith-Burge atomic form factors.



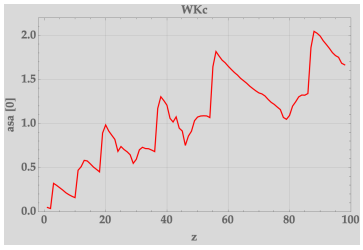
(b) Earl J. Kirkland atomic form factors.



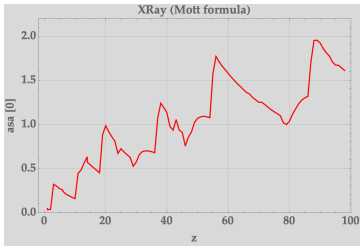
(c) Peng-Ren-Dudarev-Whelan atomic form factors.



(d) Weickenmeier-Kohl atomic form factors.



(e) Weickenmeier-Kohl (with core absorption) atomic form factors.



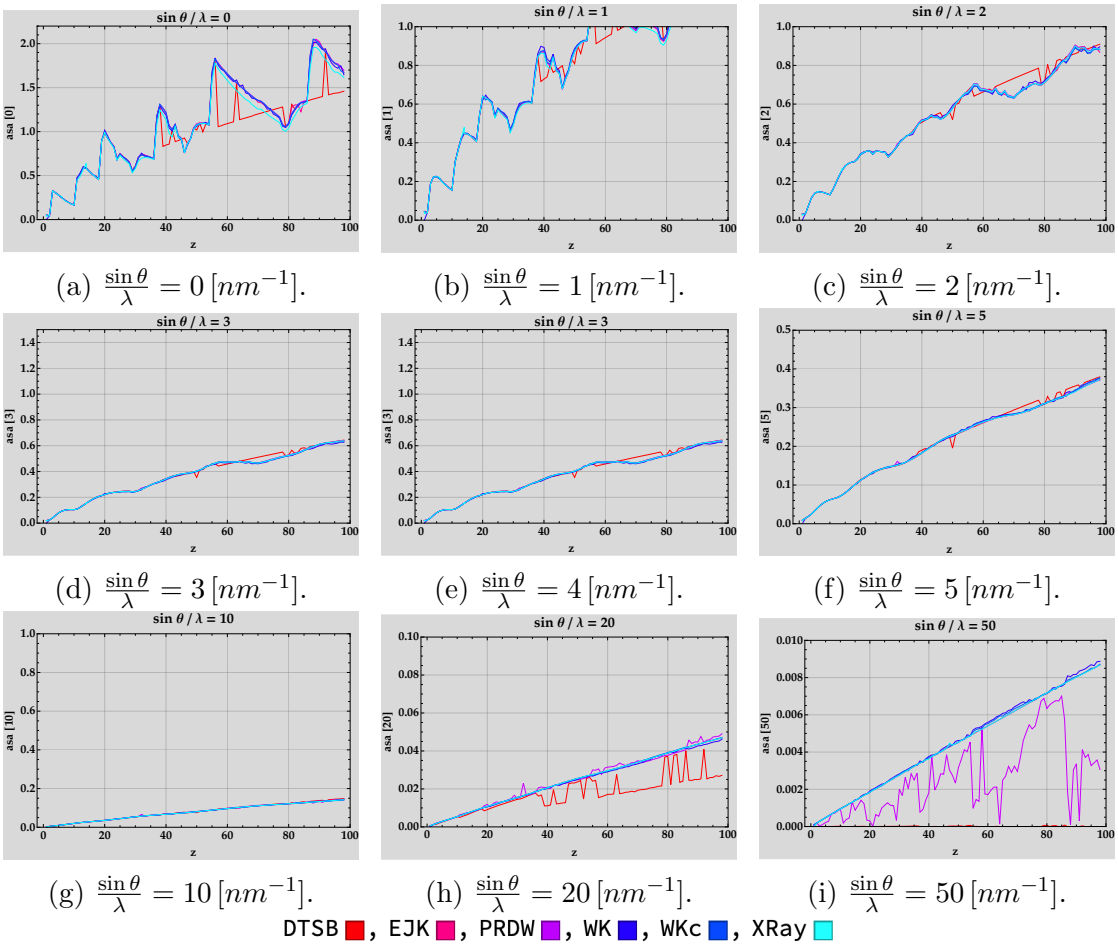
(f) X-Ray (Mott formula) atomic form factors.

(g) A particular AFF source is selected using these radio buttons.

Figure 140: Comparison of the **E**lectron **S**cattering **A**mplitudes of the different references at $\frac{\sin\theta}{\lambda} = 0$.

Fig. **??** compares the electron scattering amplitudes from the different references for selected $\frac{\sin\theta}{\lambda}$ values. It shows that the **EJK**, **WK**, **WKc** and **XRay** plots are pretty similar for all elements and the selected $\frac{\sin\theta}{\lambda}$ values.

Fig. 143 plots the scattering angle θ as a function of the reciprocal distance **s** for selected accelerating voltages.



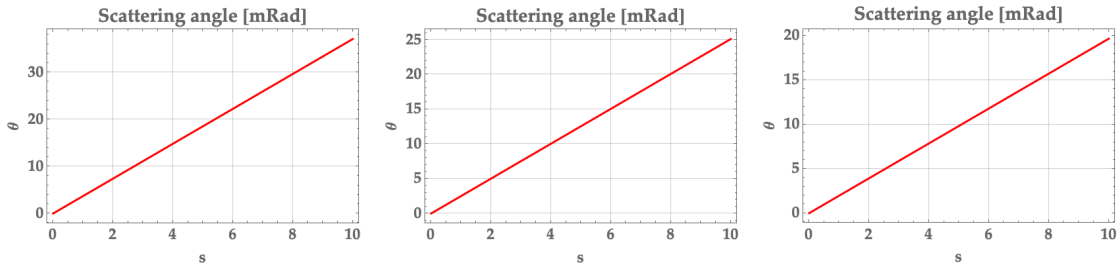
(a) $\frac{\sin\theta}{\lambda} = 0\,[nm^{-1}]$. (b) $\frac{\sin\theta}{\lambda} = 1\,[nm^{-1}]$. (c) $\frac{\sin\theta}{\lambda} = 2\,[nm^{-1}]$.

(d) $\frac{\sin\theta}{\lambda} = 3\,[nm^{-1}]$. (e) $\frac{\sin\theta}{\lambda} = 4\,[nm^{-1}]$. (f) $\frac{\sin\theta}{\lambda} = 5\,[nm^{-1}]$.

(g) $\frac{\sin\theta}{\lambda} = 10\,[nm^{-1}]$. (h) $\frac{\sin\theta}{\lambda} = 20\,[nm^{-1}]$. (i) $\frac{\sin\theta}{\lambda} = 50\,[nm^{-1}]$.

Figure 141: AFF sources.

Figure 142: Comparison of the **E**lectron **S**cattering **A**mplitudes of the different references at selected $\frac{\sin\theta}{\lambda}$ values .



(a) 100 kV. (b) 200 kV. (c) 300 kV.

Figure 143: Scattering angle $[mRad]$ as a function of s $[nm^{-1}]$ for selected accelerating voltages $[kV]$. Note the factor 2 for the conversion nm^{-1} to mRad.

29 Structure factors dialogue

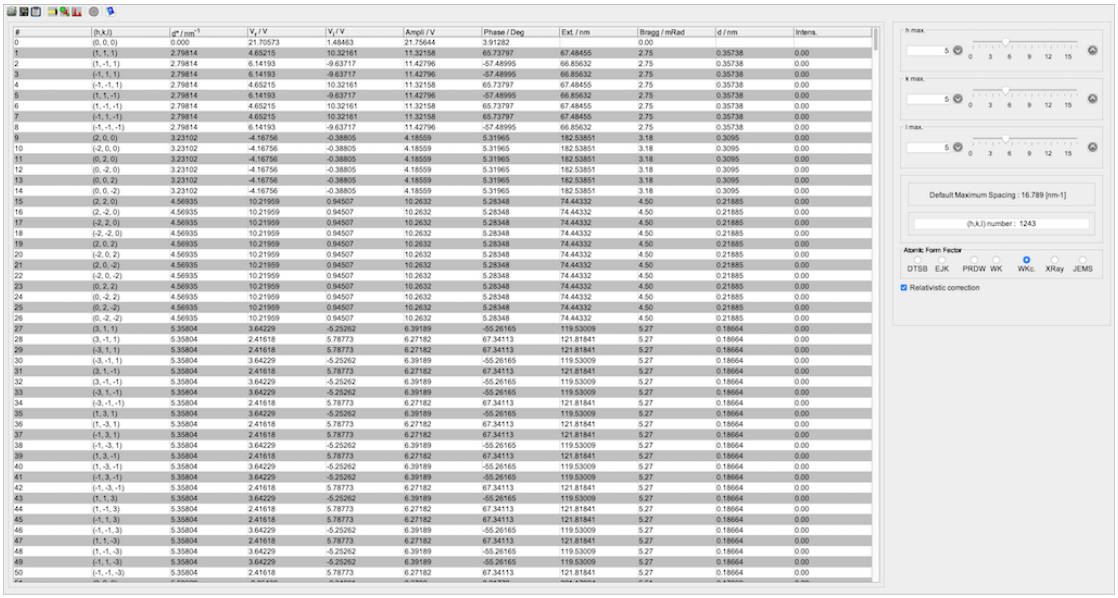
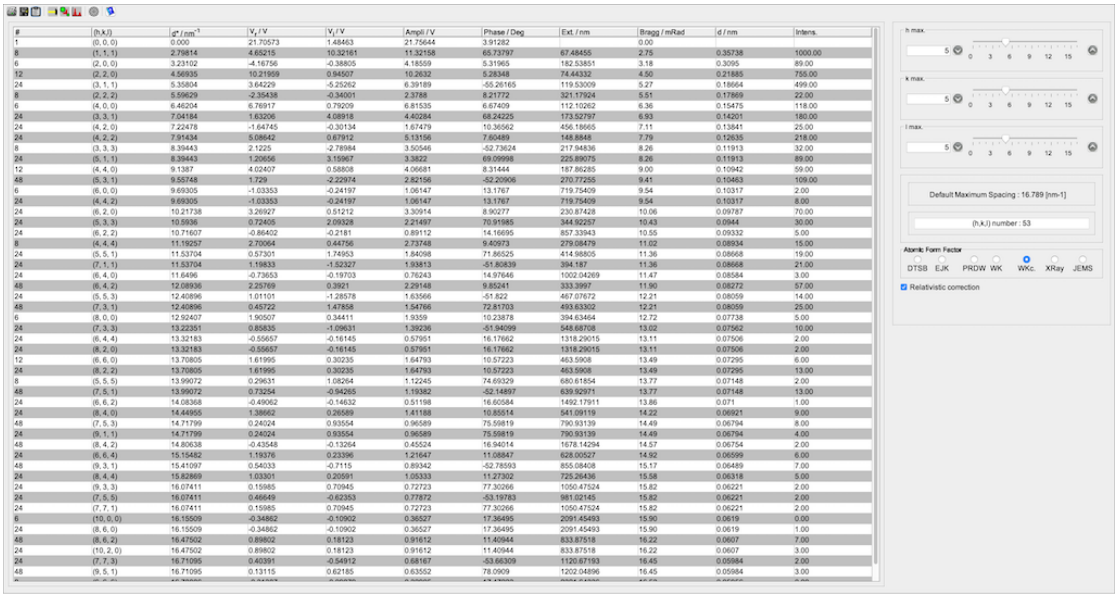


Figure 144: Table of ZnTe structure factors.

29.1 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the dialogue to the clipboard.
- : make a table with different maximum (hkl) indices.
- : reduce the table (Fig. 159).
- : open electron powder pattern frame(Fig. 135).
- : open rings pattern frame (Fig. 136).
- : display a help file.



#	(h,k,l)	q^2 / nm^{-2}	V_r / V	V_i / V	Ampli / V	Phase / Deg	Ext. / nm	Bragg / mRad	d / nm	Intens.
1	(0, 0, 0)	0.000	21.70573	1.48463	21.75644	3.91282		0.00		
8	(1, 1, 1)	2.79814	4.65215	10.32161	11.32158	65.73797	67.48455	2.75	0.35738	1000.00
6	(2, 0, 0)	3.23102	-4.16756	-0.38805	4.18559	5.31965	182.53851	3.18	0.3095	89.00
12	(2, 2, 0)	4.56935	10.21959	0.94507	10.2632	5.28348	74.44332	4.50	0.21885	755.00
24	(3, 1, 1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	499.00
8	(2, 2, 2)	5.59629	-2.35438	-0.34001	2.3788	8.21772	321.17924	5.51	0.17869	22.00
6	(4, 0, 0)	6.46204	6.76917	0.79209	6.81535	6.67409	112.10262	6.36	0.15475	118.00
24	(3, 3, 1)	7.04184	1.63206	4.08918	4.40284	68.24225	173.52797	6.93	0.14201	180.00
24	(4, 2, 0)	7.22478	-1.64745	-0.30134	1.67479	10.36562	456.18665	7.11	0.13841	25.00
24	(4, 2, 2)	7.91434	5.08642	0.67912	5.13156	7.60489	148.8848	7.79	0.12635	218.00
8	(3, 3, 3)	8.39443	2.1225	-2.78984	3.50546	-52.73624	217.94836	8.26	0.11913	32.00
24	(5, 1, 1)	8.39443	1.20656	3.15967	3.3822	69.09998	225.89075	8.26	0.11913	89.00
12	(4, 4, 0)	9.1387	4.02407	0.58808	4.06681	8.31444	187.86285	9.00	0.10942	59.00
48	(5, 3, 1)	9.55748	1.729	-2.22974	2.82156	-52.20906	270.77255	9.41	0.10463	109.00
6	(6, 0, 0)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	2.00
24	(4, 4, 2)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	8.00
24	(6, 2, 0)	10.21738	3.26927	0.51212	3.30914	8.90277	230.87428	10.06	0.09787	70.00
24	(5, 3, 3)	10.5936	0.72405	2.09328	2.21497	70.91585	344.92257	10.43	0.0944	30.00
24	(6, 2, 2)	10.71607	-0.86402	-0.2181	0.89112	14.16695	857.33943	10.55	0.09332	5.00
8	(4, 4, 4)	11.19257	2.70064	0.44756	2.73748	9.40973	279.08479	11.02	0.08934	15.00
24	(5, 5, 1)	11.53704	0.57301	1.74953	1.84098	71.86525	414.98805	11.36	0.08668	19.00
24	(7, 1, 1)	11.53704	1.19833	-1.52327	1.93813	-51.80839	394.187	11.36	0.08668	21.00
24	(6, 4, 0)	11.6496	-0.73653	-0.19703	0.76243	14.97646	1002.04269	11.47	0.08584	3.00
48	(6, 4, 2)	12.08936	2.25769	0.3921	2.29148	9.85241	333.3997	11.90	0.08272	57.00
24	(5, 5, 3)	12.40896	1.01101	-1.28578	1.63566	-51.822	467.07672	12.21	0.08059	14.00
48	(7, 3, 1)	12.40896	0.45722	1.47858	1.54766	72.81703	493.83302	12.21	0.08059	25.00
6	(8, 0, 0)	12.92407	1.90507	0.34411	1.9359	10.23878	394.63464	12.72	0.07738	5.00
24	(7, 3, 3)	13.22351	0.85835	-1.09631	1.39236	-51.94099	548.68708	13.02	0.07562	10.00
24	(6, 4, 4)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00
24	(8, 2, 0)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00
12	(6, 6, 0)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	6.00
24	(8, 2, 2)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	13.00
8	(5, 5, 5)	13.99072	0.29631	1.08264	1.12245	74.69329	680.61854	13.77	0.07148	2.00
48	(7, 5, 1)	13.99072	0.73254	-0.94265	1.19382	-52.14897	639.92971	13.77	0.07148	13.00
24	(6, 6, 2)	14.08368	-0.49062	-0.14632	0.51198	16.60584	1492.17911	13.86	0.071	1.00
24	(8, 4, 0)	14.44955	1.38662	0.26589	1.41188	10.85514	541.09119	14.22	0.06921	9.00
48	(7, 5, 3)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	8.00
24	(9, 1, 1)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	4.00
48	(8, 4, 2)	14.80638	-0.43548	-0.13264	0.45524	16.94014	1678.14294	14.57	0.06754	2.00
24	(6, 6, 4)	15.15482	1.19376	0.23396	1.21647	11.08847	628.00527	14.92	0.06599	6.00
48	(9, 3, 1)	15.41097	0.54033	-0.7115	0.89342	-52.78593	855.08408	15.17	0.06489	7.00
24	(8, 4, 4)	15.82469	1.03301	0.20991	1.05333	11.27302	725.26436	15.58	0.06318	5.00
24	(9, 3, 3)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00
24	(7, 5, 5)	16.07411	0.46649	-0.62353	0.77872	-53.19783	981.02145	15.82	0.06221	2.00
24	(7, 7, 1)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00
8	(10, 0, 0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	0.00
24	(8, 6, 0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	1.00
48	(8, 6, 2)	16.47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	7.00
24	(10, 2, 0)	16.47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	3.00
24	(7, 7, 3)	16.71095	0.40391	-0.54912	0.68167	-53.66309	1120.87193	16.45	0.05984	2.00
48	(9, 5, 1)	16.71095	0.13115	0.62185	0.63552	78.0909	1202.04896	16.45	0.05984	3.00

Figure 145: Table of non-equivalent ZnTe structure factors and their multiplicity.

30 Miscellany menu

The **Miscellany** menu offers possibilities to load .ems images or super-cells (.xyz, .cel formats) and to generate various models of crystal structures.

30.1 Miscellany menu items

The menu items allow to:

- **Load image** : load .ems images (Fig. 146).
- **Load super-cell** : load model structure in .xyz or .cel formats (Fig. 147).
- **Make void** : create a void in a structure (Fig. 148).
- **To core-shell** : create core-shell particles (Fig. 149).
- **To particle** : create spherical or facetted particles (Fig. 151).
- **To precipitate** : create a precipitate in a matrix (Fig. 152).
- **To slices** : slice a crystal structure (Fig. 154).
- **To triclinic** : duplicate and rotate a crystal structure (Fig. 156).

30.1.1 Load image

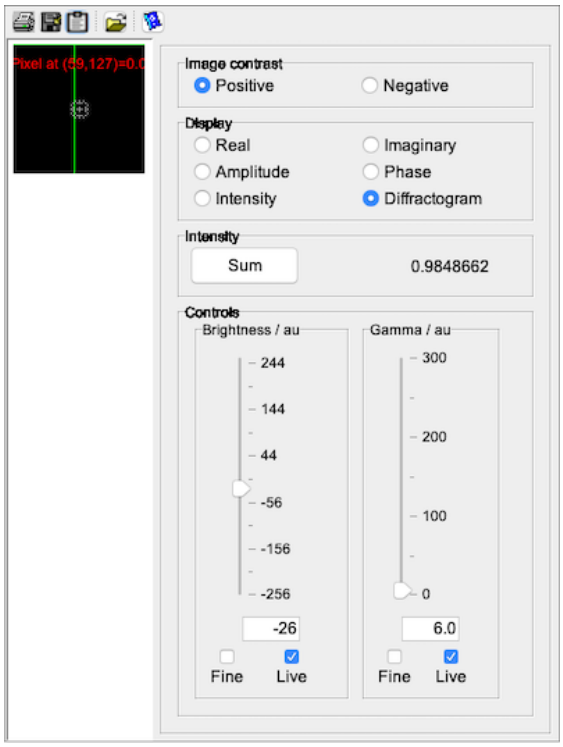


Figure 146: Miscellany menu **Load image** frame.

30.1.2 Load super-cell

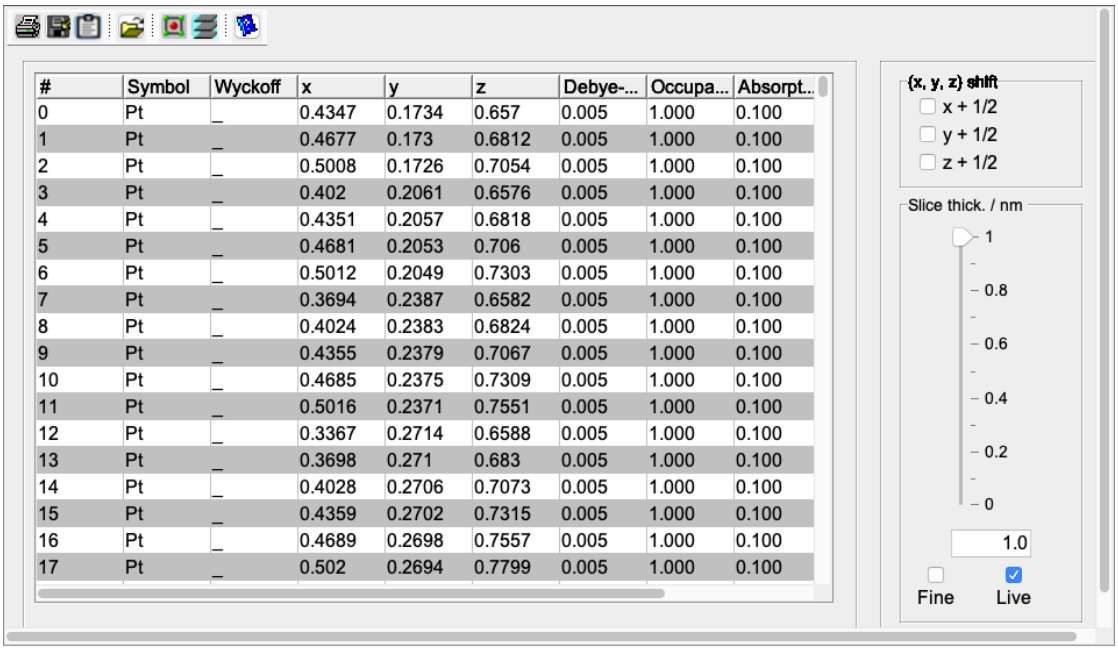


Figure 147: Miscellany menu **Load super-cell** frame.

30.1.3 Make void

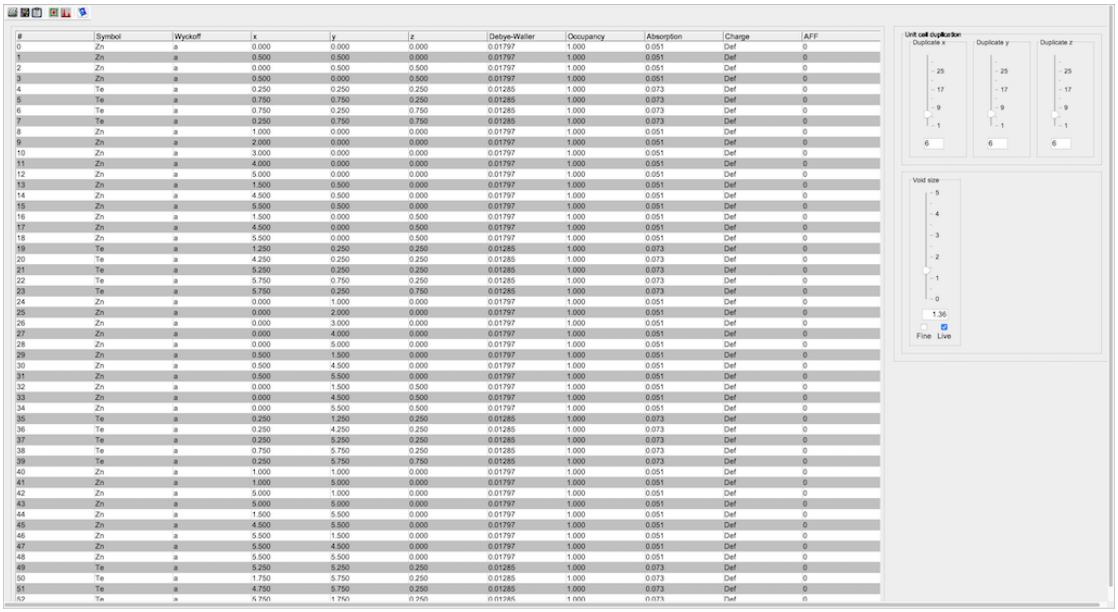


Figure 148: Miscellany menu **Make void** frame.

30.1.4 To core-shell

Frame (Fig. 149) allows to create core-shell (spherical) particles. Regular .txt crystal structures are loaded for the core (here Au, duplicated $n_x \times n_y \times n_z$ times and the shell (here SiO_2 duplicated $n'_x \times n'_y \times n'_z$ times). The particle is placed in a box and the model can be sliced into thinner sub-slices ready for multislice calculations.

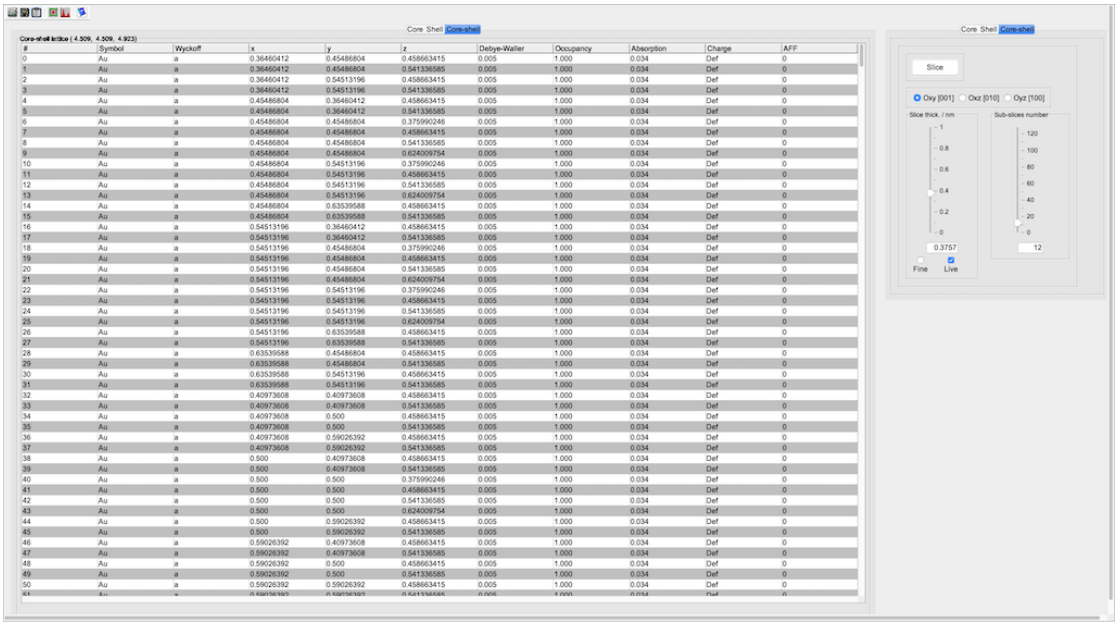
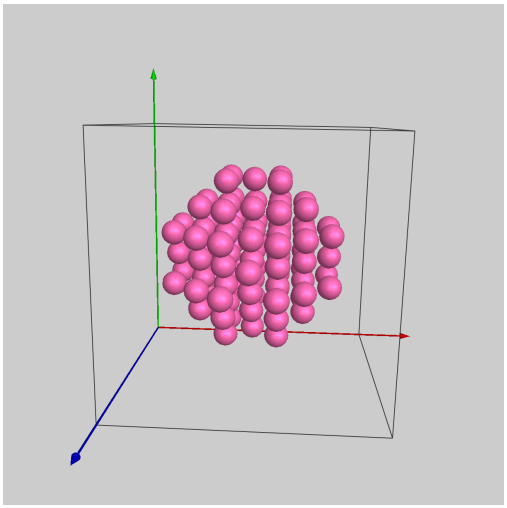
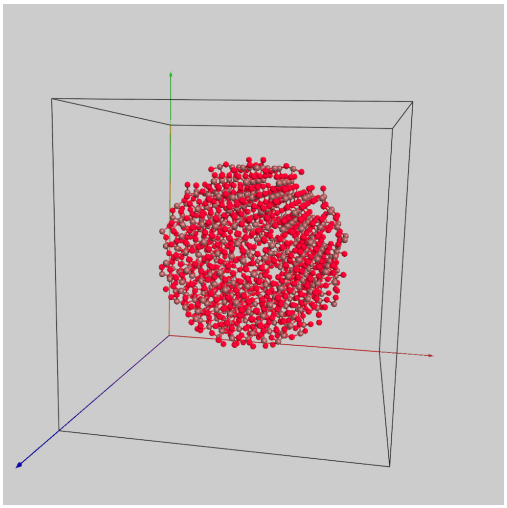


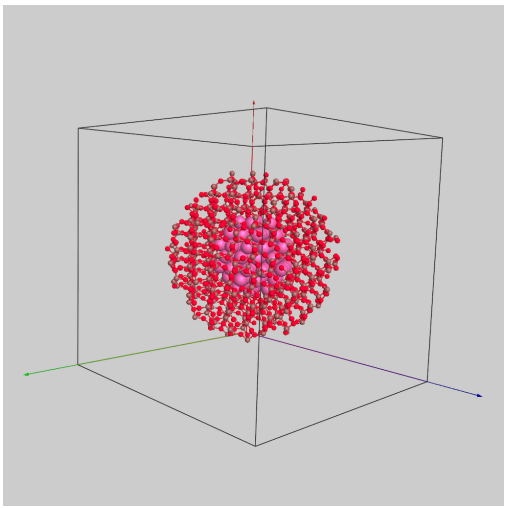
Figure 149: Miscellany menu **To core-shell** frame.



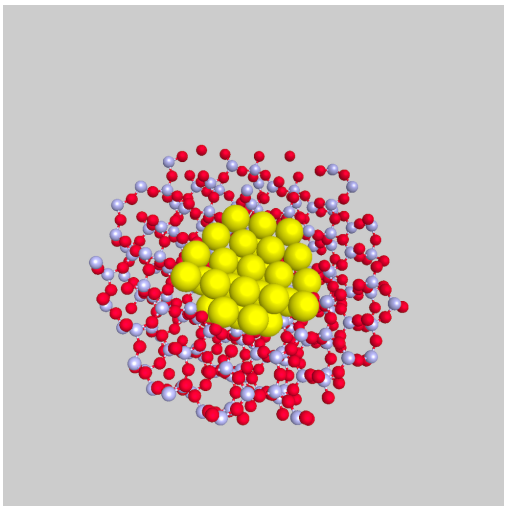
(a) Au core view.



(b) SiO_2 shell view.



(c) Core-shell particle view.



(d) Cut of the $AuSi_2$ particle.

Figure 150: To core-shell 3D-views. The model is embedded in a box of dimensions large enough to avoid "wrap around" artefacts during the multislice image calculation.

30.1.5 To particle

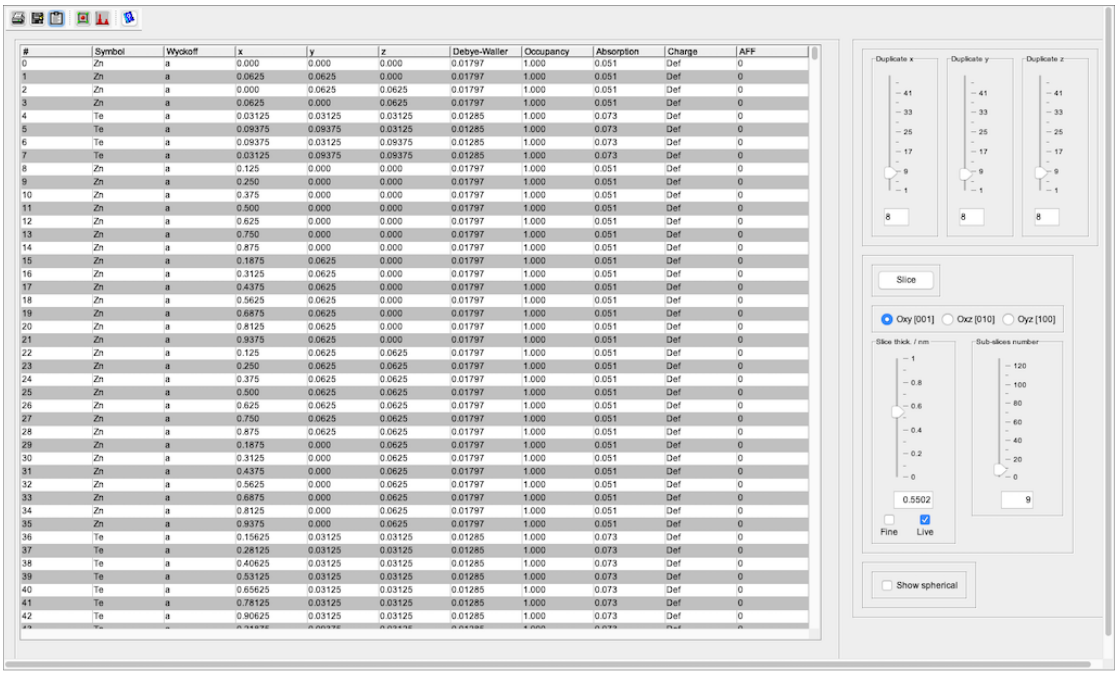


Figure 151: Miscellany menu **To particle** frame.

30.1.6 To precipitate

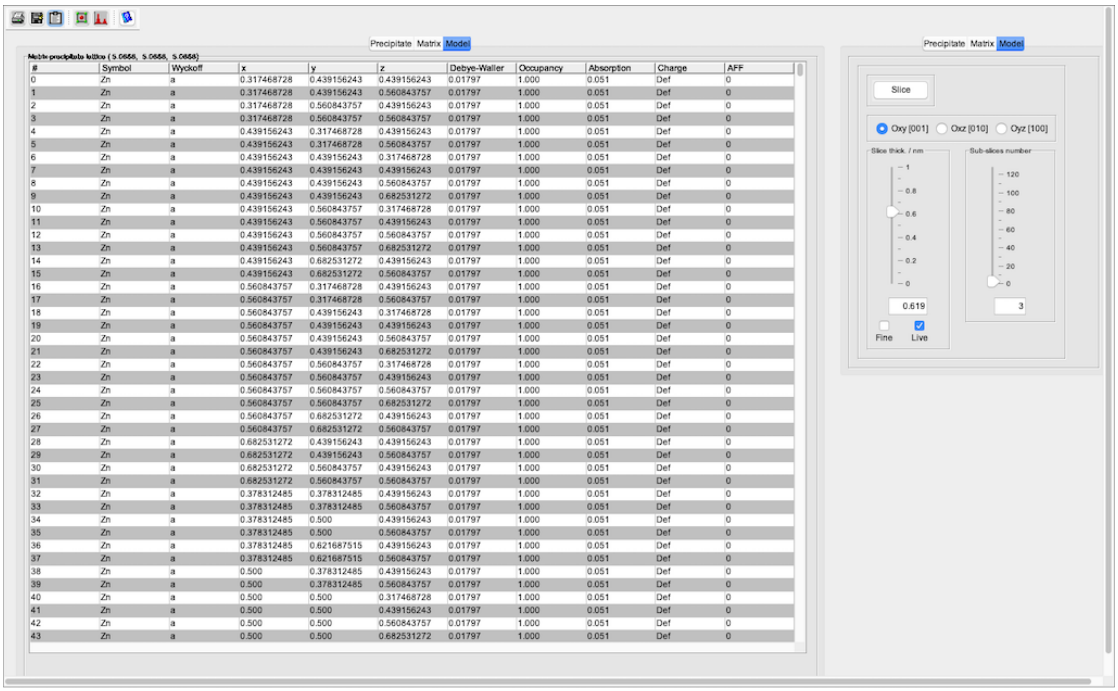
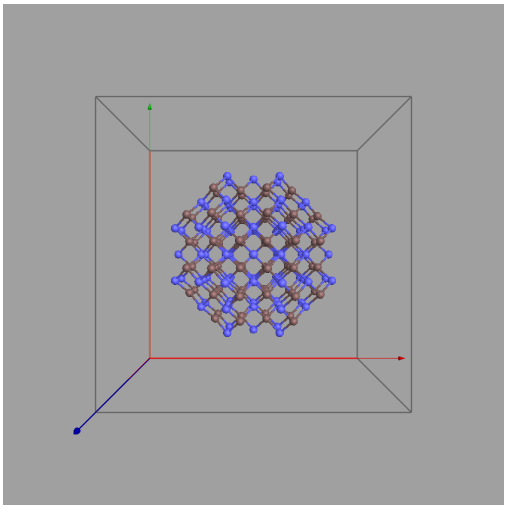
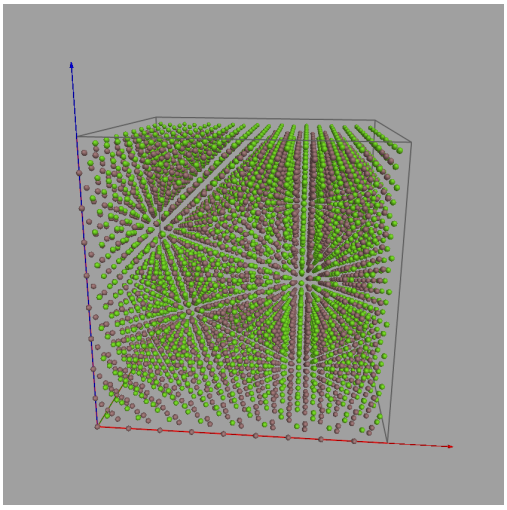


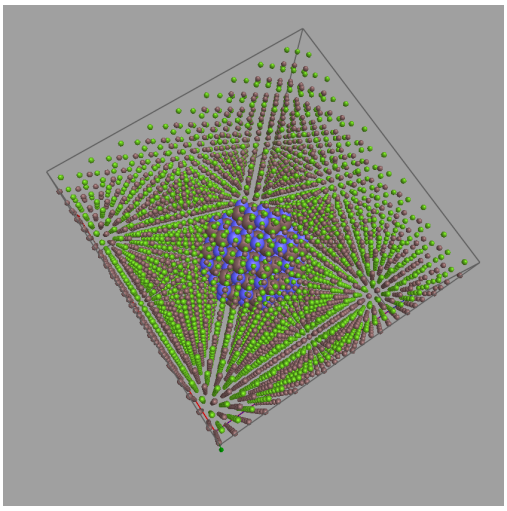
Figure 152: Miscellany menu **To precipitate** frame.



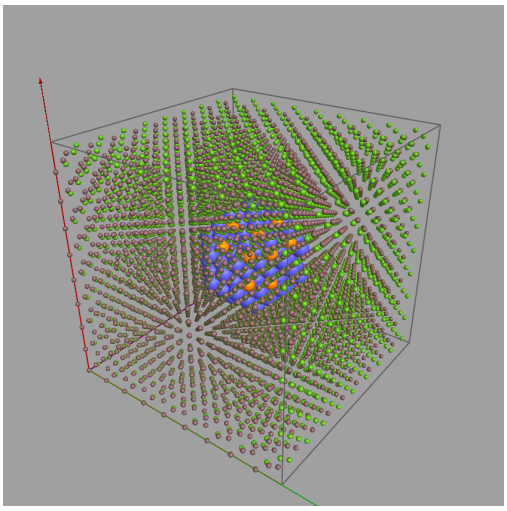
(a) Precipitate 3D-view.



(b) GaAs matrix 3D-view.



(c) ZnTe Precipitate in GaAs matrix 3D-view.



(d) Cut of the $AuSi_2$ particle.

Figure 153: To precipitate 3D-views. The model is embedded in a box of dimensions large enough to avoid "wrap around" artefacts during the multislice image calculation.

30.1.7 To slices

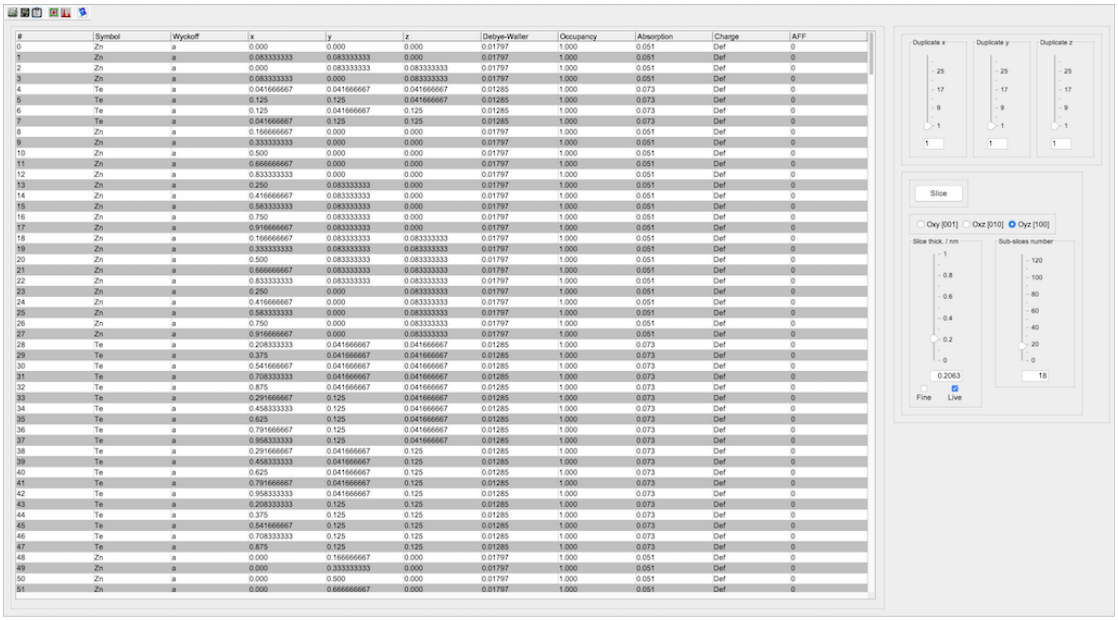
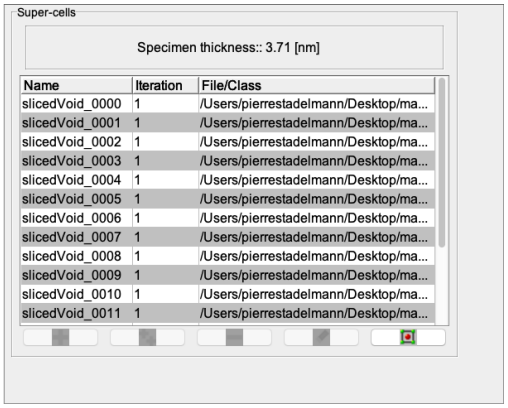
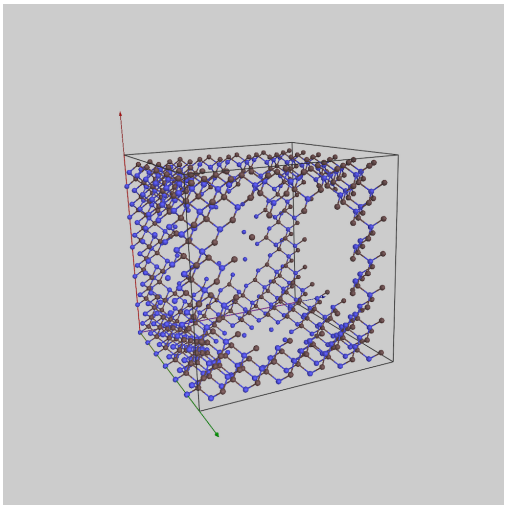


Figure 154: Miscellany menu **To slices** frame.



(a) Table of slices.



(b) 3D-view of a slice.

Figure 155: Table of slices and 3D-view of a single slice or the stack of slices.

30.1.8 To triclinic

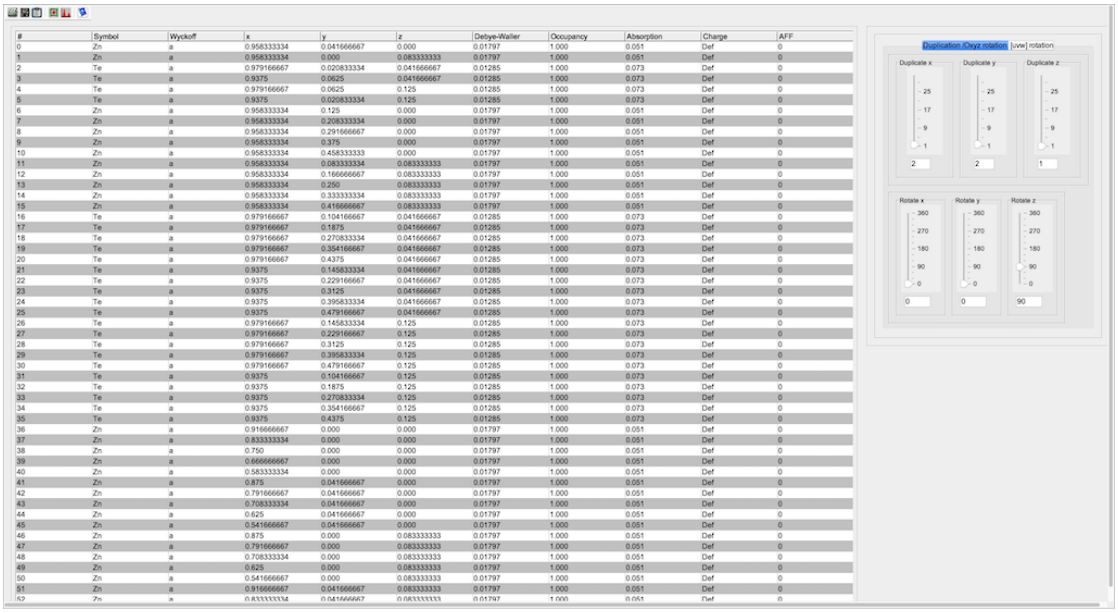
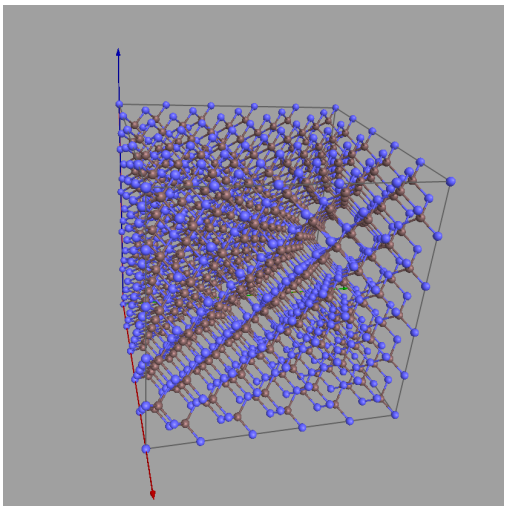
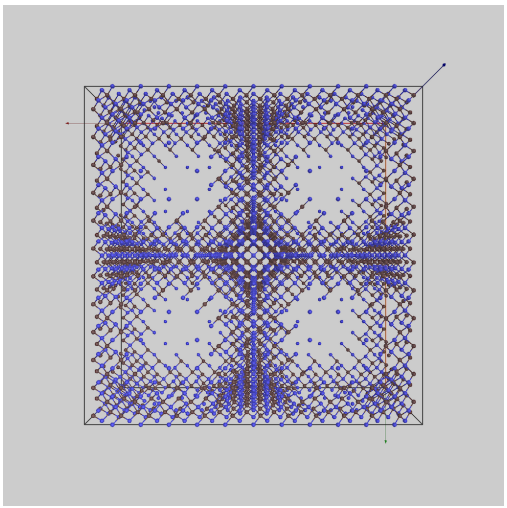


Figure 156: Miscellany menu **To triclinic** frame.



(a) To triclinic model 3D-view.



(b) Duplicated void model 2x2x1

Figure 157: To triclinic simple model and duplicated void model 3D-view.

31 Thickness

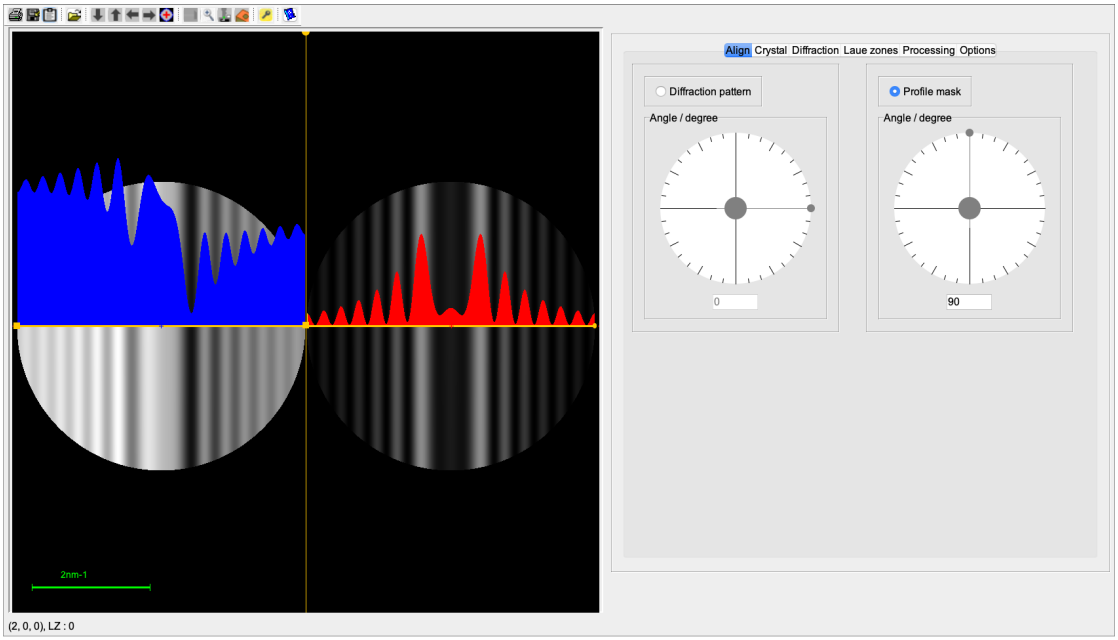


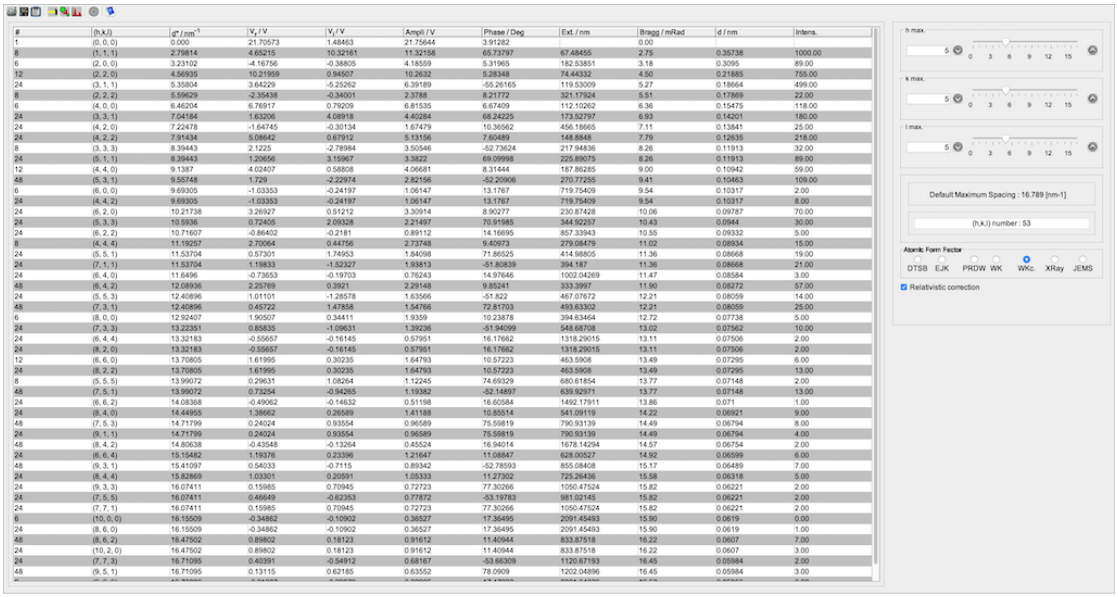
Figure 158: Thickness measurement.

31.1 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the frame to the clipboard.
- : load a CBED image.
- : move the **C**enter of the **L**aue **C**ircle (CLC) down.
- : move the CLC up.
- : move the CLC left.
- : move the CLC right.
- : make a table with different maximum (hkl) indices.
- : reduce the table (Fig. 159).

-  : display a powder pattern (Fig. 116).
-  : display a ring pattern (Fig. 136).
-  : display a help file.



#	[h,k,l]	d^* / nm^{-1}	V$_r$ / V	V$_i$ / V	Ampli / V	Phase / Deg	Ext. / nm	Bragg / mRad	d / nm	Intens.
1	(0, 0, 0)	0.000	21.70573	1.48463	21.75644	3.91282		0.00		
8	(1, 1, 1)	2.79814	4.65215	10.32161	11.32158	65.73797	67.48455	2.75	0.35738	1000.00
6	(2, 0, 0)	3.23102	-4.16756	-0.38805	4.18559	5.31965	182.53851	3.18	0.3095	89.00
12	(2, 2, 0)	4.56935	10.21959	0.94507	10.2632	5.28348	74.44332	4.50	0.21885	755.00
24	(3, 1, 1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	499.00
8	(2, 2, 2)	5.59629	-2.35438	-0.34001	2.3788	8.21772	321.17924	5.51	0.17869	22.00
6	(4, 0, 0)	6.46204	6.76917	0.79209	6.81535	6.67409	112.10262	6.36	0.15475	118.00
24	(3, 3, 1)	7.04184	1.63206	4.08918	4.40284	68.24225	173.52797	6.93	0.14201	180.00
24	(4, 2, 0)	7.22478	-1.64745	-0.30134	1.67479	10.36562	456.18665	7.11	0.13841	25.00
24	(4, 2, 2)	7.91434	5.08642	0.67912	5.13156	7.60489	148.8848	7.79	0.12635	218.00
8	(3, 3, 3)	8.39443	2.1225	-2.78984	3.50546	-52.73624	217.94836	8.26	0.11913	32.00
24	(5, 1, 1)	8.39443	1.20656	3.15967	3.3822	69.09998	225.89075	8.26	0.11913	89.00
12	(4, 4, 0)	9.1387	4.02407	0.58808	4.06681	8.31444	187.86285	9.00	0.10942	59.00
48	(5, 3, 1)	9.55748	1.729	-2.22974	2.82156	-52.20906	270.77255	9.41	0.10463	109.00
6	(6, 0, 0)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	2.00
24	(4, 4, 2)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	8.00
24	(6, 2, 0)	10.21738	3.26927	0.51212	3.30914	8.90277	230.87428	10.06	0.09787	70.00
24	(5, 3, 3)	10.5936	0.72405	2.09328	2.21497	70.91985	344.92257	10.43	0.0944	30.00
24	(6, 2, 2)	10.71607	-0.86402	-0.2181	0.89112	14.16695	857.33943	10.55	0.09332	5.00
8	(4, 4, 4)	11.19257	2.70064	0.44756	2.73748	9.40973	279.08479	11.02	0.08934	15.00
24	(5, 5, 1)	11.53704	0.57301	1.74953	1.84098	71.86525	414.98805	11.36	0.08668	19.00
24	(7, 1, 1)	11.53704	1.19833	-1.52327	1.93813	-51.80839	394.187	11.36	0.08668	21.00
24	(6, 4, 0)	11.6496	-0.73653	-0.19703	0.76243	14.97646	1002.04269	11.47	0.08584	3.00
48	(6, 4, 2)	12.08936	2.25769	0.3921	2.29148	9.85241	333.3997	11.90	0.08272	57.00
24	(5, 5, 3)	12.40896	1.01101	-1.28578	1.63566	-51.822	467.07672	12.21	0.08059	14.00
48	(7, 3, 1)	12.40896	0.45722	1.47858	1.54766	72.81703	493.63302	12.21	0.08059	25.00
6	(8, 0, 0)	12.92407	1.90507	0.34411	1.9359	10.23878	394.63464	12.72	0.07738	5.00
24	(7, 3, 3)	13.22351	0.85835	-1.09631	1.39236	-51.94099	548.68708	13.02	0.07562	10.00
24	(6, 4, 4)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00
24	(8, 2, 0)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00
12	(6, 6, 0)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	6.00
24	(8, 2, 2)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	13.00
8	(5, 5, 5)	13.99072	0.29631	1.08264	1.12245	74.69329	680.61854	13.77	0.07148	2.00
48	(7, 5, 1)	13.99072	0.73254	-0.94265	1.19382	-52.14497	639.92971	13.77	0.07148	13.00
24	(6, 6, 2)	14.08368	-0.49062	-0.14632	0.51198	16.60584	1492.17911	13.86	0.071	1.00
24	(8, 4, 0)	14.44955	1.38662	0.26589	1.41188	10.85514	541.09119	14.22	0.06921	9.00
48	(7, 5, 3)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	8.00
24	(9, 1, 1)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	4.00
48	(8, 4, 2)	14.80638	-0.43548	-0.13264	0.45524	16.94014	1678.14294	14.57	0.06754	2.00
24	(6, 6, 4)	15.15482	1.19376	0.23396	1.21647	11.08847	628.00527	14.92	0.06599	6.00
48	(9, 3, 1)	15.41097	0.54033	-0.7115	0.89342	-52.78593	855.08408	15.17	0.06489	7.00
24	(8, 4, 4)	15.82869	1.03301	0.20591	1.05333	11.27302	725.26436	15.58	0.06318	5.00
24	(9, 3, 3)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00
24	(7, 5, 5)	16.07411	0.46649	-0.62353	0.77872	-53.19783	981.02145	15.82	0.06221	2.00
24	(7, 7, 1)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00
6	(10, 0, 0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	0.00
24	(8, 6, 0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	1.00
48	(8, 6, 2)	16.47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	7.00
24	(10, 2, 0)	16.47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	3.00
24	(7, 7, 3)	16.71095	0.403391	-0.549112	0.68167	-53.66309	1120.87193	16.45	0.05984	2.00
48	(9, 5, 1)	16.71095	0.13115	0.62185	0.63552	78.0909	1202.04896	16.45	0.05984	3.00

Figure 159: Table of non-equivalent ZnTe structure factors and their multiplicity.

32 Perspective

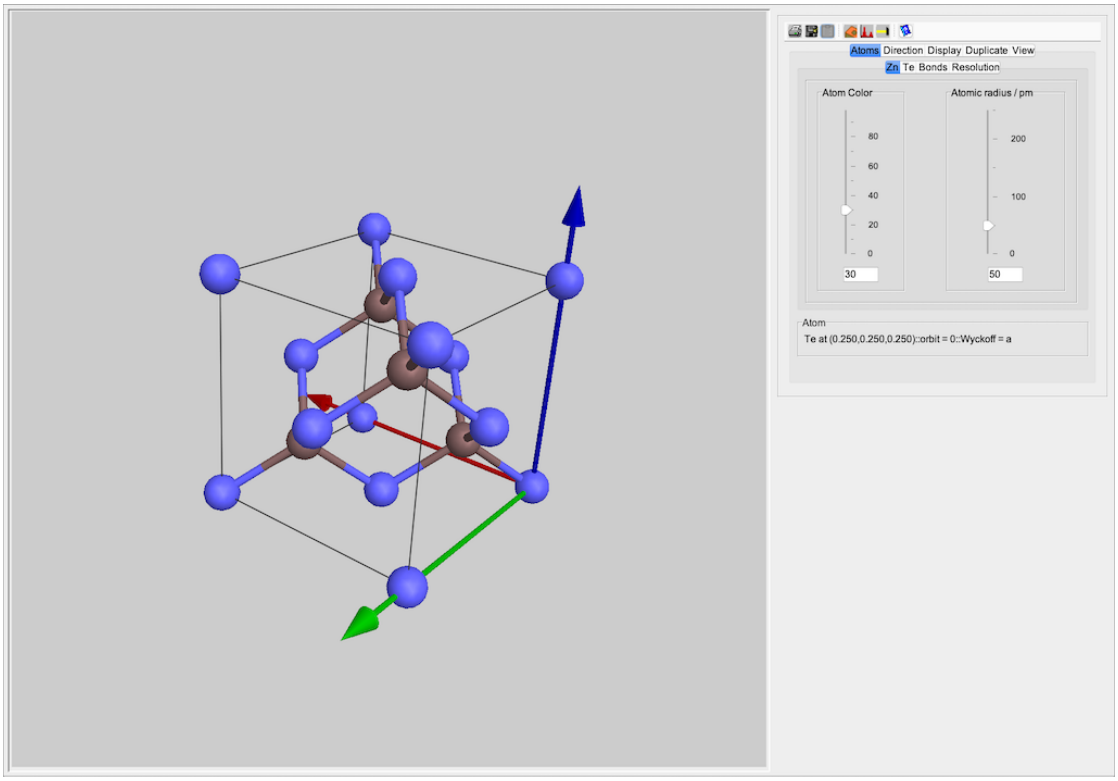


Figure 160: ZnTe perspective view.

32.1 Popup menu

The popup menu (Fig. 161) associated with the view allows to transfer the view to the clipboard as well as to save, print, create a Mathematica notebook or generate a powder pattern. It controls also the creation of the movies.

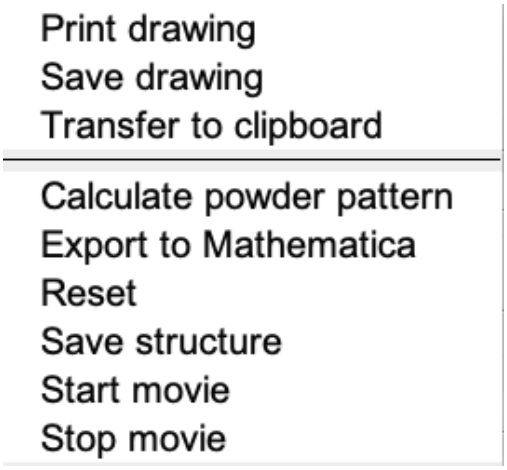
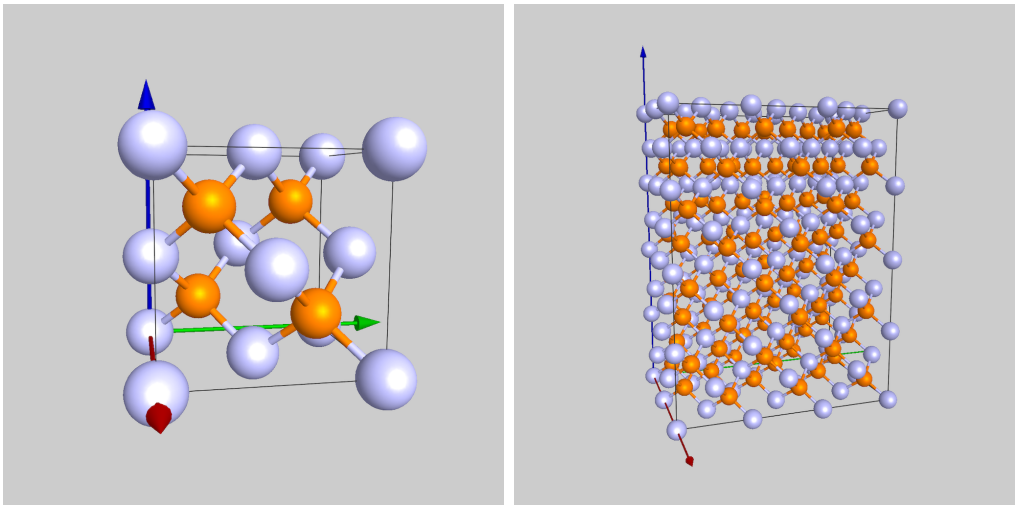


Figure 161: 3-D view popup menu.

32.2 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the frame to the clipboard.
- : open the **Specimen** dialogue (Fig. 84a).
- : display a **P**owder pattern (Fig. 116).
- : duplicate the unit cell $n_x \times n_y \times n_z$ (Fig. 162b).
- : display a help file.



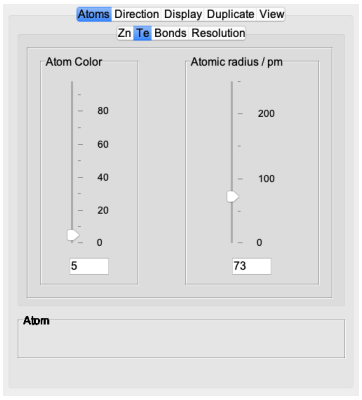
(a) ZnTe 3D-view. (b) ZnTe 2 x 3 x 4 unit cells 3D-view.

Figure 162: 3-D view of ZnTe models.

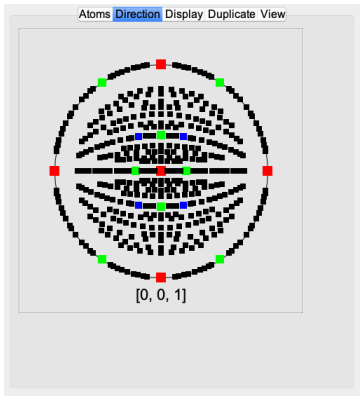
32.3 Tabs

3-D view controls are collected in the following tabs in order to define:

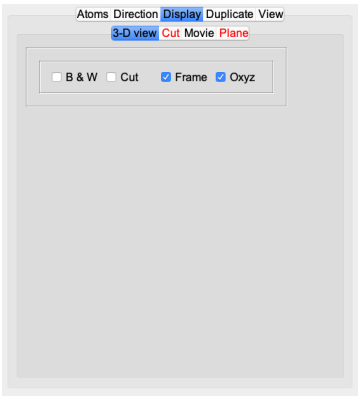
- **Atoms** : the atoms colour and size as well as bonding and resolution (Fig. 163a).
- **Direction** : the viewing direction (Fig. 163b).
- **Display** : the 3-D perspective details (Fig. 163c).
- **Duplicate** : the model duplication (Fig. 163d).
- **View** : the view type (Fig. 163e).



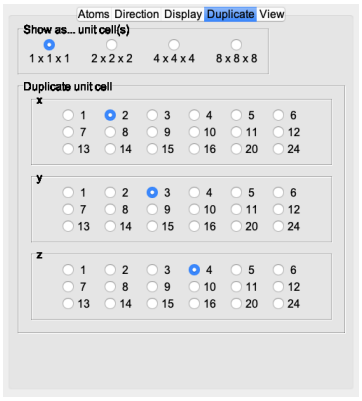
(a) Atoms.



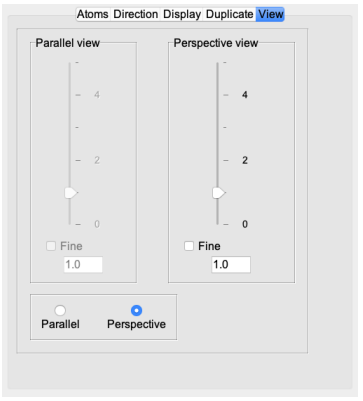
(b) Viewing direction.



(c) Display details.



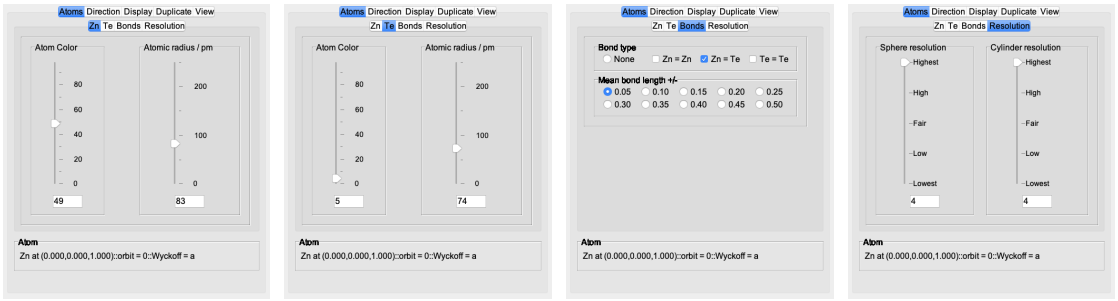
(d) Duplicate controls.



(e) View type (parallel or perspective).

Figure 163: Controls of 3D-perspective.

The **Atoms** and **Display** tabs are organized in sub-tabs that control the colour and size of the atoms as well as the bonding and resolution of the views (Figs. 164a, 164b, 164c, 164d, 164e, 164f, 164g, 164h). They allow, for example, to create **B**lack & **W**hite figure (165a) or to look at (hkl) planes (Fig. 165b).



(a) Zn colour and size.

(b) Te colour and size.

(c) Define the bonding of ZnTe.

(d) Resolution of the spheres and bonds.

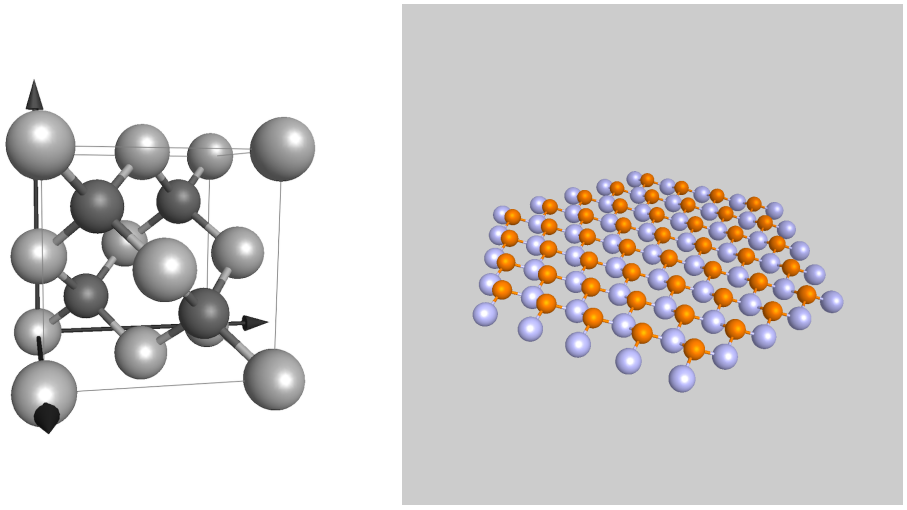
(e) 3D-view details.

(f) Cut thickness and distance to middle of model (when **Cut** check-box is selected).

(g) Movie controls.

(h) Cut plane selection (when **Cut** check-box is selected).

Figure 164: Atoms and Display Tabs.



(a) B & W ZnTe model. (b) ZnTe (111) plane.

Figure 165: Modified 3-D views.

33 Indexing SAED patterns

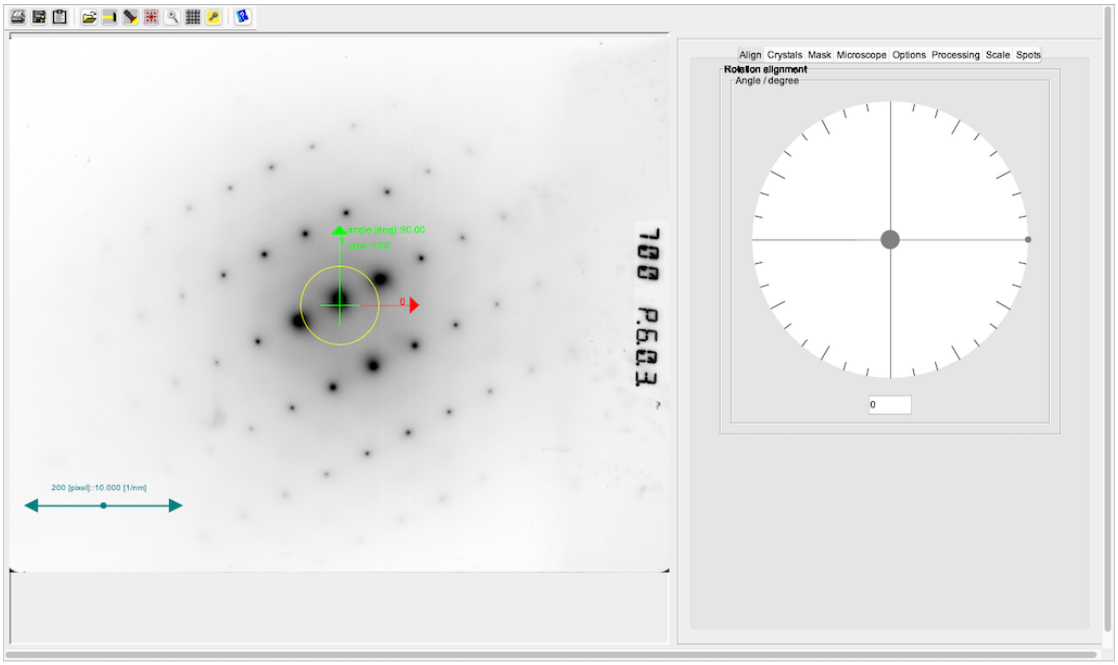


Figure 166: Indexing SAED patterns.

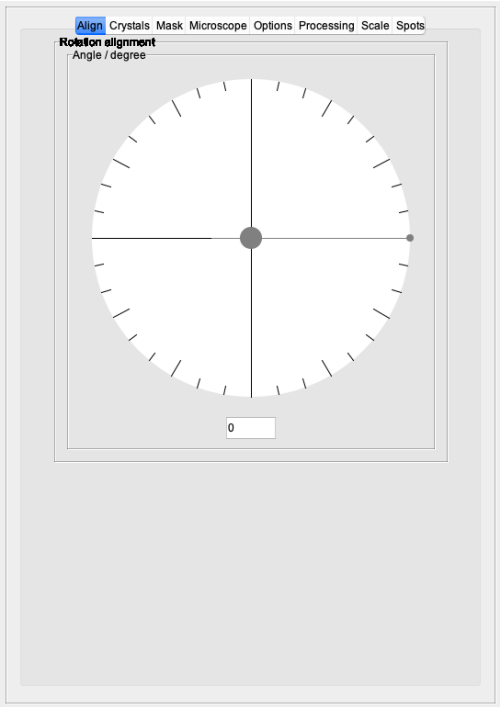
33.1 Tool buttons

The tool buttons allow to:

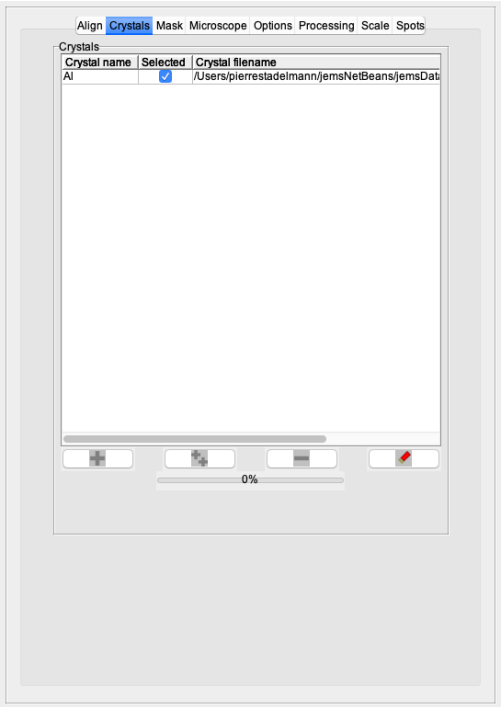
- : print the image.
- : save the image.
- : transfer the frame to the clipboard.
- : open an image.
- : process image.
- : start indexing process.
- : show diffractogram (when an HRTEM image has been loaded).
- : magnify part of image.
- : tabulate the image.

-  : open keeper dialogue (Fig. 90).
-  : display a help file.

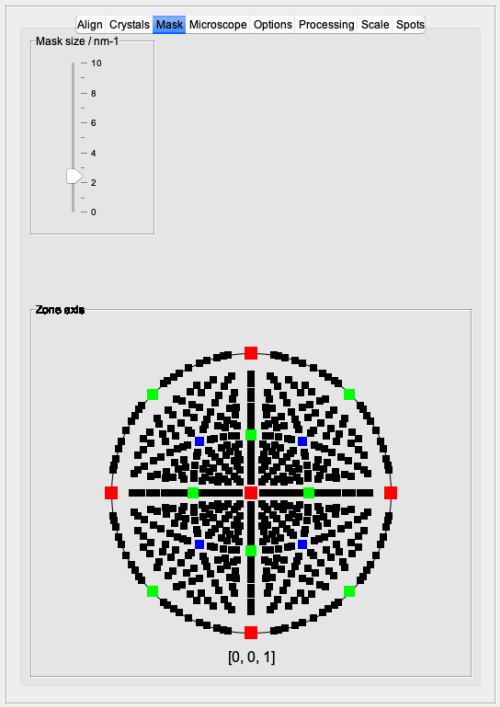
33.2 Tabs



(a) Rotation of the spot indexing mask.



(b) Table of the crystal files selected for the indexing.



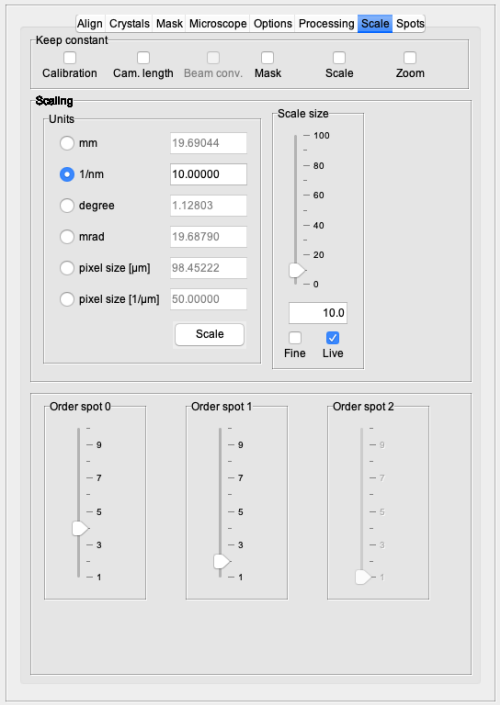
(c) Mask showing the spots selected for indexing.

(d) Controls of the microscope parameters.

Figure 167: Controls and tabs of SAED patterns indexing.

(a) Options to control the indexing process, in particular the number of spots used by the indexing.

(b) Image processing tab.



(c) Controls to set the scale of the experimental SAED pattern or diffractogram.

(d) Controls to define the spot distances and angles.

Figure 168: Controls and tabs of SAED patterns indexing.

33.3 Example

The image processing tab is available in several jems frame. It can be used to automatically identify the center of spots on diffraction patterns (Fig. 169).

(a) GaN experimental diffraction pattern.

(b) Image contrast is inverted.

(c) Peaks are listed in the peaks table.

(d) Peaks are identified.

(e) The circle are centred on SAED spots (.)

(f) Binarizing the experimental image can help figure out where the spots are located.

Figure 169: Indexing SAED to identify and list the diffraction spots.

34 ADF imager

The **ADF imager** frame is shown on Fig. 170. It allows to calculate **B**right-**F**ield, **D**ark Field, **HAADF** as well as **S**ector **D**etector images. The ADF imager moves a probe on a projected structure and integrate the scattered signal on an annular detector that is controlled using the **ADF detector** dialogue (Fig. 171). When large super-cells are imaged it is very useful to define the parent unit cell crystal and imaging zone axis (Fig. 172c) since the diffraction pattern of the detector dialogue will be created using the unit cell.

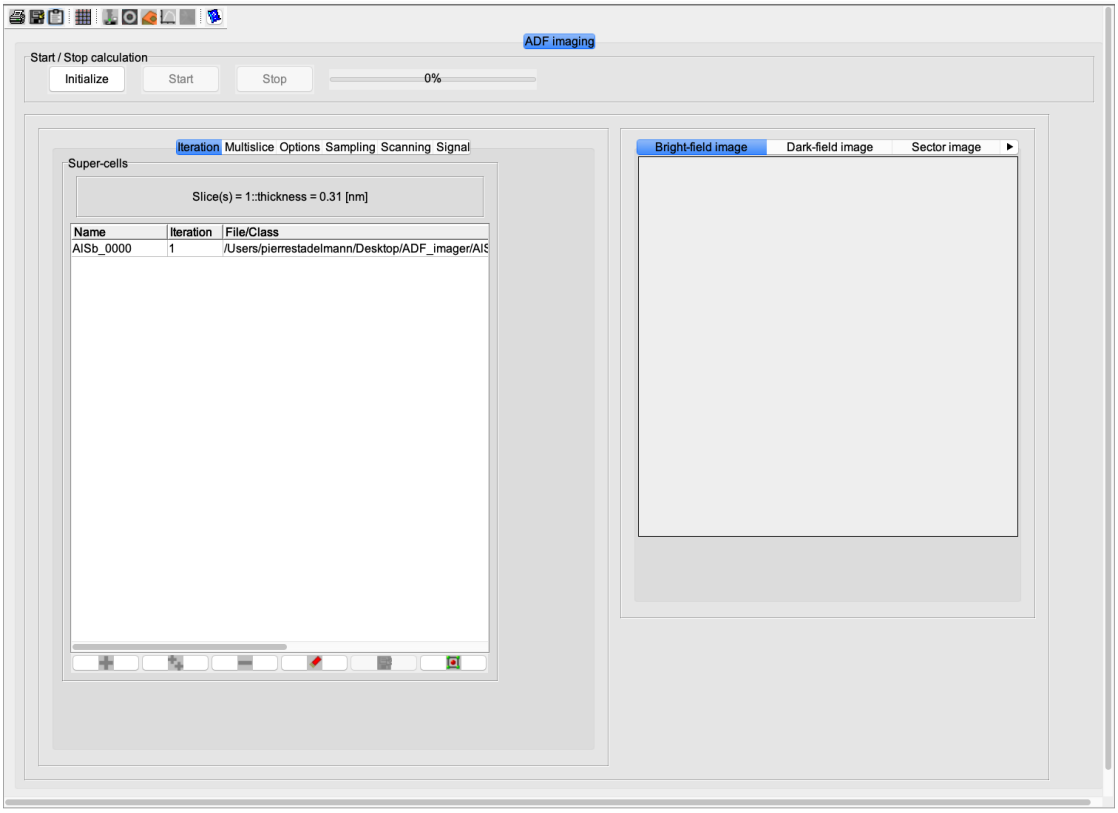


Figure 170

The ADF simulation computes 4 **B**right and **D**ark images at once. The size of the first bright or dark field detector is selected (Fig. 171) and the size of the three supplementary ones is increased by 5, 10, 15, 20 or 25 milliradians.

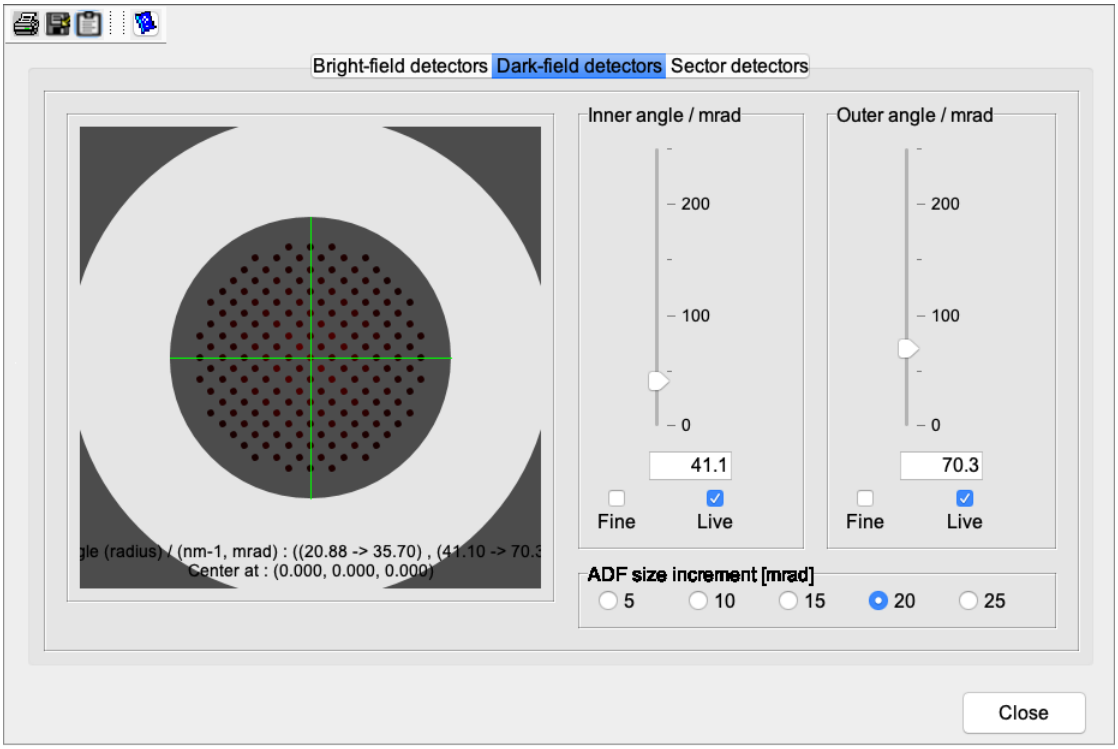


Figure 171: The **ADF detector** dialogue allows to set the size and position of the **B**right and **D**ark field detectors as well as the **S**ector detector.

34.1 Tool buttons

The tool buttons of the HRTEM imager allow to:

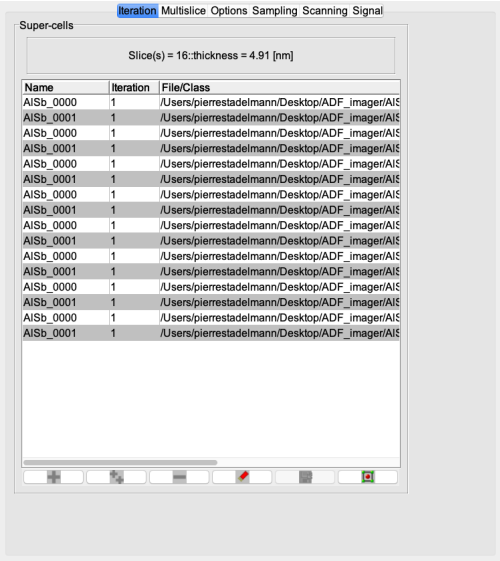
- : print the selected ADF image tab.
- : save the selected ADF image tab.
- : transfer the ADF frame to the clipboard.
- : display the interpolated ADF image and allows tabulating the selected ADF image.
- : open the **Microscope dialogue** (Fig. 108).
- : open the **ADF detector** dialogue (Fig. 171).
- : open the **Specimen** dialogue (Fig. 84a).
- : open the **Transfer function frame** (Fig. 97).
- : open the image contrast controls.

-  : open the associated help dialogue.

34.2 Tabs

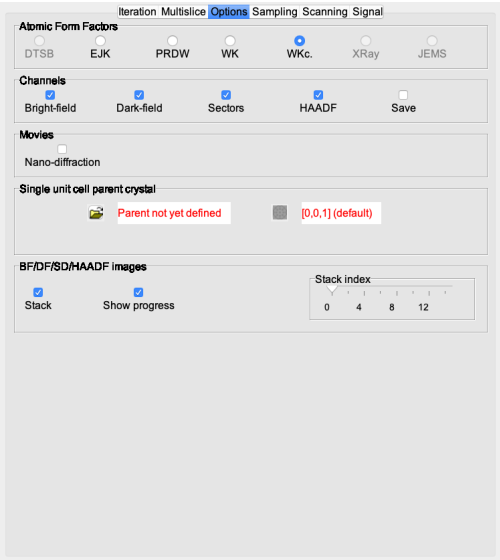
The imaging controls are organised in several tabs aimed at:

- **Iteration** : defining the super-cells stack (Fig 172a).
- **Multislice** : (Fig 172b)
- **Options** : (Fig 172c).
- **Sampling** : (Fig 172d).
- **Scanning** : (Fig 172e).
- **Signal** : (Fig 172f).

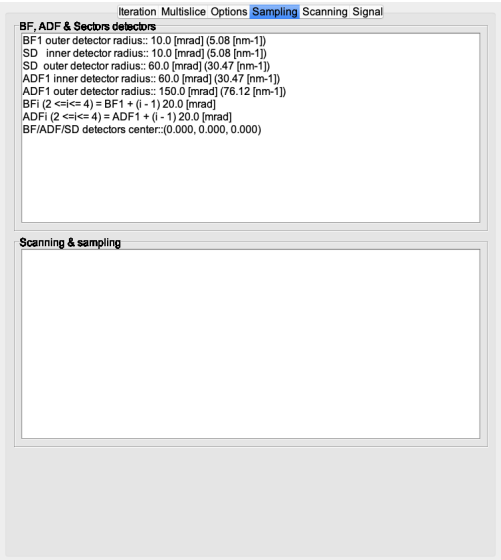


(a) Stack of super-cells and total specimen thickness.

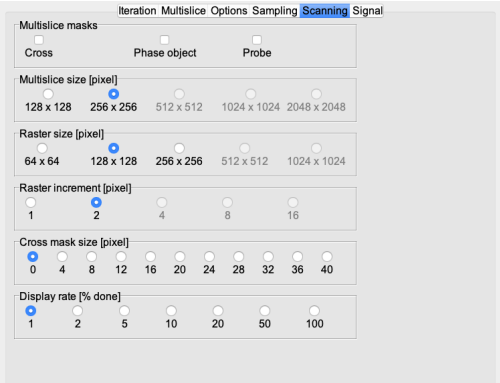
(b) Controls the potential generation method (**A**nalytic recommended), the multislice sampling and approximation, the optical potential calculation (not necessary when WK or WKc AFF are selected) and the Frozen lattice approximation and configurations number.

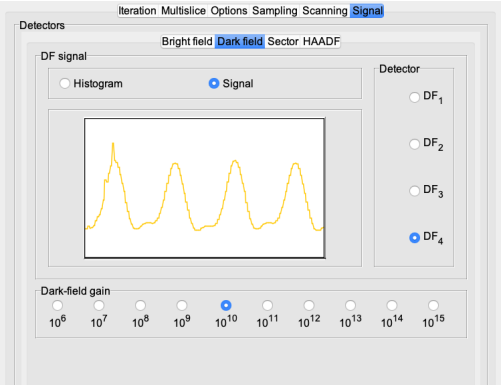


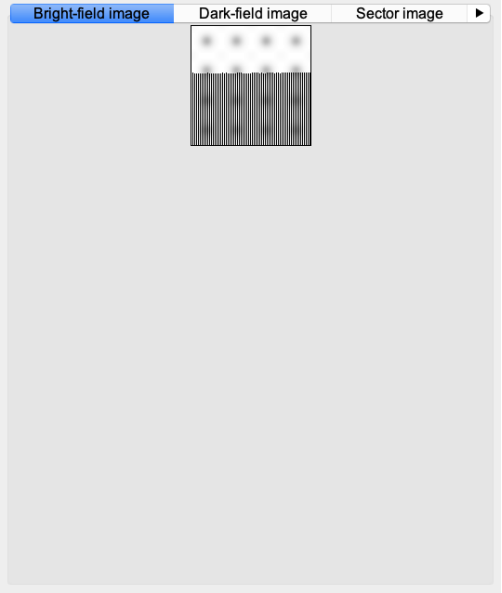
(c) Selects **A**tomic **F**orm **F**actors source, allows **B**right, **D**ark, **S**ector or **HAADF** image calculation and when checkbox **Save** is selected saves all the calculated images.



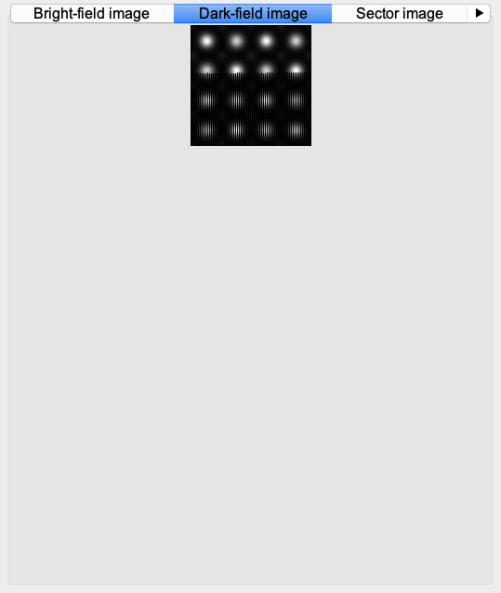
(d) Displays information about the detectors sizes and the maximum scattering angle of the multislice calculation.



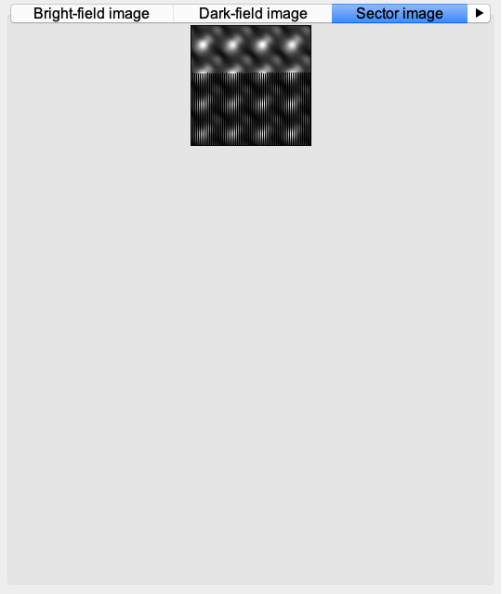




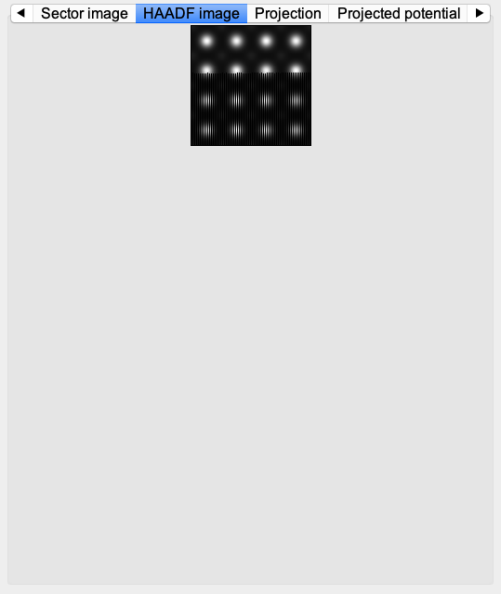
(a)



(b)

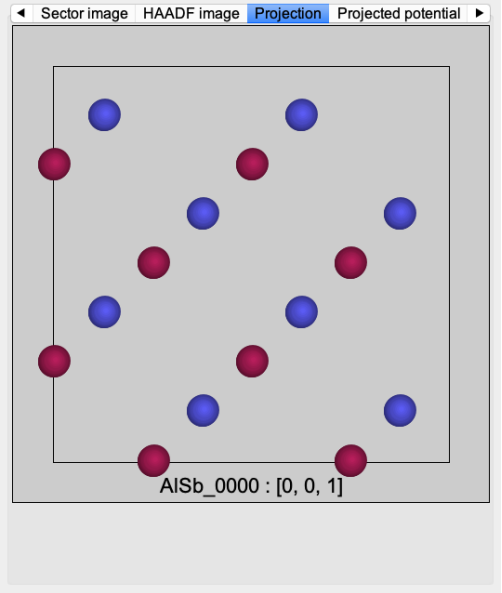


(c)

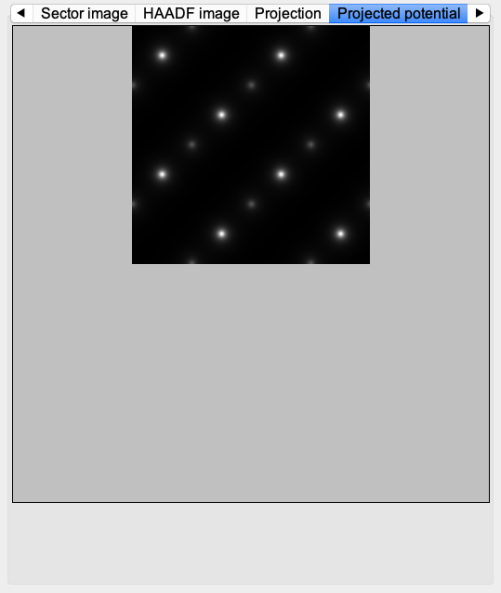


(d)

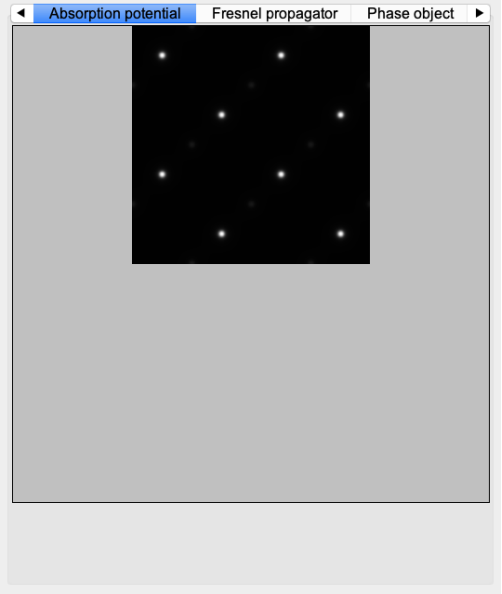
Figure 173: **Bright field**, **Dark field**, **Sector** and **HAADF** image tabs.



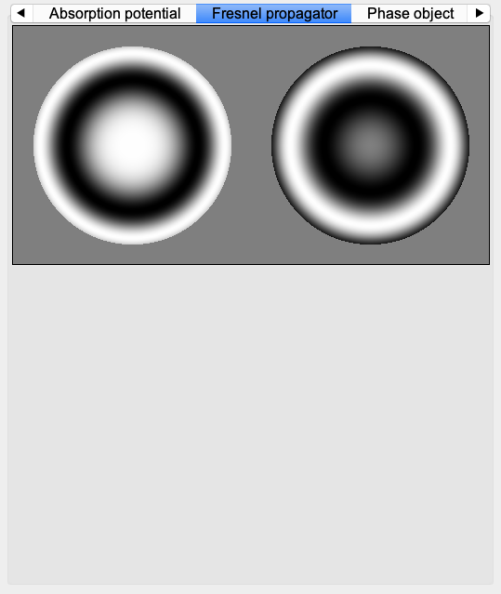
(a)



(b)

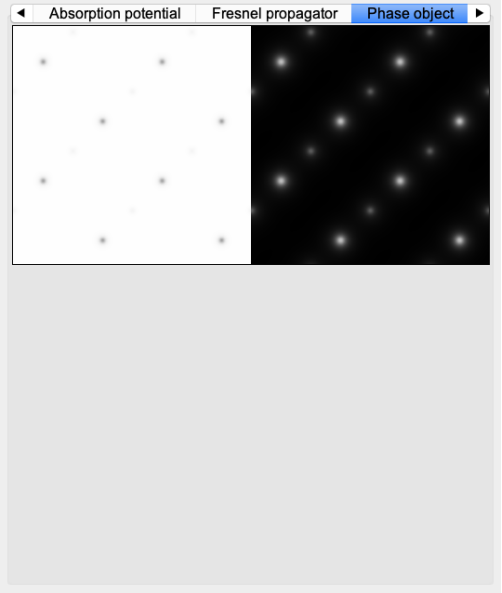


(c)

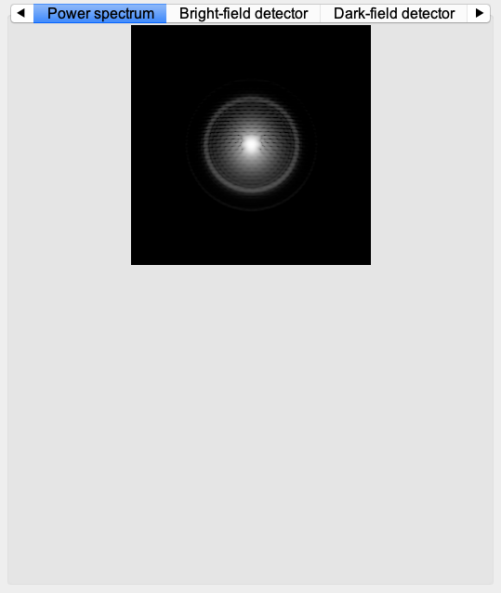


(d)

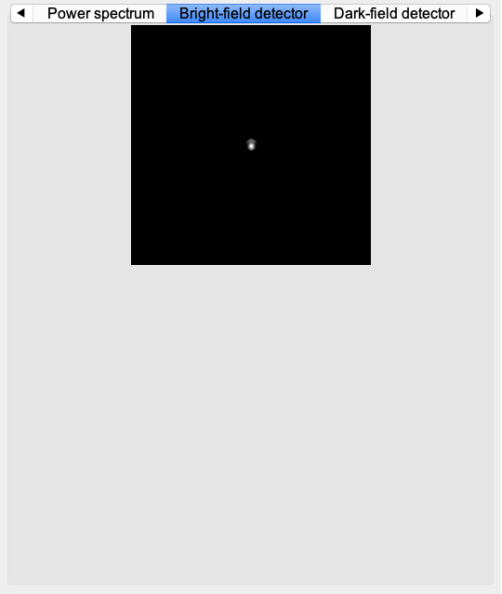
Figure 174: **Projection**, **Projected potential**, **absorption potential**, **Fresnel propagator** image tabs.



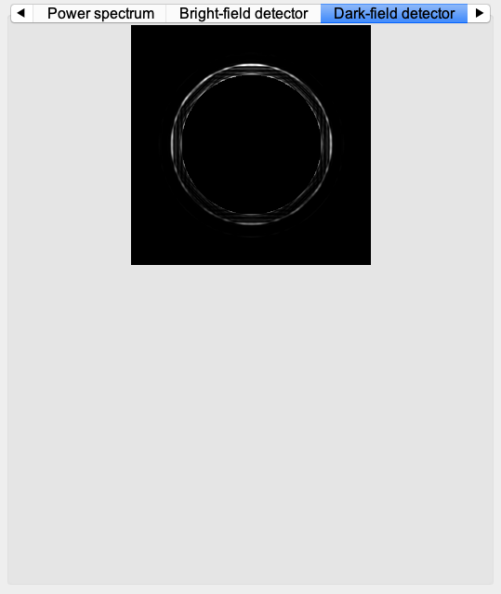
(a)



(b)

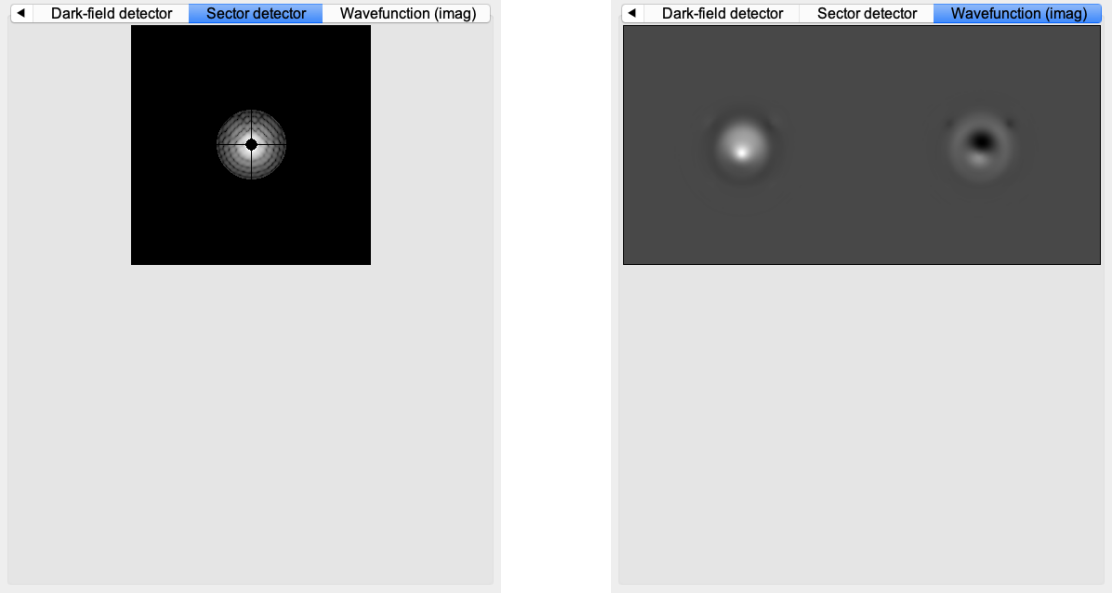


(c)



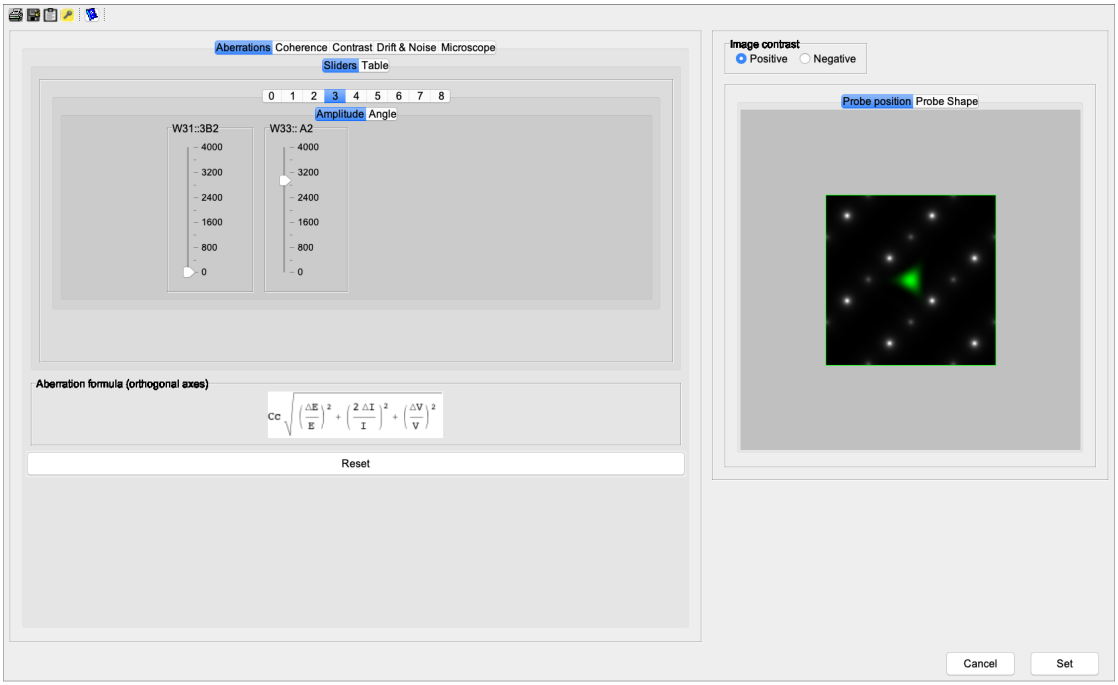
(d)

Figure 175: **Phase object**, **Power spectrum**, **Bright field detector**, **Dark field detector** image tabs.

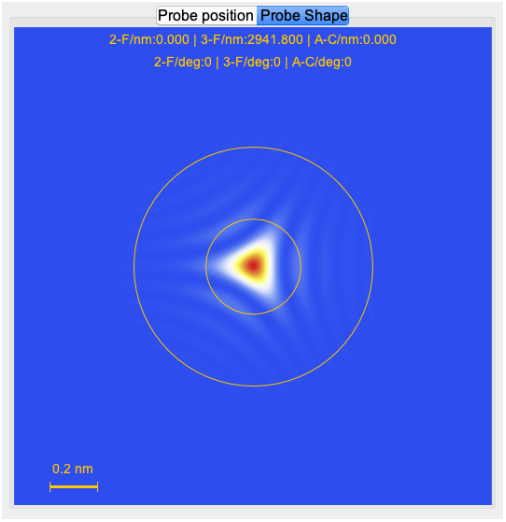


(a) (b)

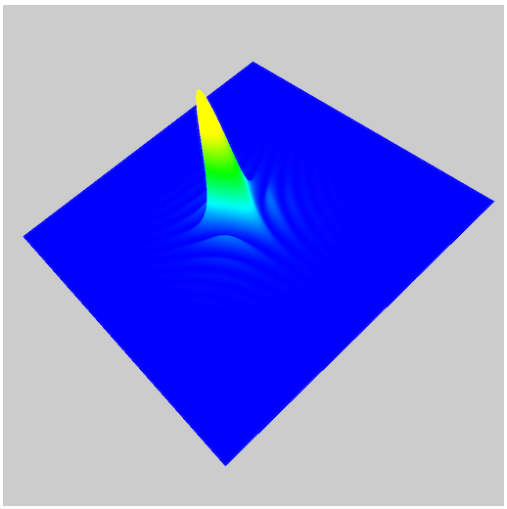
Figure 176: **Dark field detector** and **Wave-function** image tabs.



(a) Probe dialogue with probe shown on projected potential image.



(b)



(c)

Figure 177: **Probe** dialogue and **Aberrated probe** shape 2-D and 3-D (3-fold astigmatism.

The wave-front aberration W_{ij} defines the i^{th} power of the radial angle and the

j^{fold} azimutal angle [36].

[36]The chromatic aberration is W_{00}.

35 Probe imager

The **Probe imager** dialogue sets the probe position and properties (shape) before starting any ADF image calculation (Fig. 178). Depending on the size of the scanned area with respect to the size of the ADF calculation, the probe position will be placed at the middle of the projected potential image or at the middle of the scanned area (Fig. 181a). When smaller than the calculation size the position of the scan area is selectable using the pointer. The probe shape (Fig. 181b) is displayed and its shape changes according to the aberrations, coherence or microscope settings [37].

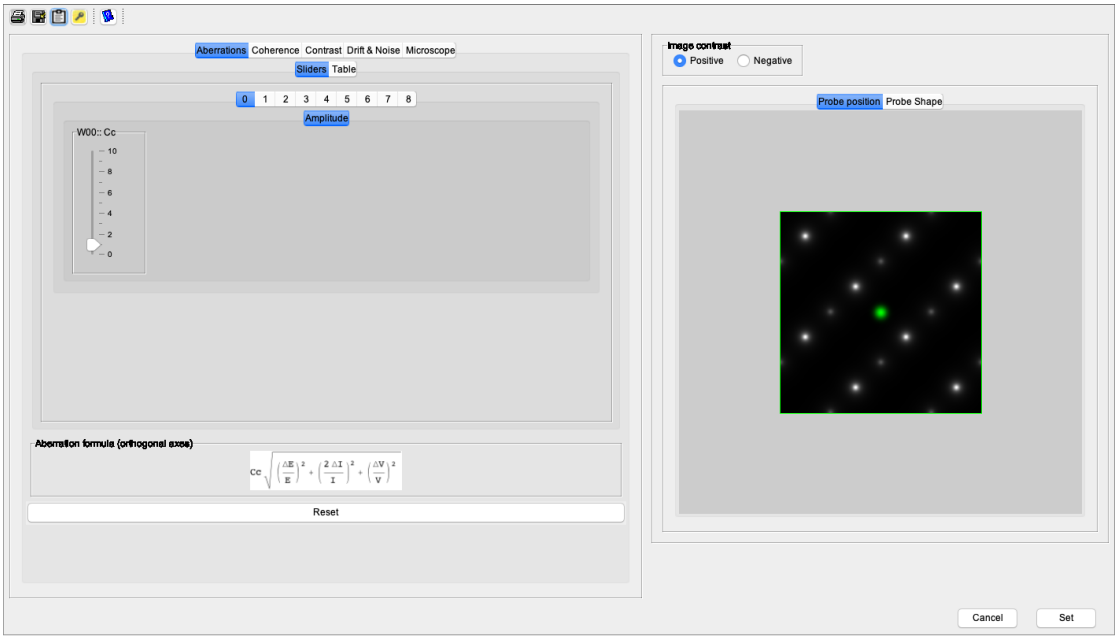


Figure 178: Probe imager dialogue.

Closing the dialogue will start the ADF image calculation.

35.1 Tool buttons

The tool buttons allow to:

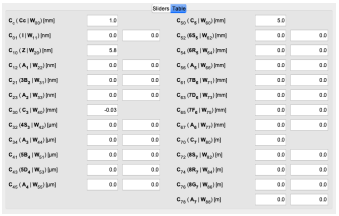
[37] The **Reset** button resets the aberrations and other settings to their default value

-  : print either the probe position or probe shape image.
-  : save the probe position or probe shape image.
-  : transfer the frame to the clipboard.
-  : open the **Keeper** dialogue.
-  : display a help file.

35.2 Tabs

The probe shape and position depends on the aberrations, coherence and several microscope settings that are collected in the following tabs:

- **Aberrations** : to set the aberrations from order 0 (chromatic aberration) to 8 (Fig. 179a) [38].
- **Coherence** : to set the coherence of the illumination (Fig. 180a).
- **Drift&Noise** : to set the **T** **M**agnetic noise and vibration (Fig. 180c).
- **Microscope** : to set the aperture diameter, accelerating voltage and virtual source size (Fig. 180d).



(a) Aberrations table. 3-fold astigmatism in Krivanek (C_{34}), Haider (A_3) and wave-front (W_{44}) notations.

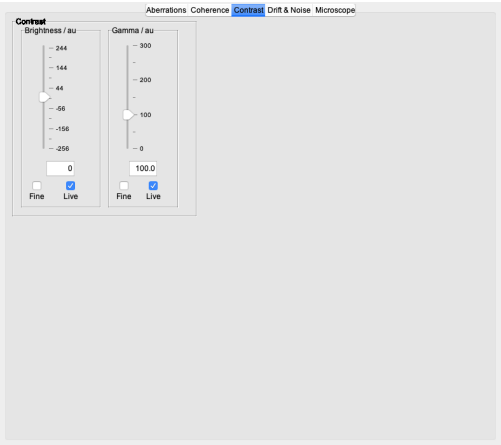
(b) Sliders to set the amplitude of $W_{4i}, i = (0, 2, 4)$ aberrations.

(c) Sliders to set the angle of $W_{4i}, i = (2, 4)$ aberrations.

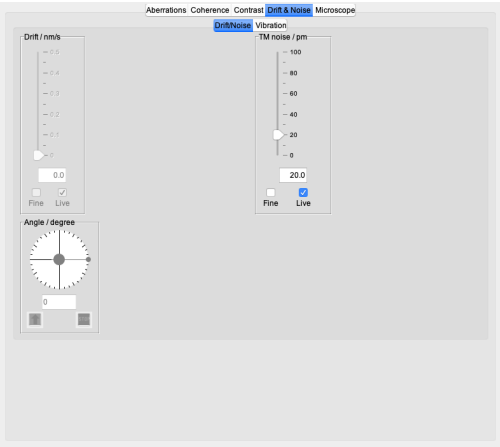
Figure 179: Probe aberrations.

[38] The formula of a particular aberration (in orthogonal axes) is displayed when its value is modified either using the table or the sliders.

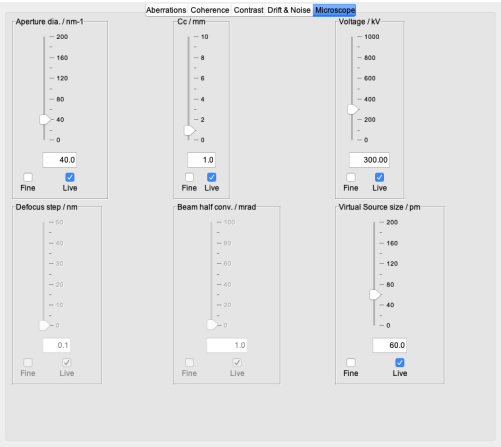
(a) Coherence settings of the microscope illumination.



(b) Contrast tab to modify the contrast of the probe image.



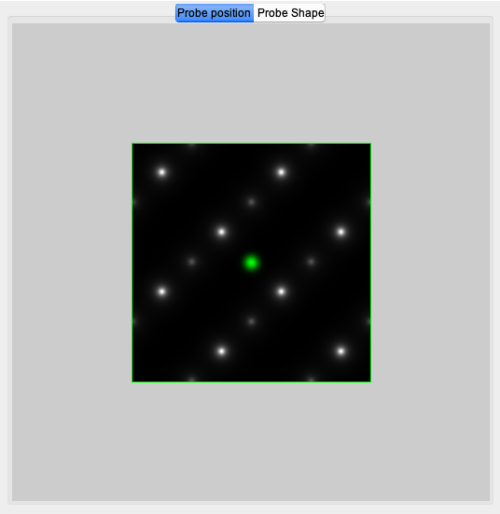
(c) **T**hermal **M**agnetic noise and vibration settings.



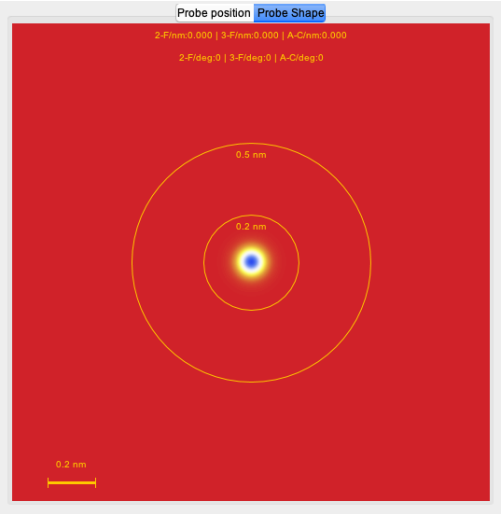
(d) Probe defocus is set using the W_{20} control (Fig. 179a).

Figure 180: Coherence, Contrast, Drift&Noise, Microscope settings.

The probe position image offers a popup menu that allows to save, print and transfer the image to the clipboard. The popup attached to the probe image allows to create a stack of defocused probe images (Fig. 182a) showing the probe shape either along the O_z axis or laterally along the O_x or O_y axes and to display the probe profile and labelled circles (Fig. 182b).

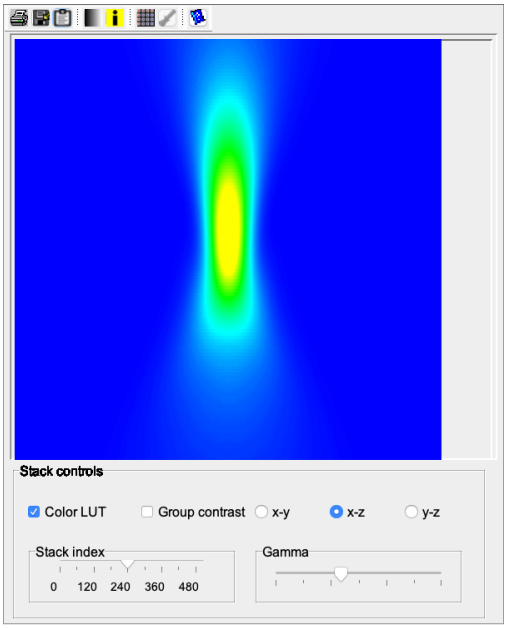


(a) The probe position is placed at the center of the scanned area (controlled by pointer).

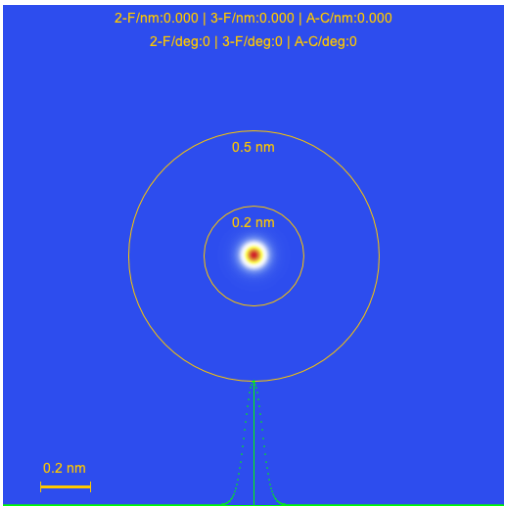


(b) Probe shape is defined using the controls collected in the left tabs.

Figure 181: Probe position and probe shape.



(a) Lateral view of the probe shape as a function of defocus, defocus step 0.1 nm and optimum defocus (-0.03 nm) at the middle of the 512 images stack.



(b) Probe profile and labelled circles.

Figure 182: Lateral probe view and probe profile (obtained using the attached popup menu).

Index