jems GUI

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List of Tables

1 Introduction

This document describes jems Graphical User Interface (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 Modulation Transfer Functions 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 Orientation Relationships between matrix and precipitates (Fig. 26c).
- 6. jemsMicroscopes.txt : the characteristics of the microscope defined using the Parameters \rightarrow Microscope dialogue (Fig. 108).
- 7. jemsPreferences.txt : the jems running preferences defined using the Parameters \rightarrow 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 $[\mu m]$.
- 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 below¹.

NA |Default camera+LA |Default camera+PS|24+R0|1024+C0|1024+M0|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+R0|1024+C0|1024+C0|1024+M0|1+A1|0.28980445861816406+A2|0.6512896418571472+A3|0.013287605717778206+A4|0.04561830684542656+B1|0.45493492+B2|0.912

¹First 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.

			V 🔤 Cubic	
			Name jemsData	NEX ann
			Jernswacc	Jov.ahh
			🗉 Ag.txt 🛛 🔄 Application	er 28, 2019 3:58 PM
> 🚞 AFF	23 Nov 2019 at 10:13	Folder	🗉 Al.txt 🖉 Macintosh	HD
> 🚞 Cubic	12 Nov 2015 at 19:58	Folder	Al14Ca12O33.00	ruesuay, pecember 15, 2020 5:2
> 🚞 Experimental	12 Nov 2015 at 19:58	Folder	Al2Ca3Si3O12Grossularite tyt	Wednesday, December 7, 2022 7:
> 🚞 Hexagonal	12 Nov 2015 at 19:58	Folder		Wednesday, December 7, 2022 7
> 🗖 ICSD	12 Nov 2015 at 19:58	Folder	E Al2MgO4.txt	Wednesday, January 13, 2021 3:
> 🚞 MathematicaCode	13 Jun 2016 at 15:30	Folder	AIAs.txt	Wednesday, January 13, 2021 3:
> 🚞 Miscellaneous	12 Nov 2015 at 19:58	Folder	E AlAs B3 tyt	Tuesday, December 15, 2020 4:1
> 🚞 Monoclinic	13 Jun 2016 at 15:30	Folder		Tuesday, December 10, 2020 4.1
> 🛅 MTF	12 Nov 2015 at 19:58	Folder	E AlCo3 L12.txt	Thursday, July 28, 2022 5:48 PM
> 🚞 Orthorhombic	13 Jun 2016 at 15:30	Folder	■ AlGaAs.txt	Tuesday, December 15, 2020 4:2
> D SuperCell	13 Jun 2016 at 15:30	Folder	E AlMaZn Jm3 txt	Wednesday, January 13, 2021 3
> 🛅 Test	13 Jun 2016 at 15:30	Folder		
> 🚞 Tetragonal	13 Jun 2016 at 15:31	Folder	⊫ AIP.txt	Tuesday, February 7, 2017 7:04 P
> ThicknessMeasurement	13 Jun 2016 at 15:31	Folder	AISh txt	Friday April 17 2020 8:04 PM
> 🚞 Triclinic	13 Jun 2016 at 15:31	Folder		
> 🛅 Trigonal	13 Jun 2016 at 15:31	Folder	$(1) \cap 1 + 1 + 0$	1 / 1 /
			(b) Cubic data tile	s access nath (Ma-

(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 $\sim /jems$).
- 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.



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 "~ /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 factor², 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 , z У , -у у rps|1|-x , z rps|2|-x rps|3|x -y x -z rps|4|z у rps|5|z -x rps|6|-z rps|7|-z х rps|8|y rps|9|-y z rps|10|y rps|11|-y -z rps|12|y x rps|13|-y -x rps|14|y rps|15|-y z х , rps|16|x z rps|17|-x z у У

²Not 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 folder³. 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|sss.yyyy
licenseLicense Code
uniqueID|Unique ID

³This 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).
- $\mathbf{LA}|$: label.
- AV : maximum accelerating voltage [kV].
- \mathbf{CS} : 3^{rd} order spherical aberration coefficient [mm].
- C5| : 5th 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 \blacksquare 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 300 T+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 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|0.0+CC|2.2+ES|1.5+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|0.7+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 HT+LA|Zeiss Libra 200 FE-HT+AV|200.0+CS|0.2+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|Libra 200 Cs-cor.+LA|Zeiss Libra 200 FE Cs-corrected+AV|200.0+CS|0.2+C5|0.0+CC|1.2+ES|0.7+LS|5.0+TM|0.0+VS|5.0+HC|1.0 NA|Libra 200 Gs-cor.+LA|Zeiss Libra 200 FE Cs-corrected+AV|200.0+CS|0.2+C5|0.0+CC|1.2+ES|0.7+LS|5.0+TM|0.0+VS|5.0+HC|1.0 NA|Jel 2000 FEC+LA|Hitachi 2000 field emission+AV|200.0+CS|1.2+C5|0.0+CC|1.4+ES|0.6+LS|5.0+TM|0.0+VS|5.0+HC|1.0 NA|Jeol 2100F+LA|Jeol 2100 field emission+AV|200.0+CS|1.2+C5|0.0+CC|1.4+ES|0.8+LS|1.0+TM|0.0+VS|5.0+HC|1.0 NA|Jeol 2100F+LA|Jeol 2100 field emission+AV|300.0+CS|0.0+CC|1.2+ES|0.8+LS|0.0+TM|0.0+VS|5.0+HC|1.0 NA|Jeol 2100F+LA|Jeol 2100 field emission+AV|300.0+CS|0.0+CC|0.0+CC|1.2+ES|0.8+LS|0.8+LS|0.1+TM|20.0+VS|5.0+HC|1.0 NA|Jeol 3010+LA|Jeol 3010 LaB6 emission+AV|300.0+CS|0.0+CC|0.0+CC|1.2+ES|0.8+LS|5.0+TM|0.0+VS|5.0+HC|1.0 NA|Jeol 4000 EX+LA|Jeol 4000 LaB6 emission+AV|300.0+CS|0.0+CC|0.0+CC|1.2+ES|0.8+LS|5.0+TM|0.0+VS|5.0+HC|1.0 NA|Jeol 4000 EX+LA|Jeol 4000 LaB6 emission+AV|200.0+CS|0.0+CC|0.2+LS|5.0+TM|0.0+VS|5.0+HC|1.0 NA|Jeol 4000 EX+LA|Jeol 4000 LaB6 emission+AV|200.0+CS|0.0+CC|0.2+LS|5.0+TM|0.0+VS|5.0+HC|1.0 NA|Jeol 400 EX+LA|JeOl 2000 LaB6 emission+AV|200.0+CS|0.0+CC|0.2+LS|0.6+LS|0.0+TM|0.0+

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** \rightarrow **Preferences** dialogue \rightarrow **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

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

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

	jems console
/Users/pierrestadelmann/jemsConsole.txt jems started at Sat Feb 19 09:01:38 CET 2022	
The atomic form factors stored in file "/Users/pierrestadelmann/jems/j	emsAFF.txt" have been loaded!
> Host data <	
Platform : Mac OS X	
Host : Imac.home Unique ID : DGKLN0HQF8JC	
> License data <	
Date : Fri Feb 18 14:30:36 CET 2022	
Platform : Mac OS X	
Host : imac.home	
Unique ID : DGKLN0HQF8JC	
Serial : 4556.2020	
License . Djijelik / Olojezuk dykudj4	

(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.



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:

- $\mathbf{\hat{E}}$: load a crystal structure in .txt format.
- \blacksquare : print the atoms table.

- 🖼 : save the atoms table in .txt format.
- 🔲 : transfer a frame or dialogue to the clipboard.
- **I**: **Build** a crystal structure (Fig. 11).
- 😤 : open the **Atom** dialogue (Fig. 17).
- 🖆 : open the Regular Point System (RPS) code dialogue (Fig. 20).
- $\mathbf{\Phi}$: open the **Space-group** dialogue (Fig. 19).
- 🗰 : tabulate the Atomic Form Factors (AFF) (Fig. 18).
- **III** : plot Selected Area Electron Diffraction 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 Contrast Transfer Function (CTF) and Optical Transfer Function (OTF) (Fig. 97).
- Le : plot Powder pattern (line position) for electron, neutron and X-Ray (Fig. 116).
- L: open the **Microscope** dialogue (Fig. 108).
- **Q** : open the **Apertures** dialogue (Fig. 79).
- Solution : show the Wave-front aberrations dialogue (Fig. 96).
- 🗟 : show the **Specimen** dialogue (Fig. 84a).
- III : open the Crystallographic calculator (Fig. 110).
- III : open the **Keeper** dialogue (Fig. 90).
- $^{\mbox{$\scriptstyle 0$}}$: display a **H**elp file.

The **Help** tool button ($^{(0)}$) 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

 $^{^5\}mathrm{Depending}$ 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).

# Atom	Wyckoff	x	у	z	D-W	Occ.	Absorp.	Charge	
0 AI	а	0.000	0.000	0.000	0.005	1.000	0.034	Def	С
1 AI	а	0.500	0.500	0.000	0.005	1.000	0.034	Def	С
2 AI	а	0.500	0.000	0.500	0.005	1.000	0.034	Def	С
3 AI	а	0.000	0.500	0.500	0.005	1.000	0.034	Def	С
4 Fe	b	0.500	0.500	0.500	0.005	1.000	0.047	Def	С
5 Fe	b	0.000	0.000	0.5	Print tal	ble		əf	С
6 Fe	b	0.000	0.500	0.0	Save to	blo		əf	С
7 Fe	b	0.500	0.000	0.0				əf	С
8 Fe	b	0.250	0.250	0.2	Iransfe	er to cli	pboard	əf	С
9 Fe	b	0.750	0.750	0.750	0.005	1.000	0.047	Def	С
10 Fe	b	0.250	0.750	0.750	0.005	1.000	0.047	Def	С
11 Fe	b	0.750	0.250	0.250	0.005	1.000	0.047	Def	С
12 Fe	b	0.750	0.250	0.750	0.005	1.000	0.047	Def	С
13 Fe	b	0.250	0.750	0.250	0.005	1.000	0.047	Def	С
14 Fe	b	0.750	0.750	0.250	0.005	1.000	0.047	Def	С
15 Fe	b	0.250	0.250	0.750	0.005	1.000	0.047	Def	С

(a) Popup menu left panel.



Print Save

Export to Mathematica Label atoms Show cell frame Show powder pattern Show projected potential image Show HAADF image Show SAED pattern Show TDS potential image Show WPOA image Transfer to clipboard [UVW] orientation

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.

⁶It 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).



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



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



(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** \rightarrow **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 button selects the structure and closes the dialogue (Fig. 9).

It is then necessary to confirm the **CIF** structure space-group settings since nonconventional 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.

		Triclinic Mo	noclinic Orthorh	ombic Tetragor	nal Trigonal He	xagonal Cubic	
			Hexagona	al axes Rhombo	ohedral axes		
Trigonal space-	groups::Hexagon	al R 'obverse se	tting' (triple cell)				
	○ P 3	O P 31	O P 32	🔿 R 3	OP-3	🔿 R -3	P 3 1 2
	O P 3 2 1	O P 31 1 2	🔿 P 31 2 1	O P 32 1 2	O P 32 2 1	OR32	P 3 m 1
	○ P 3 1 m	O P 3 c 1	O P 3 1 c	🔘 R 3 m	🔾 R 3 c	🔿 P-31 m	○ P -3 1 c
	○ P -3 m 1	○ P -3 c 1	🔿 R - 3 m	🔘 R -3 c			
Hexagonal lattic	ce parameters						
		a / nm					
		0.5	5741 🛇 🛇	M Y I Y	1.1.1.1.1	00	
			0	5 1	0 15 2	20	
		c/nm					
				. V	1 1 1 1		
		1.3	8588 🛛 🛇 🖉 🛛	5 1	0 15 2	20 20 20	
uivalent reflection	e						
{(h.k.l):(-h-k.h.l):	。 (kh-k.l):(-kh.l)	::(-h.h+k.l):(h+k	-k.l)}				
((-)	(,						

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

4 Crystal builder

The Crystal Builder (CB) is started using menu item Crystal \rightarrow 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:

- $\stackrel{\frown}{\Longrightarrow}$: print the crystal structure drawing.
- \blacksquare : save the crystal structure drawing.
- \blacksquare : transfer the frame to the clipboard.
- $\mathbf{\Phi}$: open the space-group dialogue (Fig. 19).

- \mathbf{L} : 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).



4.2 Tabs



Figure 13: Crystal builder \rightarrow **Atoms** tabs.

4.3 Atoms table's tool buttons

The tool buttons of the atom table allow to:

- $\textcircled{\bullet}$: define a new atom position.
- = : delete the selected atom.
- \checkmark : erase all the atoms.
- \square : modify the selected atom.
- \blacksquare : save the atoms table as a .txt file⁷.

The \bigoplus and \square 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).



Figure 14: Crystal builder \rightarrow Cut, Drawing, Duplicate & View tabs.

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



group description.

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

(c) Point group description.

Figure 15: Crystal builder \rightarrow **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 \rightarrow 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. Atomic Form 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.

	Atom Coordinates					
Atom coordinates	Wyckoff position: P b a a:54					
	a b c d e f Atom charge					
	○ -2 ○ -1 ○ Def ○ +1 ○ +2 ○ +3 ○ +4 ○ +5 ○ +6 ○ Val					
0.000 @ @ 0.25 0.5 0.75 1 @ @	Atomic Form Factor DTSB EJK PRDW WK WKc. XRay JEMS					
Z :						
Dahoa - Waller						
0.005 0 0 0.025 0.05 0.075 0.1 0 0						
Occupancy :						
1.000 @ @ 0 0.25 0.5 0.75 1 @ @						
Absoration :						
	Aller					
	Reset Cu_					

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



The tool buttons of the atom dialogue allow to:

- 🖺 : transfer the dialogue to the clipboard.
- III: display the AFF tables (Fig. 18). ^{8, 9, 10, 11}
- 🧏 : display a help file.

 $^{^8\}mathrm{From}$ Doyle-Turner, Smith-Burge (DTSB), Acta Cryst. **A24** (1968) 390, Acta Cryst. **15** (1962) 182.

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

 $^{^{10}\}mathrm{L.}$ Peng et al. (PRDW), Acta Cryst.
A52 (1996) 257.

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

tent.	Z	0[1]	a [2]	0 [3]	a [4]	0 [1]	6 [2]	p [b]	(b [4]
	1	0.00427	0.00957	0.00802	0.00209	4.17218	16.05892	26.78365	69.4564.3
	2	0.01217	0.02616	-0.00884	0.01841	1.83008	7.20225	16.13585	18,75551
	3	0.00251	0.03576	0.00968	0.0257	0.0262	2.00907	10.80597	130.49226
	4	0.01596	0.02959	0.04024	0.01001	0.38968	1.99208	46.80913	108.84167
	0	0.03652	0.0114	0.00677	0.01506	0.50627	3.68297	27.90586	74.96296
	0	0.04102	0.04911	0.00296	0.00061	0.41335	10.98289	34.80286	177.19113
	7	0.04123	0.0574	0.06529	0.00373	0.29792	7.84094	22.58809	72.59254
		0.03547	0.03133	0.10865	0.01615	0.17964	2.00890	11.79972	38.02912
	9	0.03967	0.07225	0.09581	0.00/92	0.16403	3.96612	12.43963	40.05053
	10	0.02597	0.02197	0.13/62	0.05394	0.09101	0.41253	5.02463	17.52794
	11	0.03283	0.08858	0.11688	0.02516	0.06008	2.07182	7,6444	146.00%52
	12	0.03833	0.17124	0.03649	0.04134	0.07424	2.87177	18.06729	97.00854
	13	0.04388	0.17743	0.00047	0.03957	0.05086	2.53/52	30.43883	98.26737
	14	0.03812	0.17833	0.0628	0.09605	0.05396	1,86461	22.54263	72,43144
	10	0.04166	0.17817	0.09479	0.04463	0.05364	1.6/5	24.45354	04.35204
	10	0.04003	0.58346	0.12218	0.03753	0.05214	1,460793	23.35091	53.596.76
	17	0.04245	0.17645	0.10014	0.03011	0.0404.3	1.15677	19.04091	04.00700
	18	0.05011	0.55667	0.17074	0.04358	0.07991	1.014.36	15.67109	39.60819
	19	0.04058	0.17582	0.20943	0.02922	0.03352	0.82964	14.13679	200.97722
	20	0.04001	0.17410	0.20966	0.05497	0.02289	0.71288	11.10914	1.35.0239
	21	0.09685	0.14777	0.20981	0.04852	0.12527	1.34248	12.43524	131.71112
	22	0.06667	0.17356	0.2271	0.05957	0.05198	0.86467	10.59984	103.56776
	23	0.05118	0.16791	0.267	0.06476	0.03786	0.5716	8.30305	91.78068
	24	0.03204	0.1846	0.30764	0.05052	0.0024	0.44931	7.92251	86.64258
1	25	0.03866	0.17782	0.31329	0.06898	0.01836	0.41203	6.73736	76.30466
	26	0.05455	0.1666	0.33208	0.06943	0.03947	0.43294	6.26864	71.2947
5	27	0.05942	0.17472	0.34423	0.06828	0.03962	0.43253	6.05175	68.72437
	28	0.06049	0.566	0.37302	0.07109	0.03558	0.39976	5.3666	62,46894
1	29	0.08034	0.15838	0.40116	0.05467	0.05475	0.45736	5.38252	60.43276
	30	0.02948	0.192	0.42222	0.0748	0.00137	0.26535	4.4804	54,26088
•	31	0.16157	0.32976	0.18964	0.06148	0.10455	2.18391	9.04125	75.16958
0	32	0.16184	0.35705	0.17618	0.07133	0.0989	2.06856	9.89926	68.13783
1	33	0.0619	0.18452	0.416	0.12793	0.01642	0.32542	3.51888	44.50604
,	34	0.15913	0.41583	0.13385	0.10549	0.07669	1.89297	11.31584	46.32082
	35	0.16514	0.41202	0.129	0.13209	0.08199	1.76568	9.87254	38.1064
	36	0.15798	0.41181	0.14254	0.14987	0.06939	1.53446	8.98025	33.04365
>	37	0.16535	0.44674	0.24245	0.03161	0.07044	1.59236	17.53592	215.26198
	38	0.16039	0.4447	0.24661	0.0584	0.06199	1,41265	14.33812	152.80257
	39	0.16619	0.44376	0.25613	0.06797	0.06364	1.34205	13.66551	125.72522
	40	0.16794	0.44505	0.27188	0.07313	0.06565	1,25292	13.09355	109.50252
5	41	0.16552	0.45008	0.30474	0.06161	0.05921	1.15624	13.24924	98.69958
9	42	0.17327	0.44679	0.32441	0.06143	0.06162	1.11236	12.76149	90.92026
	43	0.16424	0.45046	0.33749	0.07766	0.05081	0.99771	11.28925	84.28943
1	44	0.1875	0.44919	0.36323	0.05388	0.0512	1.08672	12.23172	85.27316
	45	0.16081	0.45211	0.40343	0.0614	0.04562	0.85252	10.51121	74.53949
	46	0.16599	0.43951	0.41478	0.08142	0.04933	0.79381	9.30944	41.17414
	47	0.16547	0.44658	0.45401	0.05959	0.04481	0.75608	9.34354	67.91975
	48	0.17154	0.43689	0.46392	0.07725	0.04867	0.71518	8.40595	64.244
	49	0.15752	0.44821	0.48186	0.08596	0.03672	0.64379	7.83687	73.37281
	50	0.15732	0.44563	0.48507	0.10948	0.03308	0.60931	7.04977	64.83582
	51	0.16971	0.42742	0.48779	0.13653	0.04023	0.58192	6.29247	55.57061
	52	0.14927	0.43729	0.49444	0.1644	0.02842	0.50687	5.60835	48,28004
	53	0.18053	0.44724	0.48163	0.15995	0.0383	0.5834	6.4755	47.0882
	54	0.13141	0.43855	0.50035	0.22299	0.02097	0.41007	4.52105	37.18178
	55	0.31397	0.55648	0.39828	0.04852	0.02813	1,45053	15.05933	100 4883

Figure 18: Tables of the Atomic Form Factors.

4.5 Crystal builder \rightarrow 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.
	Triclinic Monoclinic Orthorhombic Tetragonal Trigonal Hexagonal Cub	xc av			Triclinic M	onoclinic Orthorn	ombic Tetracon	Trigonal Hexad	onal Cubic		
	Conventional space-orpups				Con	wentional snace-o	muns Non-con	entional space or			
rhombic spece-groups (a * indic	ates centric setting)		Orthorhom	nbic space-groups (a * i	indicates centric s	setting)					
P222	○ P21212 ○ P212121 ○ C2221 ○ C222	F222 01222	 16 	P222	17	P 2 2 2 1	18	P 21 21 2	01	P 21 21 21	
○ I 21 21 21 ○ P m m 2	OPmc21 OPcc2 OPma2 OPca21	Pnc2 Pmn21	20	C 2 2 21	21	C 2 2 2	22	F222	02	3 1222	
OPba2 OPna21	OPnn2 OCmm2 OCmc21 OCcc2	Amm2 Aem2	24	1212121	25	Pmm2	26	Pmc21	0 2	7 Pcc2	
🔿 Ama2 👘 🔿 Aea2	○Fmm2 ○Fdd2 ○Imm2 ○Iba2 ○	Ima2 Pmmm	28	Pma2	29	Pca21	0 30	Pnc2	0 3	1 Pmn21	
O'Pnnn O Pccm	⊖ "Pban ⊖ Pmma ⊖ Pnna ⊖ Pmna ⊖	Pcca OPbam	32	Pba2	33	Pna21	0.34	Pnn2	0 3	5 C m m 2	
Pccn OPbcm	⊖Pnnm ⊖*Pmmn ⊖Pbcn ⊖Pbca ⊖	Pnma OCmcm	0.36	Cmc21	37	Geo2	38	Amm2	B 03	A A A A A A A A A A A A A A A A A A A	
Cmce OCmmn	n OCccm OCmme O*Ccce OFmmm ("Fddd Olmmm	0.40	Ama2	A1	A	A2	Emm2		Edd2	_
lbam Olbca	○ Imma			lmm2		lba2		Ima2		Ree	_
nomble space-groups (alternate	a non-centric setting)		0.44	10		Deer		Timaz		Pana	_
	⊃Pnnn ○Pban ○Pmmn ○Ccce ○Fddd		40	Pana	48	Peem	000	Poan		Pmma	_
ombic lattice parameters			0.52	Pnna	0 00	Pmna		Peca		Poam	_
	a / nm		56	Pcch	5/	Pocm	58	Pnnm		Pmmn	_
	0.619 0 0		0 60	Pbcn	61	Pbca	62	Pnma	0 06	3 Cmcm	_
	0 5 10 15 20		64	Cmce	○ 65	Cmmm	0 66	Ccom	06	7 Cmme	
	b/nm		68	*Ccce	69	Fmmm	070	*Fddd	07	1 Immm	
			072	Ibam	○ 73	Ibca	074	Imma	0		
	0.619 0 0 5 10 15 20 0 0										
	c / m										
	0.619 00 5 10 15 20 00										
				Orthorho	mbic space-grou	ps (alternate non-ce	entric setting)				
alast an Bandana				0.48	Pnnn	50	Pban	59	Pmmn	0	
SIGHT, FOR COURSE				68	Cone	0.70	Eddd	6			
,k,J);(h,-k,J)}							1000				

(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.
- III: display the space-group general and special positions as well as its pointgroup (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** \rightarrow **System** \rightarrow **RPS** code or tool button is only available from the main jems window (Fig. 20) ¹².

The tool buttons of the RPS code dialogue allow to:

- \blacksquare : 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.

nunc / non-centurc setung No	⊖ Yes		
yatal system & lattice parameters	Add/Delete/Clear n	ps code	
Triclinic Monoclinic Orthorhombic Tetragonal Trigonal Hexagonal Cubic		0 0	1 🥜
a / nm	DDC code Bot		
0.610 0.0	KPS COOL INST	L V	7
0 5 10 15 20	x	y	7
	-X	-V	z
	-x	ý	-Z
	x	-y	-Z
	z	x	У
	z	-X	-y
	-z	-x	У
	-Z	x	-y
	У	z	x
	-y	z	-x
	у	-Z	-X
	-у	-Z	x
	у	x	z
	-у	-X	z
	У	-X	-z
	-у	x	-Z
	x	z	У
	-X	z	-y
	-X	-Z	У
	x	-Z	-y
	Z	У	x
	Z	-y	-x
	-Z	У	-X
	RPS code status	_M	v
	11 0 000 04100	I::rps code number :	24
ubelont reflections			
where the second s	k (b))		

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

- III: 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:

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

Add The 🕀 tool button opens the RPS code editor dialogue (Fig. 21a). The Done adds a new code and 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 (c) jems does not check the (or entering the code di- new code validity \rightarrow 3-D rectly) to define a new code view of the updated unit-(x, y + 1/4, z - 1/2).



cell.

Figure 21: RPS code editor.

¹³For example in case of phase transformation.

5 SAED patterns

Plotting Selected Area Electron Diffraction patterns (SAED) is activated by either the **Drawing** \rightarrow **Diffraction** menu item or the tool button \blacksquare . The SAED frame (Fig. 22) shows the SAED pattern of the crystal structure shown in (Fig. 3) along the selected [uvw] zone axis.

Collection data: 10 000, 0 000, 0 000) 2019 anti: [0, 0, 1]	Avalance Crystal / matrix Diffraction Lation Laue zones Options Orientation I 1 10 10 11
Fe3AI (136 reflections) AV/kV:300.000, CL/mm:1000, ZA:[0, 0, 1], FN:[0, 0, 1]	

Figure 22: SAED patterns frame.

5.1 Tool buttons

The tool buttons of the SAED frame allow to:

- \blacksquare : print the SAED pattern.
- 📑 : save the SAED pattern.
- \bullet \blacksquare : transfer the frame to the clipboard.
- \overleftrightarrow : load an experimental SAED pattern.

- \blacksquare : move the Center of the Laue Circle (CLC) down.
- **1** : move the CLC up.
- 🖛 : move the CLC left.
- \blacksquare : move the CLC right.
- O: reset the CLC to (0,0,0) reflection.
- $\mathbf{\tilde{y}}$: search the closest zone axis.
- L: 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).
- III: 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).

0.0.1											
ematical reflections	s list	Mi Malt	Amelikuda	Obaca daa	liel on t	(Hell am	10/00	d(a. a0)	I ave more	Devis on f	Palacit 1
2.0.0)	-A 16756	-0 38805	A 18550	-174 68035	3 23102	0.3095	1,000	0.000000	0	-0.01028	o exected
	-4.10730	0.300/0	4.10009	-174.00030	3,23102	0.3095	1,000	180,000	0	-0.01020	100
1 2 0)	4 16756	-0.38805	4 18559	-174 68035	3 23102	0.3095	1,000	90.000	0	-0.01028	1010
0.2.0)	-4.16756	-0.38805	4 18559	-174.68035	3 23102	0.3095	1,000	90.000	0	-0.01028	100
(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	100
(2, 2, 0)	10.21959	0.94507	10.2632	5 28348	4.56935	0.21885	1.41421	135,000	0	-0.02055	1010
(2.2.0)	10.21050	0.94507	10.2632	6 29349	4.66026	0.21995	1.41421	45,000	0	-0.02055	100
(0,4,0)	6 76917	0.79209	6.81535	6.67409	6,46204	0.15475	2 000	90.000	0	-0.04111	1010
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	toue
(4 0 0)	6 76917	0.79209	6.81535	6.67409	6.46204	0 15475	2 000	0.000000	0	-0.04111	frame
(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	toue
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 05681	8 31444	9.1387	0.10942	2.82843	45,000	0	-0.08221	true
(44.0)	4.02407	0.58808	4.06681	8.31444	9.1387	0.10942	2.82843	135,000	0	-0.08221	true
(-44.0)	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
(06.0)	-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
(62.0)	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
26.0)	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
(4, -6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	123.69007	0	-0.1336	true
(-4, -6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	56.30993	0	-0.1336	true
(-6, -4, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	33.69007	0	-0.1336	true
(4, 6, 0)	-0.73653	-0.19703	0.76243	-165.02354	11,6496	0.08584	3.60555	56.30993	0	-0.1336	true
(6, -4, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	146.30993	0	-0.1336	true
(6, 4, 0)	-0.73653	-0.19703	0.76243	-165.02354	11.6496	0.08584	3.60555	146.30993	0	-0.1336	true
(4, 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	finue

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).



Figure 25: First 6 tabs of SAED plotting controls.

 $^{^{14}\}mathrm{Only}$ 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 pattern center, i.e. the center of the (0, 0, 0) reflection.

¹⁵The 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 \rightarrow Move center selected.



(c) SAED drawing with HOLZ reflections and lines.



(b) 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.



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



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.



(b) Acceptance angle slider and its popup menu.

The source of the Atomic Form Factors (AFF) is selected using the radio buttons of Fig. 30b. The source is described by a little tip text.



(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 \blacksquare tool button. The deviation should be set to a low value (~ 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** \rightarrow **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:

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

- S: 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.
- \blacksquare : tabulate the (h, k, l) reflections (Fig. 37).
- \blacksquare : open the toolbox with context dependent controls.
- 🖉 : open the **Keeper** dialogue (Fig. 90).
- 🚾 : reset the wave-front aberrations and imaging conditions.
- $^{\mbox{$\scriptstyle 0$}}$: open the associated help dialogue.

272 884 688 1 949

remartical reflection	Itr/nm2	LII / nm2	Amoli Volt	Phase Dec.	lial /em	26.0.0.0	Set(1+a.n/K.n)	Strong	Laue 200e	CRED 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
01.0)	4.17602	0.55147	6.33582	7.52268	2.66738	0.000000	1.000	¥95	0	0.000000
1.0.0)	4.17602	0.55147	6.33582	7.52268	2.66738	0.000000	1.000	¥05	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	V05	0	0.000000
(11.0)	3.63556	0.53031	5.52623	8,29899	3.77224	0.000000	1.000	¥95	0	0.000000
1,1,0)	3.63556	0.53031	5.52623	8.29899	3.77224	0.000000	1.000	VPS	0	0.000000
(-1, 1, 0)	3.63556	0.53031	5.52623	8,29899	3.77224	0.000000	1.000	¥05	0	0.000000
(2.0.0)	12.5745	1.00713	18.97427	4.57924	5.33476	0.000000	1,000	¥95	0	0.000000
-2.0.0)	12.5745	1.00713	18.97427	4.57924	5.33476	0.000000	1.000	V05	0	0.000000
02.01	12.5745	1.00713	18.97427	4.57924	5.33476	0.000000	1.000	¥95	0	0.000000
0.2.0)	12.5745	1.00713	18.97427	4.57924	5.33476	0.000000	1.000	V05	0	0.000000
21.0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	V05	0	0.000000
(-1.2.0)	2.57044	0.48372	3.93414	10.65756	5.96444	0.000000	1.000	VPS	0	0.000000
1.2.01	2.57044	0.48372	3 03414	10.65758	5.08444	0.000000	1.000	1005	0	0.000000
2.1.0)	2.57044	0.48372	3.93616	10.65756	5.06444	0.000000	1,000	105	0	0.000000
(12.0)	2.57044	0.48372	3,93414	10.65756	5.96444	0.000000	1,000	V05	0	0.000000
(-2.1.0)	2.57044	0.48372	3 93414	10.65756	5 95444	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	105	0	0.000000
(1.2.0)	2.57044	0.48972	3.03414	10.65758	5.00444	0.000000	1 000	100	0	0.000000
(2,2,0)	0.01473	0.88616	13,62471	5,61421	2 54448	0.000000	1,000	905	0	0.000000
(-2.2.0)	9.01473	0.53616	13.62471	5,61421	7.54448	0.000000	1,000	900	0	0.000000
(2.2.0)	9.01473	0.88616	13,62471	5.61421	7 54448	0.000000	1,000	105	0	0.000000
(22.0)	0.01473	0.88616	12 42471	5.61421	7.5///8	0.000000	1,000	100	0	0.000000
(2, -2, 0)	1.84044	0.4458	2 86148	19.65220	8.00213	0.000000	1,000	905	0	0.000000
(0,0,0)	1.84044	0.4458	2.86148	13.65220	8.00213	0.000000	1,000	900	0	0.000000
(3, 0, 0)	1.84044	0.4458	2 00140	13.55220	8.00213	0.000000	1,000	1000	0	0.000000
0.0.0)	1 84044	0.4458	2.05148	13 66220	8.00213	0.000000	1,000	100	0	0.000000
(0, 3, 0)	4 79704	0.49655	2.00140	10.00229	8.43400	0.000000	1,000	905	0	0.000000
(1,0,0)	1 72704	0.43611	2.68055	14 16400	8.43400	0.000000	1,000	yes	0	0.000000
(-1 -3 0)	1 72704	0.43611	2.68055	14 16400	8.43400	0.000000	1,000	905	0	0.000000
(-1,-3,-0)	1 72704	0.43611	2.68055	14 16400	8.43400	0.000000	1,000	900	0	0.000000
(3, 4, 6)	1 72704	0.43611	2.68055	14 16400	8.43400	0.000000	1 000	100	0	0.000000
(5, 1, 0)	1 72704	0.43611	2.68055	14 16400	8.43400	0.000000	1,000	905	0	0.000000
(1,-3,0)	1.72704	0.43611	2.68055	14.16400	8.43499	0.000000	1,000	905	0	0.000000
(3, 1, 0)	1 72704	0.43611	2.68055	14 16400	8.43400	0.000000	1,000	900	0	0.000000
(3,-1,0)	1.44120	0.40036	2.05050	16.85570	0.61737	0.000000	1,000	100	0	0.000000
(2.3.0)	1.44120	0.40936	2 25353	15.85570	0.64737	0.000000	1,000	905	0	0.000000
(2, -3, 0)	1.44420	0.40936	2 26363	10.00079	9,61737	0.000000	1,000	905	0	0.000000
3.2.00	1.44120	0.40936	2 25 363	15 85570	0.61737	0.000000	1,000	905	0	0.000000
3,2,0)	1.44120	0.40936	2 26363	15 85570	0.61737	0.000000	1,000	1000	0	0.000000
3.3.00	1.44120	0.40036	2 25363	10.00079	0.61737	0.000000	1,000	905	0	0.000000
(3, 3, 0)	1.44420	0.40036	2 26363	46.86670	0.64737	0.000000	1,000	yes	0	0.000000
(e, 0, w)	1.444.20	0.40036	2,20303	10.03079	0.64737	0.000000	1,000	905	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.



Beam half conv. / mrac

100

80

60

40

20

0

Fine

1.0

Live



(c) CBED panel.

тсс

50

40

30

-- 20

10

2.2

Fine Live

Envelope

Coherent

10

80

60

40

20

1.0

✓
Live

Fine

(b) Channeling panel.

Illumination Iteration



(d) HREM map panel.



(f) Tilt table panel.

Defocus / nm : 9.41

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 Bloch-Wave (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 Transmission Cross Coefficients.
- 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, Thermal Magnetic 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 Thermal Magnetic noise (TM).
- Yellow: thermal magnetic noise ²⁰.

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

¹⁷When placing the pointer (mouse) on the transfer function drawing, the defocus is modified using the keyboard arrow keys \uparrow and \downarrow

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

¹⁹The 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 (b) Popup associated with the imaging model. transfer function



(c) Starting defocus (d) Defocus series [nm] (minimum), de- size and duplication focus step [nm]. of unit cell image.

	0		
Crystal Reference Mag. Options Reference Start after 2 0 2 40 03 100 Number	Cystal Proteine Mar Cytore Refectors Na Options & Atomic columns & Monage Arrightade O Intensity & Phase	Crysta Frances May Crysta Frances May Crystal Refections Assess From France DT58 E.K. PROW WK WK WG, XRay JEMS Page 10 Page 1	Crystal Hickness Map Cythons References Nameer 20 © 0 00 130 130 200 200 ©
$0 \otimes 1 22 41 41 41 01$	Perciproves		Bohara sakolar Ni Bahara Natedoni Nunter: 0 Storrg : 0 Week: 0

menu

(e) Minimum crys- (f) Plot and map op- (g) HREM map iter- (h) Reflections numtal thickness [nm], tions. ation options. ber and Bethe apnumber of iterations, proximation. thickness increment

[nm].

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 aberra- (b) Defocus $[nm] 3^{rd}$ and (c) Image shift [nm] and tions [nm] and objective 5^{th} order spherical aberra- phase shift [deg]. aperture size $[nm^{-1}]$ tions [mm].

Figure 41



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



(b) Specimen vibration [nm].

Figure 42

When the MTF of the camera Modulation Transfer Function (MTF) has been measured it is possible to introduce its effect in the HRTEM image simulation. This requires to enable the **Plot** \rightarrow **Image** check box (**Iteration** \rightarrow **Map** \rightarrow **Plot** \rightarrow **Image**). When HRTEM image calculation is completed select the panel (**HREM map** \rightarrow **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.

 $^{^{21}\}mathrm{To}$ 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 .

²²A 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).



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



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



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



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



(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).



(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.



(b) Tool box of **Map** context to change 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 Convergent Beam Electron Diffraction (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.



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

🖸 Shov	v Area	Gam	ma 🔽 i	ZOLZ	Linear 💿	Log
LACBED op	tions					
LACB	ED	S	ave		Shift	
Atomic Form	n Factor					
DTSB	EJK	PRDW	wĸ	WKc.	XRay	JEMS

(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.



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

Strong reflections Number	-	
53 (0 50 100 150	200 250
Bloch-wave select	ion	
All	۵	Bethe
Reflections		
Number: 0	Strong : 0	Weak:0
iterations/HOLZ shift		
Performed : 0	Total : 0	FOLZ volt. [kV] : 277.321

(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.

			1-56-1	10		
1st LZ						
01	2	05	0 10	0 20	0 50	10 ²
O 2 10 ²	\odot 5 10 ²	\odot 10 ³	O 10 ⁴	\odot 10 ⁵	\odot 10 ⁶	10 ⁷
2nd LZ						
01	<u>2</u>	05	0 10	0 20	0 50	10 ²
O 2 10 ²	○ 5 10 ²	$\odot10^3$	O 10 ⁴	○ 10 ⁵	O 10 ⁶	0 10 ⁷
3rd LZ						
01	<u>2</u>	05	0 10	0 20	0 50	10 ²
C 2 10 ²	O 5 10 ²	$\odot10^3$	○ 10 ⁴	\odot 10 ⁵	\odot 10 ⁶	○ 10 ⁷
4th LZ						
01	<u> </u>	05	0 10	0 20	0 50	10 ²
O 2 10 ²	\odot 5 10 ²	$\odot10^3$	○ 10 ⁴	\odot 10 ⁵	$^{\circ}$ 10 ⁶	_ 10 ⁷
5th LZ						
01	<u> </u>	05	0 10	0 20	0 50	0 10 ²
O 2 10 ²	O 5 10 ²	$\odot 10^3$	O 10 ⁴	O 10 ⁵	O 10 ⁶	O 10 ⁷

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

68 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.

Figure 50: CBED controls tabs.

Editable	Real	Imaginary	Amplitude	Phase
🗹 (0, 0, 0)	54.67317	3.73953	54.80091	3.91282
🖸 (-1, 1, 1)	6.14193	-9.63717	11.42796	-57.48995
🖸 (1, -1, 1)	6.14193	-9.63717	11.42796	-57.48995
🖸 (1, -1, -1)	4.65215	10.32161	11.32158	65.73797
🗹 (-1, 1, -1)	4.65215	10.32161	11.32158	65.73797
🗹 (0, 0, -2)	-4.16756	-0.38805	4.18559	-174.68035
🛛 (0, 0, 2)	-4.16756	-0.38805	4.18559	-174.68035
🗹 (-2, 2, 0)	10.21959	0.94507	10.2632	5.28348
🛛 (2, -2, 0)	10.21959	0.94507	10.2632	5.28348
🗹 (1, -1, 3)	2.41618	5.78773	6.27182	67.34113
🗹 (-1, 1, 3)	2.41618	5.78773	6.27182	67.34113
🖸 (1, -1, -3)	3.64229	-5.25262	6.39189	-55.26165
🗹 (-1, 1, -3)	3.64229	-5.25262	6.39189	-55.26165
🗹 (2, -2, -2)	-2.35438	-0.34001	2.3788	-171.78228
🗹 (-2, 2, -2)	-2.35438	-0.34001	2.3788	-171.78228
2 (2, -2, 2)	-2.35438	-0.34001	2.3788	-171.78228

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



(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:

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

- Map, Plot, Projection tabs controls.
- 🖾 : open the **Transfer function** frame (Fig. 97).
- 🚾 : reset the wave-front aberrations and imaging conditions.
- $^{\mbox{0}}$: 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: High Angle Annular Dark Field 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 be- (b) Phase object function of (c) Projected potential of a tween slices (4×4) unit a slice (4×4) unit cells. slice (4×4) unit cells.. cells.



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



(f) HAADF image.



(g) HAADF probe dialogue.



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



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



2 unit cells, $4 \ge 4$ images).

(i) HREM image maps (2 x (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 \rightarrow Options \rightarrow Others & Plot \rightarrow 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).

(d) Nano-diffraction tab.



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



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



(e)



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

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

Nano-diffraction

tern, projected model.

pat-

The images and maps dimension (width, height) are set in the **Parameters** \rightarrow **Preferences** \rightarrow **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 $1 \times 1 [nm^2]$ 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 $10 \times 10 \ [nm^2]$ 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** \rightarrow **HOLZ reflections** tab (Fig. 57a). Some of the controls are put in a sub-tab **Multislice** \rightarrow **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** \rightarrow **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 Beset button erases the Phase Object Function (POF). The POF images can be saved for futur use or loaded in order to redo a calculation.

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

Include					Reset	
humber of sub-slices					resor	
1		2		3	0 4	
0 6		8		9	0 12	
0 16		18		24	0 32	
0 48		64		128	0 256	
Show						
Projected potential	Slices potential				Wavefunction	
Wave or reflection plot						
Potential generation						
Analvtic		Direct			Fourier	
Phase object manager						
Load phase-object			Sav	/e phas	e-object	
,,,,,,,,,						

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

France letting	HOLZ refle	ections Frozen la	ttice		
Frozen lattice		Temperatu	ire (K)		
Bicubic	Enable	0	400	800	

(b) Multislice \rightarrow Frozen lattice tab controlling atom displacement and potential interpolation.

Figure 57: **HREM** \rightarrow **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).

nns CLC selector Coherence Dark field Defocus DefocusSeries Drift & Noise Holography Imaging ► Silders Table	Wave-function display Real Imaginary Amplitude Phase Power specrum I Positive Negative
0 1 2 3 4 5 6 7 8	Image display
0:: Cc	Image Diffractogram
- 10	Image CTE Wavefunction
- 0 - 0 - 0	AuGu3_112.Thomass 4.6, delica: 102.intensity
amula (arthogonal axes) $Ce \sqrt{\left(\frac{\Delta E}{E}\right)^2 + \left(\frac{2\Delta I}{2}\right)^2 + \left(\frac{\Delta V}{V}\right)^2}$	2525
Reset	
	0000

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

8.1 Tool buttons

The tool buttons of the HRTEM imager allow to:

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

- 📋 : transfer the HRTEM frame to the clipboard.
- \cong : open a wave-function (.ems file).
- 🔳 : set the default gray LUT.
- **L**: open the **Microscope** dialogue (Fig. 108).
- 🖉 : open the **Keeper** dialogue (Fig. 90).
- \bullet \blacksquare : reset the aberrations.
- atural: open the associated help dialogue.



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



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

Figure 60: HRTEM imager, right tabs.



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

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.

²⁴The maximum aberration order is defined in **Parameters** \rightarrow **Preferences** \rightarrow **Imaging** \rightarrow **Others** tab.

²⁵The 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.

²⁷When placing the pointer (mouse) on the transfer function drawing, the defocus is modified using the keyboard arrow keys \uparrow and \downarrow .

²⁸The defocus series can be loaded and imaged using menu item **Imaging** \rightarrow **Load** \rightarrow **Stack**. ²⁹The **Stretch** option increases the image contrast.



(a) Aberrations are defined using sliders.



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



(e) Illumination coherence.



Camera MTF Aberrations	CLC selector	Coherence	Dark field	Defocus	DefocusSeries	Drift & Noise	Holography >
			Sliders Ta	ble			
$C_{c} (Cc W_{00}) [mm]$	1.0		с	₅₀ (C ₅ W	60) [mm]	5.0	
$\mathbf{C}_{01}(\mathbf{I} \mathbf{W}_{11})$ [nm]	0.0		0.0 C	₅₂ (65 ₅ V	(₆₂) [mm]	0.0	0.0
$\mathbf{C}_{10} (\mathbf{Z} \mathbf{W}_{20}) [\text{nm}]$	9.4		с	₅₄ (6R ₅ V	V ₆₄) [mm]	0.0	0.0
$\mathbf{C}_{12} (\mathbf{A}_1 \mathbf{W}_{22}) [\text{nm}]$	0.0		0.0 C	₅₆ (A ₅ W	66) [mm]	0.0	0.0
$C_{21} (3B_2 W_{31}) [nm]$	0.0		0.0 C	₆₁ (78 ₆ V	V ₇₁) [mm]	0.0	0.0
$\mathbf{C}_{23}^{}(\mathbf{A_2}^{} \mathbf{W}_{33}^{})[\mathrm{nm}]$	0.0		0.0 C	₆₃ (7D ₆ V	V ₇₃) [mm]	0.0	0.0
$\boldsymbol{C}_{30}(\boldsymbol{C}_{3} \boldsymbol{W}_{40})[mm]$	-0.03		с	₆₅ (7F ₆ W	(₇₅) [mm]	0.0	0.0
${f C}_{32}({f 4S}_3 {f W}_{42})[\mu m]$	0.0		0.0 C	₆₇ (A ₆ W	77) [mm]	0.0	0.0
$\mathbf{C}_{34}(\mathbf{A_3} \mathbf{W}_{44})[\mu\mathrm{m}]$	0.0		0.0 C	₇₀ (C ₇ W	₈₀) [m]	0.0	
$\mathbf{C}_{41} (\mathbf{5B}_4 \mathbf{W}_{51}) [\mu m]$	0.0		0.0 C	₇₂ (85 ₇ V	(₈₂) [m]	0.0	0.0
${\bf C}_{43}({\bf 5D}_{4} {\bf W}_{53})[\mu{\rm m}]$	0.0		0.0 C	₇₄ (8R ₇ V	V ₈₄) [m]	0.0	0.0
${f C}_{45}({f A}_{4} {f W}_{55})[\mu m]$	0.0		0.0 C	₇₆ (8G ₇ V	V ₈₆) [m]	0.0	0.0
			с	₇₈ (A ₇ W	₈₈) [m]	0.0	0.0
Aberration formula (orthogo	nal axes)						
		$ce \sqrt{\left(\frac{\Delta E}{E}\right)}$	$^{2} + \left(\frac{2 \bigtriangleup I}{I}\right)$	$\Big)^2 + \Big(\frac{\bigtriangleup v}{v}\Big)$)2		
			Reset				

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



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



(a) Dark field condition.



(c) Defocus setting.



(b) CTF in dark field condition.

W20 (defocus) / nm	Defocus step / nm	Defocus series size
- 300	- 50	- 100
	-	-
- 100	- 40	- 80
¢.	-	-
100	- 30	- 60
-	-	-
300	- 20	- 40
-		-
500	- 10	- 20
700	<u> </u>	<u> </u>
9.4	0.1	1
Fine Live	Fine Live	Fine Live
aries options		
Save ems	Save	html
efocus series		
Start		Stop

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

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



(a) Drift & Noise.



(c) Biprism voltage and orientation.



(d) HRTEM image in holography mode.

(b) Vibration.



(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.





(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.

³⁰The 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

	Aberrations Coherence Drift & Noise	Imaging Microscope	Display images as
tress & Contrast	Contrast Law	Orange Law	O Positive Negative
gniness / au	Contrast / au	Gamma / au	
- 244		- 300	HAADF Image Probe Intensity
- 144	- 4	-	
		- 200	
- 44			
L 56	- 2		
		Ç- 100	
156			
	* - 0	1 - 0	
0	1.0	100.0	
	 Image: Image: Ima		
ne Live	Fine Live	Fine Live	
erion & oste			
ge X-tiling	Image Y-tiling	% noise level	
- 30	- 30	- 100	
		- 60	
- 20	- 20	- 60	
		- 40	
- 10	- 10		
P		- 20	
- 0	- 0	-0	
-			
0	6	0.0	

Figure 68: HRSTEM imager.

9.1 Tool buttons

The tool buttons allow to:

- $\textcircled{\sc iso}$: print the HAADF image.
- 🖼 : save the HAADF image.
- \blacksquare : transfer the dialogue to the clipboard.
- \cong : open a saved multislice HAADF intensity image ($xxxSTEM_nnnn.ems$).
- **I** : set the default gray **LUT**.
- L: open the Microscope dialogue (Fig. 108).
- 🕗 : open the **Keeper** dialogue (Fig. 90).
- \bullet \blacksquare : reset the wave-front aberrations and imaging conditions.
- 🧖 : display a help file.

Controls and images tabs 9.2

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).





()		
(slider	controls).	
	Aberrations Coherence Drift & Noise In	aging Microscope
Ingritions, Contrast & Gamma	Contrast / au	Gamma / au



. - 120 40.0 Fine Live 40 30 20 10 Live

(f) Microscope settings.

Figure 69: HRSTEM imager controls.

(e) Imaging settings.

The images tabs allow to display:

(d) Drift & Noise settings.

• **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.



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).



intensity with the object in-

tensity.

by convolution of the probe 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).



Figure 72: Effect of source size change.

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



Figure 73: Imaging ${\bf x}$ & ${\bf y}$ image-tiling.

10 Camera MTF

The measurement of the camera Modulation Transfer Function (MTF) requires to load several images of the camera noise pattern (Fig. 74). This procedure measures what is called the Noise Transfer Function. 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.

- \blacksquare : transfer the frame to the clipboard.
- 🗁 : open a noise pattern image (Fig. 76a).
- I: start the fitting procedure (requires at least 2 images).
- \blacksquare : 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, (b) Camera normalized
 (c) Camera PSF.
 parameters of fitting proce- MTF.
 dure, MTF fitting model selection.

Figure 75: Crystal MTF \rightarrow 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 \times 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.

Col :	1024	Default col sizes 256 512 0 1024 2048 4096
Row :	1024	Default row sizes 256 512 1024 2048 4096
Offset :	0	Default data offsets • 0 0 2 4 8
-Signed ty Byte Unsigne	pes Short II id types- te Short I	tteger Float Double Endian type Big C Little

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

Fit Parameters							
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				
В	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				
10	1 07925	0.00222	0.09512				

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

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



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:

- \bullet \blacksquare : 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) Large Angle Convergent Beam Diffraction (LACBED) or Dark Field (DF) aperture.





Figure 81: HRTEM images with different objective aperture settings.



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



(a) Acceptance angle and camera length.



(c) SAED or LACBED aperture on axis.



(b) Beam convergence and deviation.



(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]

Foil normale

Done

.

Figure 85: Use the arrows tool buttons to move the Center of the Laue Circle (CLC).



(a) Small deviation \rightarrow small number of reflections.

(b) Large deviation \rightarrow 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 $[1, 1, 2] \rightarrow \text{tilt}$ 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) First Order Laue Zone.

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



Figure 89

13 Keeper dialogue

Crystal	Aberrations	ADF imager	Diffraction	Imaging	Kikuchi indexing	Iteration-BW	Iteration-CBED	
	Cr	ystal path		rrestad	lelmann/jemsDocs/je	emsGUI/structure	es/AuCu3.txt	
Zone axi	s / [u,v,w]			[0, 0, 1]				
Entrance	foil normale / [u	ı,v,w]		[0, 0, 1]				
Exit foil n	ormale / [u,v,w]			[0, 0, -1	1			
3D-cut pl	ane / (h,k,l)			(0, 0, 1))			
3D-cut o	rigin / nm			0.0				
3D-cut th	ickness / nm			1.0				

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:

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

- 🖼 : print the current parameters.
- \blacksquare : 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.

Crystal Aberrations	ADF imager	Diffraction	Imaging	Kikuchi indexing	Iteration-BW	Iteration-CBED	2
		Woo	to W ₅₅ W ₆	0 to W ₈₈			
$\mathbf{W}_{00} \left(\mathbf{C}_{c} \mathbf{Cc} ight) [mm]$			1.0				
$\mathbf{W}_{11}\left(\mathbf{C}_{01}\right \mathbf{I}\right)\left[\mathbf{nm}\right]$			0.0		0.0		
$\mathbf{W}_{20}\left(\mathbf{C}_{10} \mathbf{Z}\right) [nm]$			9.41	2445			
$\mathbf{W}_{22}\left(\mathbf{C}_{12}^{} \mathbf{A_{1}}\right)\left[nm\right]$			0.0		0.0		
$W_{31}(C_{21} 3B_2)$ [nm]			0.0		0.0		
$\mathbf{W}_{33}\left(\mathbf{C}_{23}^{} \mathbf{A_{2}^{}}\right)\left[nm\right]$			0.0		0.0		
$\mathbf{W}_{40}\left(\mathbf{C}_{30} \; \mathbf{C}_{3}\right) [\text{mm}]$			-0.0	3			
$\boldsymbol{W}_{42}\left(\boldsymbol{C}_{32}^{} \right \boldsymbol{4S_3} \right) [\mu m]$			0.0		0.0		
$\boldsymbol{W}_{44}\left(\boldsymbol{C}_{34}^{} \right \boldsymbol{A}_{3}^{})\left[\mu m \right]$			0.0		0.0		
${\bf W}_{51}({\bf C}_{41}^{} {\bf 5B}_4^{})[{\rm \mu m}]$			0.0		0.0		
$\mathbf{W}_{53}\left(\mathbf{C}_{43} \:\mathbf{5D}_{4}\right)\left[\boldsymbol{\mu}\boldsymbol{m}\right]$			0.0		0.0		
$\mathbf{W}_{55}\left(\mathbf{C}_{45}^{}\right \mathbf{A}_{4}^{}\right)\left[\mu\mathrm{m}\right]$			0.0		0.0		

Crystal	Aberrations	ADF imager	Diffraction	Imaging	Kikuchi indexing	Iteration-BW	Iteration-CBED	•
			W ₀₀	to W ₅₅ W ₆	to W ₈₈			
W ₆₀ (0	C ₅₀ C ₅) [mm]			5.0				
W ₆₂ (0	65 ₂ 65 ₅) [mm]			0.0		0.0		
W ₆₄ (C ₅₄ 6R ₅) [mm]			0.0		0.0		
W ₆₆ (0	C ₅₆ A₅) [mm]			0.0		0.0		
W ₇₁ (0	C ₆₁ 7B ₆) (mm]			0.0		0.0		
W ₇₃ (0	C ₆₃ 7D ₆) (mm]			0.0		0.0		
W ₇₅ (6	C ₆₅ 7F ₆) [mm]			0.0		0.0		
W ₇₇ (0	C ₆₇ A₆) [mm]			0.0		0.0		
W ₈₀ (0	C ₇₀ C ₇) [m]			0.0				
W ₈₂ (0	C ₇₂ 8S ₇) [m]			0.0		0.0		
W ₈₄ (0	C ₇₄ 8R ₇) [m]			0.0		0.0		
W ₈₆ (0	C ₇₆ 8G ₇)[m]			0.0		0.0		
W ₈₈ (6	C ₇₈ A ₇) [m]			0.0		0.0		

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

(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 $^{32}.$

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

³²The sign of the under-defocus is defined in the **Parameters** \rightarrow **Preferences** \rightarrow **Imaging** \rightarrow **Others**.
🛩 🖼 🔠 🛯 🛸			📽 🖬 🗃 🛄 🖗			🛩 🖬 🗃 🛄 🔌	
Crystal Aberrations ADF Imager Diffraction	Imaging Kikuchi Indexing	Iteration-BW Iteration-CBED >	Crystal Aberrations ADF imager Diffraction	Imaging Kikuchi indexing Iteration-BW	Baration-CBED	Crystal Aberrations ADF imager Diffraction	Imaging Kikuchi indexing Iteration-BW Iteration-CBED +
ADF detector angles [mrad]	60.0	150.0	Center of Laue circle / (h,kJ)	(0.000, 0.000, 0.000)		Defocus step / nm	0.1
ADF center indices / (h,k,J)	(0.000, 0.000, 0.000)		Number of Laue zone (s)	0		Defocus series size	1
BF detector outer angle [mrad]	10.0		Deviation / nm-1	0.5		Image dup-x	1
			HOLZ line threshold / m//	10.0		Image dup-y	1
			Kikuchi band threshold / mV	1000.0		Noise level / %	0
			Powder line threshold / %	0.0			
			Powder size / nm	5.0			
			Spot threshold / mV	10.0			
			Zoom	1.0			
			Show dot pattern	ana			
			Show HOLZ pattern	tolse			
			Show Kikuchi patlem	tulse			
			Show ZOLZ lines	tolse			
			Set HOLZ shift	false .			
			Center of diffraction pattern	0.0			
			Contract of Contractory posterio				
		Cancel Done		Cencel	Done		Cancel Done

and HAADF detector diameters.

(a) BF, annular dark field (b) Diffraction parameters. (c) Defocus step, size of de-

focus 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.

Crystal Aberrations ADF Imager Diffraction Imaging Nikuch Indexing Terration-BW Terration-CBED	Iteration-BW Iteration-CBED Iteration-8 Angle error %	S Microscope Measuring Precession Spotindesing Vibration	◀ Instation-BW Instation-CBED Instation-MS	and the second sec
Defocus step / nm 0.1	Angle error %			Microscope Measuring Precession Spotindexing Vibration
		3	Rotation angle / degree	0.0
Defocus series size 1	Distance error %	5	Rotation center / point	416,416
Image dup-x 1	Mask origin (x, y)	0,0	Powder ring calibration	1.0
Image dup-y 1	Mask rotation / deg.	0.0	Powder ring center / point	416,416
Noise level / % 0	Mask size / rm-1	0.1		
	Pixel size / nm-1	0.024		
	Scale unit	1		
	Scale value	10.0		
	Scale tail	20,50		
	Scale head	220,50		
	Spot 0 order	1		
	Spot 1 order	1		
	Spot 2 order	1		
	Spot 0 (d / nm-1, a / deg.)	100.0, 0.0		
	Spot 1 (d / nm-1, a / deg.)	100.0.90.0		
	Spot 2 (d / nm-1, a / deg.)	104.1, 45.0		
Cancel Done		Cancel Done		Cancel Done
a) Kikuchi indexing param-	(b) Spot ir	deving parame-	(c) Paramete	ers related to ro-

eters.

ters.

tation and powder ring pattern center.

Figure 93: Kikuchi and SAED patterns indexing.



wave calculations.

(a) Parameters of Bloch- (b) Parameters of CBED (c) Parameters of multislice calculations.

calculations.

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



and azimutal increment.

and drift imaging parameters.

Figure 95: Microscope, precession and vibration parameters.

14 Wave-front aberrations dialogue



Figure 96: Wave-front aberration and Contrast Transfer Function.

14.1 Tool buttons

- 🖺 : 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

- \blacksquare : print the image panel.
- \blacksquare : save the image panel.
- \blacksquare : transfer the frame to the clipboard.
- 🔳 : reset the gray scale.
- L: open the Microscope dialogue (Fig. 108).
- **I** : make a tilt tableau (Fig. 105).
- e : open the **Specimen** dialogue (Fig. 84a).
- \blacksquare : 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.







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

(b) OTF tab.

Figure 99: Diffractogram and $\mathbf{O}\textsc{ptical}\ \mathbf{T}\textsc{ransfer}\ \mathbf{F}\textsc{unction}.$



(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.



Figure 102: Defocus and drift or noise settings.



Figure 103: Microscope and shift or tilt settings.



Figure 104: Wave-front aberrations, CTF, diffractogram and Ronchigram with 4-fold astigmatism 4 $[\mu m]$.

		Slider	s Table			
C _c (Cc W ₀₀) [mm]	1.0		C ₅₀ (C ₅ W ₆₀) [mm]	5.0		
C ₀₁ (1 W ₁₁) [nm]	0.0	0.0	C ₅₂ (6S ₅ W ₆₂) [mm]	0.0	0.0	
C ₁₀ (Z W ₂₀) [nm]	9.4		C ₅₄ (6R ₅ W ₆₄) [mm]	0.0	0.0	
C ₁₂ (A ₁ W ₂₂) [nm]	0.0	0.0	$C_{56} (A_5 W_{66}) [mm]$	0.0	0.0	
C ₂₁ (3B ₂ W ₃₁) [nm]	0.0	0.0	C ₆₁ (7B ₆ W ₇₁) [mm]	0.0	0.0	
C ₂₃ (A ₂ W ₃₃) [nm]	0.0	0.0	C ₆₃ (7D ₆ W ₇₃) [mm]	0.0	0.0	
C ₃₀ (C ₃ W ₄₀) [mm]	-0.03		C ₆₅ (7F ₆ W ₇₅) [mm]	0.0	0.0	
C ₃₂ (4S ₃ W ₄₂) [µm]	0.0	0.0	C ₆₇ (A ₆ W ₇₇) [mm]	0.0	0.0	
C ₃₄ (A ₃ W ₄₄) [µm]	0.0	0.0	C70 (C7 W80) [m]	0.0		
C ₄₁ (5B ₄ W ₅₁) [µm]	0.0	0.0	$C_{72} (8S_7 W_{82}) [m]$	0.0	0.0	
$C_{43} (5D_4 W_{53}) [\mu m]$	0.0	0.0	$C_{74} (8R_7 W_{84}) [m]$	0.0	0.0	
C ₄₅ (A ₄ W ₅₅) [µm]	0.0	0.0	C ₇₆ (8G ₇ W ₈₆) [m]	0.0	0.0	
			C78 (A7 W88) [m]	0.0	0.0	
Aberration formula (orthogor	al axes) C	$c \sqrt{\left(\frac{\Delta E}{E}\right)^2 + \left(\frac{\Delta E}{E}\right)^2}$	$\frac{2 \text{ alg}}{1} \Big)^2 + \left(\frac{\text{ ag}}{V}\right)^2$			
		R	eset			

0	0	0	0	0
0	0	•	•	¢
0	$\overline{\mathbf{o}}$	\odot	•	0
(*)	0	\odot	\bullet	0
•	۲	•	٠	٠

(a) Table of aberrations

(b) Tilt tableau.

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

		Slider	s Table		
C _c (Cc W ₀₀) [mm]	1.0		C ₅₀ (C ₅ W ₆₀) [mm]	5.0	
C ₀₁ (I W ₁₁) [nm]	0.0	0.0	C 52 (65 W 62) [mm]	0.0	0.0
C ₁₀ (Z W ₂₀) [nm]	9.4		C ₅₄ (6R ₅ W ₆₄) [mm]	0.0	0.0
C ₁₂ (A ₁ W ₂₂) [nm]	0.0	0.0	$C_{56} (A_5 W_{66}) [mm]$	0.0	0.
C ₂₁ (3B ₂ W ₃₁) [nm]	0.0	0.0	C ₆₁ (7B ₆ W ₇₁) [mm]	0.0	0.0
C ₂₃ (A ₂ W ₃₃) [nm]	800.0	60.0	C ₆₃ (7D ₆ W ₇₃) [mm]	0.0	0.0
C ₃₀ (C ₃ W ₄₀) [mm]	-0.03		C ₆₅ (7F ₆ W ₇₅) [mm]	0.0	0.0
C ₃₂ (4S ₃ W ₄₂) [µm]	0.0	0.0	C ₆₇ (A ₆ W ₇₇) [mm]	0.0	0.0
C ₃₄ (A ₃ W ₄₄) [µm]	0.0	0.0	C70 (C7 W80) [m]	0.0	
C ₄₁ (5B ₄ W ₅₁) [µm]	0.0	0.0	C72 (8S7 W82) [m]	0.0	0.0
C ₄₃ (5D ₄ W ₅₃) [µm]	0.0	0.0	$C_{74} (8R_7 W_{84}) [m]$	0.0	0.
C ₄₅ (A ₄ W ₅₅) [µm]	0.0	0.0	C76 (8G7 W88) [m]	0.0	0.1
			$C_{78} (A_7 W_{88}) [m]$	0.0	0.0
Aberration formula (orthogo	nalaxes)	$\left(\frac{\Delta E}{E}\right)^2 + \left(\frac{\Delta E}{E}\right)^2$	$\frac{2 \Delta I}{I} \bigg)^2 + \left(\frac{\Delta V}{V} \right)^2$		
		Re	eset		

(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

- \blacksquare : load a microscope table.
- 🗟 : save the table of microscopes.
- 🖺 : transfer the frame to the clipboard.
- \bigoplus : add a new microscope.
- = : delete the selected microscope.
- **I** : 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 Contrast Transfer Function with positive sign for the underfocus. The **Parameters** \rightarrow **Preferences** \rightarrow **Imaging** \rightarrow **Others** tab allows to use the opposite sign.

The **yellow** envelope introduces the effect of Thermal Magnetic Noise 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

, 2, 3]		[2, 3, 5]	
[uvw]	🔿 (hkl)	🗿 [uvw]	🔿 (hkl)
suits			
All		Angle / Deg.	19.12
Bragg / mRad	nothing to calculate	Common (hkl)	(1, 6, -4)
Cell	[0, -3, 2], [1, 0, 0], [0, 2, 3]::13	Ratio	0.58489764
Dhkl Duvw	2.232	Zone axis	nothing to calculate
To cartesian	(0.000,1.238,1.857)		
To (hkl)	(0, 2, 3)		
To [uvw]	[0, 2, 3]		
Vhkl /V	nothing to calculate		
From Weber	not hexagonal		
To Weber	not hexagonal		

Figure 110: Crystallographic calculator.

17.1 Tool buttons

The tool buttons allow to:

- \blacksquare : print the frame.
- \blacksquare : 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.

³³When the calculations are first performed with $\langle uvw \rangle$ 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].



(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.



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

a 🖪 📋					
	Center of Lau	e circle : (0.000, 0 Tilt angle / 50 n	.000, 0.000)::Zon tleg. : 0.00 m-1	e axis : [0, 0, 1]	
		•	•	•	
		•	•	•	•
	•	•	•	•	•
	•	• •	•	•	•
•	•	•	•	•	•
•	•	•	10	•	•
•		•	00	•	•
			•	•	•
				•	
		•	•	•	•
	•	•	•	•	•
	•	•	•	•	•
•	•	•	•	•	•
		•	•	•	
		•	•	•	
AV/	n kV:300.000	ot saved (a)), CL/mm:15	82 reflection 500, ZA:[0, 0	fs)), 1], FN:[0,	0, 1]

(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: $\langle uvw \rangle$ stereogram and Wulff net.

18.1 Tool buttons

- \bullet $\textcircled{\mbox{\footnotesize \mbox{\footnotesize \mbox{--}}}}$: print the stereographic projection.
- \bullet \blacksquare : save the stereographic projection.
- \bullet \blacksquare : transfer the frame to the clipboard.

- 🗵 : overlay stereograms.
- 📑 : make a table of zone axis.
- \blacksquare : open the toolbox.
- 🧖 : display a help file.

18.2Tabs



stereograms.

Figure 115: Stereogram tabs.

19 Powder pattern frame

uib.	(h,k,l)	d*/nm ⁻¹	OScatt / Deg.	Intens.	OBrado / mRad	V _r [V nm e]	V _i [V][nm][e]	Ampli. [V nm e]	d/nm	LP factor	S I	Electron diffraction	Neutron d	ffraction X-Ra	y diffractio	in
	(0, 0, 0)	0.000	0.000		0.000	21.706	1.485	21.756				Atomic Form Factor				
	(1, 1, 1)	2.798	0.316	1000	2.754	4.652	10.322	11.322	0.357	0.3574	3			0		
	(0, 0, 2)	3.231	0.365	89	3.181	-4.168	-0.388	4.186	0.310	0.3095	4	DTSB EJK PRDW	WK	WKc.	XRay	JEMS
2	(0, 2, 2)	4.569	0.516	755	4.498	10.220	0.945	10.263	0.219	0.2188	8	Onlines				
1	(1, 1, 3)	5.358	0.605	499	5.274	3.642	-5.253	6.392	0.187	0.1866	11	Options	Disekman			
	(2, 2, 2)	5.596	0.632	22	5.509	-2.354	-0.340	2.379	0.179	0.1787	12		biackman	correction		
	(0, 0, 4)	6.462	0.729	118	6.361	6.769	0.792	6.815	0.155	0.1548	16					
ł	(1, 3, 3)	7.042	0.795	180	6.932	1.632	4.089	4.403	0.142	0.142	19	Crystal diameter / nm		Voltage / kV		
1	(0, 2, 4)	7.225	0.815	25	7.112	-1.647	-0.301	1.675	0.138	0.1384	20	50		- 1000		
	(2, 2, 4)	7.914	0.893	218	7.791	5.086	0.679	5.132	0.126	0.1264	24					
	(3, 3, 3)	8.394	0.947		8.263	2.123	-2.790	3.505	0.119	0.1191	27	- 40		- 800		
	(1, 1, 5)	8.394	0.947	121	8.263	1.207	3.160	3.382	0.119	0.1191	27			000		
	(0, 4, 4)	9.139	1.031	59	8.996	4.024	0.588	4.067	0.109	0.1094	32	- 20		- 600		
3	(1, 3, 5)	9.557	1.079	109	9.408	1.729	-2.230	2.822	0.105	0.1046	35	- 30		- 000		
1	(2, 4, 4)	9.693	1.094	10	9.542	-1.034	-0.242	1.061	0.103	0.1032	36			400		
	(0, 0, 6)	9.693	1.094		9.542	-1.034	-0.242	1.061	0.103	0.1032	36	- 20		- 400		
	(0, 2, 6)	10.217	1.153	70	10.058	3.269	0.512	3.309	0.098	0.0979	40	-		1		
	(3, 3, 5)	10.594	1.195	30	10.428	0.724	2.093	2.215	0.094	0.0944	43	1-10		- 200		
	(2.2.6)	10.716	1.209	5	10.549	-0.864	-0.218	0.891	0.093	0.0933	44	Υ.		1.		
0	Int.				u youn an to	rongener						Fine Live	0 10.0	Fine Live	30.0	
40	_											40.0 50.0 60.0	0 70.0	● 80.0 ○	90.0	
20	-															

Figure 116: Powder pattern frame.

19.1 Tool buttons

The tool buttons allow to:

- \blacksquare : print the stereogram.
- \mathcal{P} : 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).

leutron wave	elength / nm	diffraction N	autron diffraction	X-Ray d	iffraction	
0.0 0.1	0.2 0.3	0.4 0.5				
0.0 0.1	0.2 0.0	0.4 0.0				
0.05						
	ata fastar					
	11Z factor					
Camera	eras		Camera			
O Po	wder camer	a 1	Powde	er camera	12	
Diame	eter / mm	5730.0	Diameter /	mm	11460.0	
aximum dista	nce / nm-1					
aximum dista	nce / nm-1 2.0	5.0	0 10.0 0	20.0	30.0	

	Electron diffraction	Neutron diffraction	X-Ray diffraction	n
	s	ources Cameras		
X-Ray source Ti Ka Ka Ka	$\begin{bmatrix} Cr & \mathbf{K}_{\alpha 1} \\ & \mathbf{K}_{\alpha 2} \\ \mathbf{K}_{\beta 1} \\ & \mathbf{K}_{\alpha} \\ \mathbf{K}_{\alpha} \\ \end{bmatrix}$ $\begin{bmatrix} Ag \\ & \mathbf{K}_{\alpha 1} \\ & \mathbf{K}_{\alpha 2} \\ & \mathbf{K}_{\beta 1} \\ & \mathbf{K}_{\alpha} \end{bmatrix}$	$ \begin{array}{c} Fe & K_{\alpha 1} \\ & K_{\alpha 2} \\ & K_{\beta 1} \\ & K_{\alpha} \end{array} \end{array} \left[\begin{array}{c} C \\ & K_{\beta 2} \\ & K_{\beta 1} \\ & K_{\alpha} \end{array} \right] \\ \hline \\ & K_{\alpha} \end{array} \right] $	$\left \begin{array}{c} \mathbf{C} \\ \mathbf{K}_{\alpha 1} \\ \mathbf{K}_{\alpha 2} \\ \mathbf{K}_{\beta 1} \\ \mathbf{K}_{\alpha } \\$	$\begin{array}{c} \kappa_{\alpha 1} \\ \kappa_{\alpha 2} \\ \kappa_{\beta 1} \\ \kappa_{\alpha} \end{array}$
Maximum distance	e / nm-1 2.0 5.0	10.0 •	20.0 30	0

(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_ nm ⁻ '	g2::(h,k,l)	Vg ₂ Volt	g_ nm ⁻ '	g1/g2	g ₂ /g ₁	(g ₁ , g ₂)	FOLZ nm ⁻¹	SOLZ nm ⁻¹	TOLZ nm
[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

- B : 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.
- $\mathbf{\mathbf{\hat{y}}}$: index a SAED pattern using the table(s).
- 🧖 : display a help file.

21 Transform unit cell dialogue

a/nm		0.3749				a/nm	oo caa	0.5301887			
		0 3749				b/nm		0 5301887			
		0.3743						0.0001007			
c/nm		0.3749				c/nm		0.6493459			
alpha / D	Deg.	90.0				alpha /	alpha / Deg. 90.0				
beta / De	eg.	90.0				beta / D	eg.	90.0			
gamma	/Deg.	90.0				gamma	/Deg.	120.0			
1.0.01	(0, 1, 0), (0, 0	41				[1 . 1 . 0]		11-2.0			
1, 0, 0 <u>]</u> ,	[0, 1, 0], [0, 0	, ıj	1	1		[1,-1,0]	[0, 1, -1][1, 1	(, IJ.:3.0	1	1	1
	Symbol	Wyckoff	X 0.000	y 0.000	2 0.00	#	Symbol	Wyckoff	X 0.000	y 0.000	Z
	Cu	a	0.000	0.000	0.00	1	Au	a	0.666667	0.000	0.
	Cu	C	0.500	0.500	0.00	2	Au	2	0.333333	0.666667	0
	Cu	c	0.500	0.000	0.50	3	Cu	c	0.000	0.500	0
	00	U	0.000	0.000	0.00	4	Cu	c	0.666667	0.833333	0.
						5	Cu	c	0.3333333	0.166667	0.
						6	Cu	c	0.500	0.000	0
						7	Cu	c	0.166667	0.3333333	0.
						8	Cu	c	0.833333	0.666667	0.
						9	Cu	с	0.500	0.500	0.
						10	Cu	с	0.166667	0.833333	0.
						11	Cu	с	0.833333	0.166667	0.

Figure 120: Transform unit cell dialogue.

21.1 Tool buttons

- B: print the dialogue.
- 🖼 : save the dialogue image.
- \bullet \blacksquare : transfer the dialogue to the clipboard.

- \blacksquare : 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

- \blacksquare : print the frame.
- a : 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° though they can be slightly lower depending on the original unit cell.

a /nm 0.619 a /nm 1.0721395 b /nm 0.619 b /nm 0.8753982 c /nm alpha / Deg. 90.0 b /nm 0.8753982 c /nm gamma / Deg. 90.0 b /nm 0.8753982 c /nm gamma / Deg. 90.0 b /nm 0.8753982 c /nm (1,0,0], [0,1,0], [0,0,1]::1 ipha / Deg. 90.0 beta / Deg. 90.0 [1,0,0], [0,1,0], [0,0,1]::1 ipha / Deg. 90.0 ipha / Deg. 90.0 [1,0,0], [0,1,0], [0,0,1]::1 ipha / Deg. 90.0 ipha / Deg. 90.0 [1,-1,1], [1,0,-1], [1,2,1]::6 ipha / Deg. 90.0 ipha / Deg. 90.0 [2, Zn a 0.000 0.500 0.500 0.500 0.500 0.500 3 Zn a 0.500 0.500 0.500 3 Zn a 0.33333 0.750 0.0 3 Zn a 0.750 0.250 0.750 0.250 0.750 5 Te a 0.416667 0.500 0.0 6 Te a 0.750 0.750 0.750 0.250 0.750 0.250 0.750 0.250 0.750 0.250 0	a / nm 0.619 a / nm 1.0721395 b / nm 0.619 a / nm 1.0721395 c / nm 0.619 a / nm 1.5162342 alpha / Deg. 90.0 alpha / Deg. 90.0 gamma / Deg. 90.0 alpha / Deg. 90.0 gamma / Deg. 90.0 alpha / Deg. 90.0 f# Symbol Wyckoff x y 0 Zn a 0.000 0.000 1 Zn a 0.000 0.000 2 Zn a 0.000 0.500 3 Zn a 0.500 0.500 3 Zn a 0.500 0.500 5 Te a 0.750 0.250 5 Te a 0.750 0.250 6 Te a 0.750 0.750 7 Te a 0.250 0.750 7 Te a 0.750 0.750 7 Te a 0.750 0.750						Orthogonal coll				<u>*</u>		Ĕ 🙋	ilett ooli					
b / nm 0.619 c / nm 0.619 c / nm 0.619 alpha / Deg. 90.0 beta / Deg. 90.0 gamma / Deg. 90.0 (1, 0, 0], [0, 1, 0], [0, 0, 1]:1 # Symbol Wyckoff x y z 0 Zn a 0.000 0.000 0.000 1 Zn a 0.000 0.500 0.500 2 Zn a 0.000 0.500 0.500 3 Zn a 0.500 0.500 0.500 5 Te a 0.750 0.250 0.250 5 Te a 0.750 0.250 0.750 7 Te a 0.250 0.750 0.750 7 Te a 0.250 0.750 0.750 1 Zn a 0.33333 0.500 0.001 6 Te a 0.750 0.750 0.750 7 Te a 0.250 0.750 0.750 1 Zn a 0.33333 0.000 0.500 1 Zn a 0.33333 0.000 0.500 1 Te a 0.416667 0.500 0.002 5 Te a 0.750 0.750 0.750 1 Zn a 0.666667 0.500 0.001 6 Zn a 0.666667 0.500 0.001 1 Zn a 0.000 0.750 0.001 1 Zn a 0.0003 0.550 0.001 1 Zn a 0.003333 0.500 0.001 1 Zn a 0.666667 0.500 0.001 2 Zn a 0.000 0.000 0.000 1 Zn a 0.0000 0.0000 0.0000 1 Zn a 0.0000 0.0000 0.0000 1 Zn a 0.0000 0	b /nm 0.619 c /nm 0.619 alpha / Deg. 90.0 gamma / Deg. 90.0 gamma / Deg. 90.0 (1, 0, 0), [0, 1, 0), [0, 0, 1]::1 # Symbol Wyckoff x y z 0 Zn a 0.000 0.000 0.000 2 Zn a 0.000 0.500 0.500 3 Zn a 0.500 0.500 0.500 3 Zn a 0.500 0.500 0.500 5 Te a 0.750 0.250 0.250 6 Te a 0.750 0.250 0.750 7 Te a 0.250 0.750 0.750 6 Te a 0.750 0.250 0.750 7 Te a 0.250 0.750 0.750 6 Te a 0.750 0.250 0.750 6 Te a 0.750 0.250 0.750 7 Te a 0.250 0.750 0.750 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.77 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.77 1 Zn a 0.666667 0.57 9 Zn a 0.08333 0.57 1 Zn a 0.500 0.750 0.750 1 Te a 0.250 0.750 0.750 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.77 1 Zn a 0.666667 0.57 9 Zn a 0.08333 0.57 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.75 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.75 1 Zn a 0.666667 0.57 9 Zn a 0.08333 0.57 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.75 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.75 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.75 1 Zn a 0.666667 0.57 9 Zn a 0.08333 0.57 1 Zn a 0.666667 0.57 9 Zn a 0.000 0.75 1 Zn a 0.666667 0.57 1 Zn a 0.66667 0.57 1 Zn a 0.750 0.75 1 Zn a 0.000 0.7 1 Zn a 0.000 0.7 1 Zn a 0.000 0.7 1 Zn a 0.000 0.57 1 Zn a 0.000 0.7 1 Zn a 0.75 0.7 1 Zn a 0.000 0.7 1 Zn a 0.7 1				721395	1.0	a/nm				19	0.61		a/nm					
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anpria / Deg. 90.0 beta / Deg. 90.0 gamma / Deg. 90.0 gama	alpha / Deg. 90.0 gamma / Deg. 90.0 gamma / Deg. 90.0 [1, 0, 0], [0, 1, 0], [0, 0, 1]::1 # Symbol Wyckoff x y z 0 Zn a 0.000 0.000 0.000 1 Zn a 0.000 0.500 0.500 2 Zn a 0.050 0.500 0.500 3 Zn a 0.500 0.000 0.500 4 Te a 0.750 0.750 0.250 6 Te a 0.750 0.750 0.250 6 Te a 0.750 0.750 0.750 7 Te a 0.250 0.750 0.750 9 Zn a 0.000 0.75 10 Te a 0.750 0.75 9 Zn a 0.000 0.75 11 Zn a 0.666667 0.57 12 Te a 0.416667 0.57 13 Te a 0.083333 0.57 14 Zn a 0.33333 0.57 15 Zn a 0.33333 0.57 16 Zn a 0.666667 0.75 17 Te a 0.416667 0.75 10 Te a 0.750 0.75 10 Te a 0.416667 0.75 11 Zn a 0.666667 0.75 12 Te a 0.416667 0.57 13 Te a 0.083333 0.57 14 Zn a 0.33333 0.57 15 Zn a 0.666667 0.75 19 Te a 0.416667 0.55 20 Te a 0.41667 0.55 20 Te a 0.416667 0.55 20 Te a 0.41667 0.55 20 Te a 0.4166				0	0.0	olpha (Deg	alpha / Deg 90.0											
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3 Zn a 0.500 0.000 0.500 0.4 Te a 0.333333 0.250 0.0 5 Te a 0.750 0.750 0.250 0.5 5 Te a 0.416667 0.000 0.00 5 Te a 0.750 0.250 0.750 0.250 5 Te a 0.416667 0.000 0.0 6 Zn a 0.666667 0.000 0.0<	3 Zn a 0.500 0.000 0.500 4 Te a 0.250 0.250 0.250 5 Te a 0.750 0.250 0.750 6 Te a 0.750 0.250 0.750 7 Te a 0.250 0.750 0.750 8 Te a 0.666667 0.00 9 Zn a 0.000 0.25 10 Te a 0.000 0.25 11 Zn a 0.000 0.25 12 Te a 0.000 0.25 13 Te a 0.083333 0.00 13 Te a 0.333333 0.00 14 Zn a 0.666667 0.25 17 Te	0 0.91	0.750	0.333333	а		2 Zn	0.500	0.500	0.000	а		Zn	2					
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5 Te a 0.750 0.250 0.750 0.250 0.750 6 Zn a 0.666667 0.000 <	5 Te a 0.750 0.250 0.750 6.250 6.6 Te a 0.416667 0.00 6.6 Zn a 0.666667 0.00 7.7 Te a 0.250 0.750 0.750 6.750 7 Zn a 0.666667 0.00 7.7 Zn a 0.666667 0.00 0.750 0.750 9 Zn a 0.000 0.75 9 Zn a 0.000 0.25 11 Zn a 0.000 0.25 12 Te a 0.000 0.25 12 Te a 0.003333 0.00 12 13 Te a 0.333333	0 0.83	0.500	0.416667	а		4 Te	0.250	0.250	0.250	а		Te	4					
66 Te a 0.750 0.250 0.750 0.750 7 Zn a 0.666667 0.000 0.4 7 Te a 0.250 0.750 0.750 7 Zn a 0.666667 0.000 0.4 8 Te a 0.000 0.750	66 Te a 0.750 0.250 0.750 0.750 7 Te a 0.250 0.750 0.750 7 Zn a 0.666667 0.00 7 Te a 0.250 0.750 0.750 7 Zn a 0.666667 0.00 7 Te a 0.250 0.750 0.750 17 Zn a 0.666667 0.00 8 Te a 0.000 0.75 9 Zn a 0.000 0.25 10 Te a 0.000 0.25 11 Zn a 0.000 0.25 11 Zn a 0.003333 0.00 0.02 12 Te a 0.083333 0.00 0.01 13 Te a 0.0333333 0.00 14 Zn a 0.333333 0.00 15 16 Zn a 0.666667 0.25 17 Te a 0.416667 0.25 17 18 Zn a 0.416667 0.25	0 0.83	0.000	0.416667	а		5 Te	0.250	0.750	0.750	а		Те	5					
7 Te a 0.250 0.750	7 Te a 0.250 0.750 0.750 8 Te a 0.666667 0.50 8 Te a 0.750 0.75 9 Zn a 0.000 0.75 9 Zn a 0.000 0.75 10 Te a 0.000 0.25 10 Te a 0.000 0.25 11 Zn a 0.000 0.25 11 Zn a 0.000 0.25 12 Te a 0.083333 0.00 13 Te a 0.083333 0.00 13 Te a 0.333333 0.00 14 Zn a 0.333333 0.00 1.5 Zn a 0.333333 0.00 1.5 1.5 Zn a 0.416667 0.25 1.7 Te a 0.416667 0.25 1.7 18 Zn a 0.416667 0.25 20 Te a	0 0.83	0.000	0.666667	а		6 Zn	0.750	0.250	0.750	а		Те	6					
8 Te a 0.750	8 Te a 0.750 0.75 9 Zn a 0.000 0.75 10 Te a 0.750 0.25 11 Zn a 0.000 0.25 12 Te a 0.000 0.25 12 Te a 0.083333 0.00 13 Te a 0.083333 0.00 14 Zn a 0.333333 0.00 15 Zn a 0.333333 0.00 16 Zn a 0.666667 0.25 17 Te a 0.416667 0.75 18 Zn a 0.666667 0.25 20 Te a 0.750 0.00 21 Te a 0.750 0.00 22 Zn a 0.750 0.00	0 0.83	0.500	0.666667	а		7 Zn	0.750	0.750	0.250	а		Те	7					
9 Zn a 0.000 0.750 0. 10 Te a 0.750 0.250 0. 11 Zn a 0.000 0.250 0. 11 Zn a 0.000 0.250 0. 12 Te a 0.083333 0.000 0.4 13 Te a 0.833333 0.000 0.4 14 Zn a 0.333333 0.000 0.4 15 Zn a 0.666667 0.250 0.4 16 Zn a 0.666667 0.750 0.4 17 Te a 0.666667 0.750 0.4 18 Zn a 0.666667 0.750 0.4 20 Te a 0.750 0.500 0.4 21 Te a 0.750 0.000 0.4	9 Zn a 0.000 0.75 10 Te a 0.750 0.25 11 Zn a 0.000 0.25 12 Te a 0.000 0.25 12 Te a 0.083333 0.00 13 Te a 0.083333 0.00 14 Zn a 0.333333 0.00 15 Zn a 0.333333 0.00 16 Zn a 0.666667 0.25 17 Te a 0.416667 0.75 18 Zn a 0.666667 0.25 20 Te a 0.416667 0.25 21 Te a 0.750 0.00 22 Zn a 0.750 0.00	0 0.75	0.750	0.750	а		8 Te												
10 Te a 0.750 0.250 0. 11 Zn a 0.000 0.250 0. 12 Te a 0.083333 0.000 0.4 13 Te a 0.833333 0.000 0.4 14 Zn a 0.333333 0.000 0.4 15 Zn a 0.666667 0.250 0.4 16 Zn a 0.666667 0.250 0.4 17 Te a 0.666667 0.750 0.4 18 Zn a 0.666667 0.750 0.4 20 Te a 0.750 0.500 0.4 21 Te a 0.750 0.900 0.4	10 Te a 0.750 0.25 11 Zn a 0.000 0.25 12 Te a 0.083333 0.00 13 Te a 0.083333 0.00 14 Zn a 0.333333 0.00 15 Zn a 0.333333 0.00 16 Zn a 0.666667 0.25 17 Te a 0.416667 0.75 18 Zn a 0.666667 0.25 20 Te a 0.416667 0.25 21 Te a 0.750 0.00 22 Zn a 0.750 0.00	0 0.75	0.750	0.000	а		9 Zn												
11 Zn a 0.000 0.250 0.1 12 Te a 0.083333 0.000 0.4 13 Te a 0.083333 0.500 0.4 14 Zn a 0.333333 0.000 0.4 15 Zn a 0.333333 0.500 0.4 16 Zn a 0.666667 0.250 0.4 17 Te a 0.666667 0.750 0.4 18 Zn a 0.666667 0.750 0.4 20 Te a 0.750 0.500 0.4 21 Te a 0.750 0.000 0.4	11 Zn a 0.000 0.25 12 Te a 0.083333 0.00 13 Te a 0.083333 0.00 14 Zn a 0.333333 0.00 15 Zn a 0.333333 0.00 16 Zn a 0.666667 0.25 17 Te a 0.416667 0.75 18 Zn a 0.666667 0.25 20 Te a 0.416667 0.25 21 Te a 0.750 0.00 22 Zn a 0.750 0.00	0 0.75	0.250	0.750	а		10 Te												
12 Te a 0.083333 0.000 0.4 13 Te a 0.083333 0.500 0.4 14 Zn a 0.333333 0.000 0.4 15 Zn a 0.333333 0.500 0.4 16 Zn a 0.666667 0.250 0.4 17 Te a 0.666667 0.750 0.4 18 Zn a 0.666667 0.750 0.4 20 Te a 0.750 0.500 0.4 21 Te a 0.750 0.900 0.4 22 Zn a 0.000 0.000 0.4	12 Te a 0.083333 0.00 13 Te a 0.083333 0.00 14 Zn a 0.333333 0.00 15 Zn a 0.333333 0.00 16 Zn a 0.666667 0.25 17 Te a 0.416667 0.75 18 Zn a 0.666667 0.25 19 Te a 0.416667 0.25 20 Te a 0.416667 0.25 21 Te a 0.750 0.00 22 Zn a 0.700 0.00	0 0.75	0.250	0.000	а		11 Zn												
13 Te a 0.083333 0.500 0.1 14 Zn a 0.33333 0.000 0.1 15 Zn a 0.33333 0.500 0.1 16 Zn a 0.666667 0.250 0.1 17 Te a 0.666667 0.750 0.1 18 Zn a 0.666667 0.750 0.1 19 Te a 0.750 0.500 0.1 20 Te a 0.750 0.500 0.1 21 Te a 0.000 0.000 0.1	13 Te a 0.083333 0.50 14 Zn a 0.333333 0.00 15 Zn a 0.333333 0.50 16 Zn a 0.666667 0.25 17 Te a 0.666667 0.75 18 Zn a 0.666667 0.25 19 Te a 0.416667 0.25 20 Te a 0.416667 0.25 21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.66	0.000	0.083333	а		12 Te												
14 Zn a 0.333333 0.000 0.4 15 Zn a 0.333333 0.500 0.4 16 Zn a 0.666667 0.250 0.4 17 Te a 0.666667 0.750 0.4 18 Zn a 0.666667 0.750 0.4 19 Te a 0.416667 0.250 0.4 20 Te a 0.750 0.500 0.4 21 Te a 0.750 0.000 0.4	14 Zn a 0.333333 0.00 15 Zn a 0.333333 0.50 16 Zn a 0.666667 0.25 17 Te a 0.416667 0.75 18 Zn a 0.666667 0.25 19 Te a 0.416667 0.25 20 Te a 0.416667 0.25 21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.66	0.500	0.083333	а		13 Te												
15 Zn a 0.333333 0.500 0.4 16 Zn a 0.666667 0.250 0.4 17 Te a 0.416667 0.750 0.4 18 Zn a 0.666667 0.250 0.4 19 Te a 0.416667 0.250 0.4 20 Te a 0.750 0.500 0.4 21 Te a 0.750 0.000 0.4	15 Zn a 0.333333 0.50 16 Zn a 0.666667 0.25 17 Te a 0.416667 0.75 18 Zn a 0.666667 0.25 19 Te a 0.416667 0.25 20 Te a 0.416667 0.25 21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.66	0.000	0.333333	а		14 Zn												
16 Zn a 0.666667 0.250 0.1 17 Te a 0.416667 0.750 0.1 18 Zn a 0.666667 0.750 0.1 19 Te a 0.416667 0.250 0.1 20 Te a 0.750 0.500 0.1 21 Te a 0.750 0.000 0.1 22 Zn a 0.000 0.000 0.1	16 Zn a 0.666667 0.25 17 Te a 0.416667 0.75 18 Zn a 0.666667 0.75 19 Te a 0.416667 0.25 20 Te a 0.416667 0.25 21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.66	0.500	0.333333	а		15 Zn												
17 Te a 0.416667 0.750 0.41667 18 Zn a 0.666667 0.750 0.41667 19 Te a 0.416667 0.250 0.41667 20 Te a 0.750 0.500 0.41667 21 Te a 0.750 0.000 0.41667	17 Te a 0.416667 0.75 18 Zn a 0.666667 0.75 19 Te a 0.416667 0.25 20 Te a 0.750 0.50 21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.58	0.250	0.666667	а		16 Zn												
18 Zn a 0.666667 0.750 0.1 19 Te a 0.416667 0.250 0.1 20 Te a 0.750 0.500 0.1 21 Te a 0.750 0.000 0.1 22 Zn a 0.000 0.000 0.1	18 Zn a 0.666667 0.75 19 Te a 0.416667 0.25 20 Te a 0.750 0.00 21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.58	0.750	0.416667	а		17 Te												
19 Te a 0.416667 0.250 0.4 20 Te a 0.750 0.500 0.4 21 Te a 0.750 0.000 0.4 22 Zn a 0.000 0.000 0.4	19 Te a 0.416667 0.25 20 Te a 0.750 0.50 21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.58	0.750	0.666667	а		18 Zn												
20 Te a 0.750 0.500 0.1 21 Te a 0.750 0.000 0.1 22 Zn a 0.000 0.000 0.1	20 Te a 0.750 0.50 21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.58	0.250	0.416667	а		19 Te												
21 Te a 0.750 0.000 0.0	21 Te a 0.750 0.00 22 Zn a 0.000 0.00	0 0.50	0.500	0.750	а		20 Te												
22 Zn a 0.000 0.000 0.	22 Zn a 0.000 0.00	0 0.50	0.000	0.750	а		21 Te												
		0 0.50	0.000	0.000	a		22 Zn												

Figure 122: Dialogue to create orthogonal cells.



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

Orthogo	nai ceii	4 54000 10												
a/nm		1.5162342												
b/nm		1.3841261												
c/nm		3.3904028												
alpha	/ Deg.	90.0												
beta /	Deg.	90.0												
gamm	a / Deg.	90.0												
[2, -1,	1], [1, 0, -:	2], [2, 5, 1]::3	0											
#	Sym	ool Wycko	ff x	у	z									
0	Те	а	0.666667	0.450	0.98									
1	Те	а	0.166667	0.450	0.98									
2	Zn	а	0.916667	0.700	0.98									
3	Zn	а	0.700	0.98										
4	Те	а	0.083333	8 0.150	0.96									
5	Те	а	0.583333	0.150	0.96									
6	Zn	а	0.333333	3 0.400	0.96									
7	Zn	а	0.833333	3 0.400	0.96									
8	Те	а	0.500	0.850	0.95									
9	Те	а	0.000	0.850	0.95									
10	Zn	а	0.750	0.100	0.95									
11	Zn	а	0.250	0.100	0.95									
12	Те	а	0.416667	0.550	0.93									
13	Te	а	0.916667	0.550	0.93									
14	Zn	а	0.166667	0.800	0.93									
15	Zn	а	0.666667	0.800	0.93									
16	Zn	а	0.083333	3 0.500	0.91									
17	Zn	а	0.583333	0.500	0.91									
18	Те	а	0.333333	8 0.250	0.91									
19	Те	а	0.833333	0.250	0.91									
20	Те	а	0.250	0.950	0.90									
21	Zn	а	0.000	0.200	0.90									
22	Zn	а	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 \times 30).

23 Image processing frame



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

iii 🖬 📖 📗																															
															8	eal															
Real part	240.00	0.047.00	047.000	047.000	247.00	040.000	247.00	047.000	047.00	240.000	247.00	047.00	247.00	247.00	047.00	247.00	247.00	047.000	247.000	247.00	047.000	247.000	247.000	047.00	247.02	247.00	047.00	247.00	246.000	047.000	247.00
205	243.00	0 247.35	249.000	247.000	247.39	243.000	247.000	247.000	247.99	249.000	247.000	246.000	247.000	247.39	246.000	247.000	247.39	247,000	247.000	247.39	247.000	247.000	247.000	247.99	247.99	247.000	247.99	247.39	240.000	247.000	247.99
207	247.99	_ 247.00	0 247.99.	. 247.000	247.000	247.000	247.000	247.99.	249.000	249.000	249.000	247.99	247.000	247.000	246.000	247.000	247.000	247.99	247.99_	247.99	247.000	247.99	247.99	247.99	247.99_	247.99	247.99	249.000	247.000	247.99	247.000
208	246.00	0 247.00	0 247.000	247.000	247.99.	249.000	247.99.	247.99.	247.99.	247.99.	247.99	247.99	247.99.	246.000	246.000	249.000	249.000	247.000	247.99	247.99.	247.000	247.000	247.99.	247.000	247.99	247.99	246.000	247.000	247.000	247.000	246.000
209	247.99	246.00	0 247.000	246.000	247.000	249.000	247.000	247.000	247.000	247.99	247.000	247.99	247.99	247.000	247.000	247.99	247.99	247.000	247.99_	247.99	247.000	247.99	247.99	247.000	247.000	247.99	247.000	247.99_	246.000	247.000	247.000
210	247.99	246.00	0 247.000	247.99.	247.99.	249.000	247.99.	247.000	247.99	247.000	247.000	247.000	247.99	247.99	247.99	247.99	247.000	247.000	247.000	247.000	247.000	247.000	247.99.	247.99	247.000	247.000	247.99	247.99	247.99	247.000	246.000
212	247.99	0 247.95	247.99	247.000	249.000	247.99	247.000	247.000	247.000	247.000	246.000	247.000	247.39	247.000	247.000	247.39	247.39	247,000	247.000	247.000	247.000	240.000	240.000	247.99	249.000	249.000	243.000	243.000	245.000	247.000	247.99
213	247.00	0 247.95	_ 247.99	249.000	247.99	247.99	247.99	247.000	247.000	247.99	247.99	247.000	247.000	247.99.	247.000	247.99	247.000	247.000	247.000	247.99	247.99	246.000	247.000	247.99	247.99	247.99	247.000	246.000	246.000	247.000	247.00
214	247.99	247.00	0 247.99	247.99	247.000	247.99.	247.000	247.99.	247.99.	247.99	247.99.	247.000	247.000	247.000	249.000	247.99	247.000	247.000	247.000	247.99.	247.99	247.000	247.000	247.99.	247.99	247.99	247.000	246.000	246.000	247.000	247.000
215	247.99	247.95	247.000	247.99.	247.000	247.99	247.99	247.99.	247.99	247.99	247.99	247.99	247.99	247.99	249.000	247.99_	247.000	247.99	247.000	247.000	247.99	247.000	247.000	247.000	247.000	247.000	247.000	247.000	247.99	247.000	247.000
216	247.99	247.00	0 246.000	247.000	247.000	247.99	247.99.	247.99.	247.99.	247.99.	247.99	247.99	247.99	247.99	247.99	247.000	247.99	247.99	247.000	247.99.	247.99	247.000	247.99.	247.000	247.000	247.99	247.99	247.99	247.99	247.000	247.000
217	247.99	247.00	0 247.000	246.000	247.000	247.99	247.99	247.99	247.000	247.000	247.000	247.99	247.39	247.000	247.000	247.39	247.39	247.39.	247.39	247.39	247.99	247.000	247.000	247,000	247.000	247.39	247.99	247.39	247.000	247.99	247.00
219	247.99	_ 247.00	0 247.000	247.99.	. 247.99.	. 247.99	247.99_	249.000	247.000	247.99	247.000	247.99	247.99_	247.99	247.000	247.99_	247.99	247.99	247.99_	247.000	247.99.	247.99	247.99	247.000	247.000	247.000	247.99	247.000	247.000	247.000	247.000
220	247.00	0 247.00	0 247.000	247.000	247.99.	247.99.	247.99.	249.000	247.000	247.99.	247.000	247.99	247.99.	247.99.	247.000	247.99	247.99	247.99	247.000	247.000	247.99.	247.99	249.000	247.99	247.000	247.000	247.000	247.000	247.000	247.99	247.99.
221	247.00	0 247.00	0 247.99.	247.000	247.000	247.99	249.000	249.000	247.99	247.99	247.000	247.000	247.99	247.99	246.000	247.99	247.000	247.99	247.99_	247.000	247.99	247.99	247.000	247.99	247.000	247.99	247.000	247.99_	246.000	249.000	249.000
222	246.00	0 247.00	0 247.000	249.000	247.000	247.99	247.99.	247.99.	247.99.	247.99	247.000	247.000	247.99	247.99	247.99	249.000	247.99	247.99	247.000	247.000	247.000	247.99	245.000	247.000	247.99	247.99	247.000	246.000	247.000	249.000	249.000
223	245.00	0 247.00	0 247.000	247.99	247.000	246.000	247.000	249.000	247.99	247.99	247.99	246.000	246.000	247.99	247.99	249.000	247.000	247.99	247.000	246.000	248.000	249.000	246.000	247.99	247.99	247.99	247.000	240.000	240.000	247.99	247.99
225	247.99	_ 247.00	0 247.000	249.000	249.000	247.99.	247.99	247.000	246.000	246.000	247.000	246.000	247.000	246.000	247.99_	247.99_	247.000	247.000	247.000	247.99	247.000	247.99_	249.000	247.99	247.99_	249.000	247.000	247.000	247.99	247.99	247.99.
226	247.00	0 246.00	0 249.000	249.000	247.000	247.000	247.000	247.99.	247.99.	249.000	247.99.	247.99	247.000	246.000	247.000	247.99	247.99	249.000	247.99	247.99.	247.99	247.000	247.000	247.99.	249.000	247.99	247.99	249.000	247.99	247.000	247.000
227	247.99	247.00	0 247.99.	. 247.99.	247.99.	246.000	247.000	247.000	247.99	249.000	247.99	247.99	247.99	247.99	247.99	247.99	249.000	247.99	247.99_	247.000	246.000	247.000	247.000	247.000	247.99_	247.99	247.000	246.000	247.99	247.99	247.99.
228	247.99	247.95	247.000	247.000	249.000	247.000	247.000	247.99.	249.000	247.99	247.99	247.99	247.99	247.99	247.99	247.99	247.99	247.99	247.99	247.99.	247.000	247.99	249.000	247.99	247.99	249.000	249.000	247.000	247.99	247.99	247.000
230	245.00	0 247.35	0 247.000	247.99	247.99	247.99	247.000	247.000	247.99	249.000	247.99	247.000	247.000	247.000	246.000	246.000	246.000	247,000	247.99	247.99	247.000	247.000	247.99	247.99	247.000	247.99	247.000	247.000	249.000	247.99	247.000
231	247.00	0 247.00	0 246.000	247.000	247.99.	247.99.	247.000	246.000	247.99.	247.99	247.000	247.99	247.99_	247.000	247.000	246.000	247.000	247.000	247.000	247.99	247.99	247.000	247.000	247.99	247.99_	247.99	247.99	247.99	246.000	246.000	247.000
232	247.00	0 247.00	0 246.000	247.99.	247.000	247.000	247.99	247.000	247.99.	247.000	247.99.	247.000	247.99	247.000	247.000	247.99	247.99	247.000	247.000	247.000	247.000	247.000	249.000	249.000	247.99	247.99	247.000	247.99	247.000	247.000	247.99.
233	247.00	0 247.95	247.000	247.99.	. 247.99.	247.000	247.99	247.99.	247.000	247.99	247.000	247,000	247.000	247.99	247.000	247.99	249.000	247.99	247.99_	247.99	247.99	247.99	247.99	247.99	247.99_	247.99	247.99	247.000	247.000	247.000	247.99
234	247.00	0 247.00	0 246.000	247.99.	247.99	247.99.	247.99	247.000	247.000	247.000	247.000	247.000	247.000	247.000	247.000	247.99	249.000	247.99	247.99	247.000	247.99	249.000	246.000	247,000	247.000	247.99	247.000	247.99	247.000	247.000	247.99
236	247.99	246.00	0 246.000	246.000	247.000	246.000	247.000	247.000	247.99	246.000	247.000	247.000	247.99	247.000	247.000	247.000	247.99	247.99	247.000	247.000	247.99	247.99	247.99	247,000	247.000	247.000	247.99	247.000	247.000	247,000	247.000
237	247.99	247.00	0 247.000	247.000	246.000	247.000	247.000	247.000	247.99	247.000	247.000	247,000	247.99	247.000	247.99	247.000	247.000	247.99	247.000	247.000	247.99	247.000	247.000	247,000	247.000	247.000	247.000	247.000	246.000	246.000	247.000
238	247.99	247.00	0 247.000	249.000	247.000	247.000	247.000	247.000	247.99.	247.99	247.99.	247.000	247.99	247.99.	247.000	247.99	247.000	247.99	247.99_	247.99.	247.000	247.99	247.99.	247.99	247.99	247.000	246.000	247.99	246.000	246.000	247.000
239	247.99	247.00	0 247.000	247.99.	247.000	247.000	247.99	247.000	247.99.	249,000	247.99.	246.000	247.000	247.99.	247.000	247.000	247.000	247.99	247.99	247.99.	246.000	247.99	247.99	247.99	247.99	247.000	247,000	247.000	247.000	246.000	246.000
240	245.00	0 247.00	0 247.99	249.000	247.000	247.99	247.99	247.000	247.99	247.000	247.000	248.000	247.000	246.000	248.000	247.99	247.000	247.000	247.000	247.000	247.000	247.000	249.000	249.000	247.000	247.000	247.000	249.000	247.000	247.000	247.99
242	247.00	0 247.00	0 247.000	247.000	247.99	247.99	247.99	247.000	247.000	246.000	247.99	247.000	247.000	247.000	247.000	247.000	247.99	247.000	246.000	246.000	247.000	247.000	247.000	247.000	247.000	247.000	247.000	247.99	247.99	247.99	247.000
243	247.00	0 247.00	0 246.000	247.000	247.99.	247.000	247.000	247.000	247.000	247.000	246.000	247.000	247.000	247.000	247.000	247.99_	247.99	247.000	246.000	246.000	247.000	247.99	247.000	246.000	247.000	247.99	247.000	247.99_	247.99	247.99	247.99.
244	246.00	0 246.00	0 247.99.	247.99.	247.99.	247.000	246.000	246.000	247.99.	247.000	247.000	247.000	247.99	247.000	246.000	246.000	247.000	247.99	247.000	246.000	247.99.	247.000	247.000	246.000	247.000	247.99	247.000	247.000	246.000	247.99	247.99.
245	247.00	0 247.00	0 247.000	246.000	247.000	247.000	247,000	247.000	247,000	246,000	246.000	247,000	247,000	246.000	247.99	247,000	246.000	247,000	246.000	246.000	247,000	247.99	247.000	247,000	247.99	247.99.	247,000	247.000	247.99.	247,000	247.000
247	246.00	0 247.00	0 247.000	247.000	246.000	247.99	247.000	247.000	247.000	249.000	246.000	246.000	247.000	247.99	247.99	247.000	247.000	247.99	247.99	247.99	247.99	247.99	247.000	247.99	247.99	247.000	247.99	247.000	247.000	247.000	247.00
248	246.00	0 247.00	0 246.000	247.000	246.000	247.000	247.000	246.000	247.99	247.000	246.000	246.000	247.99	247.99.	247.000	247.000	247.000	247.000	247.000	247.99	249.000	247.99	247.99	247.99	247.99	247.000	247.000	246.000	246.000	247.000	247.000
249	246.00	0 247.00	0 246.000	247.000	245.000	246.000	246.000	246.000	247.99	247.000	247.000	247.000	247.99	247.99	247.000	247.99_	247.99	247.000	246.000	247.000	247,000	247.000	247.99	247.99	247.99_	247.000	247.000	247.99_	247.99	246.000	247.99.
250	246.00	0 246.00	0 246.000	247.99	245.000	245.000	246.000	247.000	247.99.	247.000	247.000	247.000	247.000	247.000	245.000	246.000	247.000	246.000	246.000	247.000	247.000	247.99	247.000	247.000	247.000	249.000	247.000	246.000	247.000	246.000	247.000
251	247.00	247.00	0 246.000	247.000	247.000	246.000	246.000	247.000	247.000	247.000	247.000	247.99	247,000	247.000	246.000	246.000	247.000	246.000	247.000	247.000	247,000	246.000	247.99	247,99	247.99	247.99	246.000	244.00	247.99	247,000	247.008
253	247.99	247.00	0 246.000	247.99	247.000	246.000	245.000	247.000	247.000	246.000	246.000	247.000	246.000	246.000	247.000	247.99	247.99	247.000	247.000	247.000	247.99	247.000	247.99	247.99	247.000	247.000	247.000	247.99	247.99	247.000	247.00
254	247.00	0 247.00	0 246.000	247.99	247.000	247.000	247.000	247.000	247.000	247.000	246.000	247.000	246.000	246.000	246.000	247.99	247.99	247.000	247.99	247.99	247.99	247.000	247.99	247.99	247.99	247.99	247.000	247.000	247.99	247.000	247.000
255	246.00	0 247.00	0 247.000	247.99.	246.000	247.99	247.99_	247.000	246.000	247.99_	246.000	247.000	247.000	247.000	247.99	247.000	247.000	247.99	247.99_	247.000	246.000	247.99	247.99	247.000	247.99_	247.99	247.000	247.000	247.99	247.000	247.000
256	246.00	0 246.00	0 247.000	247.000	246.000	247.000	247.99	247.000	247.000	247.99	246.000	247.99	247.99	247.99	247.99	247.99	247.99	247.99	247.000	247.000	246.000	247.99	247.000	247.000	247.99	247.99	247.99	247.99	247.000	247.000	247.99.
257	245.00	0 246.00	0 247.000	247.000	247.000	246.000	247.000	247.99	247,000	247,000	246.000	247,000	247,000	247.000	247,000	247.99	247.99	247.99	247.000	247.000	247,000	247.99	247,000	247,000	247.99	247.99	247.99	247.99	247.99	247.99	247.99
259	246.00	0 247.00	0 247.000	246.000	247.99	247.99	247.99	247.99	247.000	247.99	247.99	247.000	247.000	247.000	246.000	246.000	246.000	247.000	249.000	247.99	247.99	247.000	247.99	247.99	247.000	247.000	247.000	246.000	247.99	247.99	247.99
																														_	

Figure 126: Table of image pixels.

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



(a) Image processing frame after action ${\bf Colorize}$.



(c) Image processing local Fourier transform $(\textcircled{\bullet})$.



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



(d) Image processing local magnifier (\mathfrak{A})

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

23.1 Tool buttons

- \blacksquare : print the image.
- 📑 : save the image.

- \blacksquare : transfer the frame to the clipboard.
- 🖻 : open an image.
- III: tabulate the image (Fig. 126).
- \mathbb{X} : select and cut part of image.
- I: apply selected process (Fig. 129b).
- 🗰 : Fourier transform part of image.
- 🚨 : show 3-D view.
- 🕄 : magnify part of image.
- \blacksquare : open the toolbox.
- ¹⁰ : 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.



(c) Peaks are listed in the peaks table.



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



(b) Image contrast is inverted.



(d) Peaks are identified.



(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 LookUp Table (Fig. 131). The table contains 56 different LUTs including **TemperatureMap** and **Thermometer-Colors** (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.

		Set 1 Set 2				Set 1 Set 2	
AlpineColors	AquamarineColors	ArmyColors	AtlanticColors	GreenPinkTones	IslandColors	LakeColors	LightTemperatureMap
AutoraColors	AvocadoColors	BeachColors	BlueGreenYellow	LightTerrain	MintColors	NeonColors	Pastel
BrassTones	Brigh/Bands	BrownGyanTones	CandyColors	PearlColors	PigeonTones	PlumColors	Rainbow
CherryTones	CMYKColors	CoffeeTones	DarkBands	RedBlueTones	RedGreenSplit	RoseColors	RustTones
DarkRainbow	DarkTerrain	O DeepSeaColors	FatColors	SandyTerrain	SiennaTones	SolarColors	SouthwestColors
FruitPunchColors	FuchsiaTones	GrayScale	GrayTones	StarryNightColors	SunsetColors	C TemperatureMap	ThermometerColors
GrayYellowColors	GreenBrownTerrain			ValentineTones	WatermelonColors		
			Done				Done

(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:

- \blacksquare : transfer the dialogue to the clipboard.
- $^{\mbox{$\scriptstyle 0$}}$: open associated help file.



(a) Biprism settings.



(b) Diffraction settings.

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



(c) Biprism rotated.

(d) Biprism rotated 90° .

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:

- \blacksquare : print the table.
- \blacksquare : save the table.
- \blacksquare : 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:

- \blacksquare : print the table.
- \blacksquare : save the table.
- \blacksquare : transfer the frame to the clipboard.
- = : make a table with different maximum (hkl) indices.
- \mathbf{a} : reduce the table (Fig. 159).
- L : display a powder pattern (Fig. 116).
- 🕲 : display a ring pattern (Fig. 136).

• 🧖 : display a help file.

iii 🖬 📋 😑	N 🗉 🔍 🔍										
	(h,k,l)	d*/nm ⁻¹	V,/V	V ₁ /V	Ampli / V	Phase / Deg	Ext./nm	Bragg / mRad	d/nm	Intens.	h max.
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	5 0 3 6 9 12 15 0
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	1 mm
24	(3, 1, 1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	499.00	* max
8	(2, 2, 2)	5.59629	-2.35438	-0.34001	2.3788	8.21772	321.17924	5.51	0.17869	22.00	6 A
6	(4, 0, 0)	6.46204	6.76917	0.79209	6.81535	6.67409	112.10262	6.36	0.15475	118.00	0 3 6 9 12 15
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	- I max.
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	50
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	Default Maximum Spacing : 16 789 (nm-1)
24	(4, 4, 2)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	8.00	a contraction of a contract of a contract of
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	(h,k,i) number : 53
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	Adomic Porm Pector
24	(7, 1, 1)	11.53704	1.19833	-1.52327	1.93813	-51,80839	394.187	11.36	0.08668	21.00	DTSB EIK DRDW WK WKC YRW IEMS
24	(6, 4, 0)	11.6496	-0.73653	-0.19703	0.76243	14.97646	1002.04269	11.47	0.08584	3.00	brob car man int mit. sitily scale
48	(6, 4, 2)	12.08936	2.25769	0.3921	2.29148	9.85241	333.3997	11.90	0.08272	57.00	Relativistic correction
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	-52.14897	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	
A	100 A AL	*******	0.040.07	0.00030	A AAAAAF	17 17000	A444 A 4444	****		A AA	

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

28 Atomic Form Factor

The Atomic Form Factors (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 Thermal Diffuse Scattering 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. A24 (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. A47 (1991) 590-597.
- WKc : A. Weickenmeier and H. Kohl, Acta Cryst. Acta Cryst. A54 (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 Atomic Scattering Amplitude 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 Dyck³⁵. 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.

 $^{^{35}\}mathrm{I}.$ Lobato and D. Van Dyck, Acta Cryst. A
70 (2014) 636-649.

	DTSB (Doyle	-Turner / Smith-Burge) EJK (E	arl J. Kirkland) PRDW	(Peng-Ren-Dudarev-Whe	lan) WK (Weickenmeie	r-Kohl phonon only) WK	ic (Weickenmeier-Kohl p	honon + core) XRay ()	(-Ray Mott formula) JEMS (Mott formula)
tomic form factors	2	Authors	[a.[1]	6.01	a [2]	6.021	a (3)	6.01	a 641	6.64
Ac	89	Smith-Burge	6.278	28.323	5.195	4.949	2.321	0.557	0.000000	0.000000
Ac	47	Dovie-Turper	2.036	61497	3.272	11.824	2.511	2.846	0.837	0.327
AL	13	Dovle-Turner	2.276	72.322	2.428	19.773	0.858	3,080	0.317	0.408
Am	95	Smith-Burne	6.378	29.156	5 4 9 5	5 102	2.495	0.565	0.000000	0.000000
Ar	18	Dovie-Turper	1 274	26.682	2 190	8.813	0.793	2 219	0.326	0.307
As	33	Dovie-Turner	2.399	45.718	2.790	12.817	1.529	2.280	0.594	0.328
A1	85	Smith-Burne	6 133	28.047	5.031	4.957	2 2 3 9	0.558	0.000000	0.000000
Au	79	Dovie-Turper	2 388	42.866	4 226	9.743	2.689	2 264	1 255	0.307
B	5	Dovle-Turner	0.945	46.444	1.312	14.178	0.419	3.223	0.116	0.377
Ra	56	Dovie-Turner	7.821	117.657	6.004	18 778	3 280	3 263	1 103	0.376
Be	4	Dovie-Turner	1 250	60.804	1.334	18.591	0.360	3.653	0.106	0.416
Bi	83	Dovle-Turner	3.841	50.261	4.679	11,999	3.192	2.560	1.363	0.318
Bk	97	Smith-Burge	6.502	28.375	5.478	4.975	2.510	0.561	0.000000	0.000000
Br	35	Dovle-Turper	2 166	33,899	2 904	10.497	1.395	2 041	0.589	0.307
c	6	Dovle-Turner	0.731	36,995	1.195	11.297	0.456	2.814	0.125	0.346
Ca	20	Dovle-Turner	4.470	99.523	2.971	22.696	1.970	4.195	0.482	0.417
Cd	48	Dovie-Turner	2.574	55.675	3.259	11.838	2.547	2 784	0.838	0.322
Ce	58	Smith-Burge	5.007	28,283	3,980	5.183	1.678	0.589	0.000000	0.000000
Cf	98	Smith-Burne	6.548	28.461	5.526	4.965	2.520	0.557	0.000000	0.000000
CI	17	Dovie-Turner	1.452	30.935	2 292	9.980	0.787	2.234	0.322	0.323
Cm	96	Smith-Burge	6.460	28.396	5.469	4.970	2.471	0.554	0.000000	0.000000
Co	27	Dovie-Turper	2 367	61.431	2 236	14 180	1.724	2 725	0.515	0.344
Cr	24	Dovle-Turner	2.307	78.405	2.334	15 785	1.823	3 157	0.490	0.364
Cs	55	Dovle-Turner	6.062	155.837	5.986	19,695	3.303	3,335	1.096	0.379
Cu	29	Dovle-Turner	1.579	62.940	1.820	12.453	1.658	2.504	0.532	0.333
Dv	66	Smith-Burne	5.332	28.888	4.370	5 198	1.863	0.581	0.000000	0.000000
Fr	68	Smith-Burge	5.436	28.655	4.437	5.117	1.891	0.577	0.000000	0.000000
Eu	63	Dovle-Turner	6.267	100.298	4.844	16.066	3.202	2,980	1.200	0.367
F	9	Dovle-Turner	0.387	20.239	0.811	6.609	0.475	1.931	0.146	0.279
Fe	26	Dovle-Turner	2.544	64.424	2.343	14.880	1.759	2.854	0.506	0.350
Fr	87	Smith-Burge	6.201	28,200	5.121	4.954	2.275	0.556	0.000000	0.000000
Ga	31	Dovle-Turner	2.321	65.602	2.486	15.458	1.688	2.581	0.599	0.351
Gd	64	Smith-Burge	5.225	29.158	4.314	5.259	1.827	0.586	0.000000	0.000000
Ge	32	Dovle-Turner	2.447	55.893	2.702	14.393	1.616	2.446	0.601	0.342
н	1	Smith-Burge	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-Burge	5.588	29.001	4.619	5.164	1.997	0.579	0.000000	0.000000
На	80	Dovle-Turner	2.682	42.822	4.241	9.856	2.755	2,295	1.270	0.307
Но	67	Smith-Burge	5.376	28.773	4.403	5.174	1.884	0.582	0.000000	0.000000
1	53	Dovle-Turner	3.473	39,441	4.060	11.816	2.522	2,415	0.840	0.298
In	49	Dovle-Turner	3.153	66.649	3.557	14,449	2.818	2,976	0.884	0.335
lr .	77	Smith-Burge	5.754	29.159	4.851	5.152	2.096	0.570	0.000000	0.000000
к	19	Dovle-Turner	3.951	137.075	2.545	22.402	1.980	4.532	0.482	0.434
Kr	36	Dovle-Turner	2.034	29,999	2.927	9.598	1.342	1,952	0.589	0.299
La	57	Smith-Burge	4.940	28.716	3.968	5.245	1.663	0.594	0.000000	0.000000
u	3	Dovle-Turner	1.611	107.638	1.246	30,480	0.326	4,533	0.099	0.495
Lu	71	Smith-Burge	5.553	28.907	4.580	5.160	1.969	0.577	0.000000	0.000000
Ma	12	Dovie-Turper	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.
- \blacksquare : transfer the dialogue to the clipboard.
- 🤨 : display a help file.

28.2 Popup menu

A Atomic Scattering Amplitude (ASA or Electron Scattering Amplitude) 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 $\mathbf{x} \mathbf{n}$: 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.



(d) Weickenmeier-Kohl atomic form factors.



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



(b) Earl J. Kirkland atomic form factors.



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



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



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

Figure 140: Comparison of the Electron Scattering Amplitudes 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.



Figure 141: AFF sources.

Figure 142: Comparison of the Electron Scattering Amplitudes of the different references at selected $\frac{\sin\theta}{\lambda}$ values.



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

	(m k D	dt (am ²]	V./V	V./V	Amoli /V	Phase / Dec	Ext (nm	Brann / mRad	d (nm	Interne	(i) h max
	(0,0,0)	0.000	21,70573	1.48463	21.75644	3.91282	EXC / HIT	0.00	di initi	a rage rag.	
	(1, 1, 1)	2.79814	4.65215	10.32161	11.32158	65.73797	67.48455	2.75	0.35738	0.00	5 🔘
	(1, 1, 1)	2 79814	6 14193	963717	11.42796	.57 48995	66,85632	2.75	0.35738	0.00	0 3 6 9 12 15
	(1.1.1)	2.79814	6 14193	-963717	11.42796	57.48995	66,85632	2.75	0.35738	0.00	
	(4, 4, 4)	2 79814	4.65215	10.32161	11.32158	65 73797	67.48455	2.75	0.35738	0.00	x max.
	(1, 1, -1)	2,79814	6.14193	-9.63717	11.42796	-57,48995	66,85632	2.75	0.35738	0.00	
	(111)	2,79814	4.65215	10.32161	11.32158	65,73797	67.48455	2.75	0.35738	0.00	5 0 3 6 9 12 15
	(-1, 1, -1)	2 79814	4.65215	10.32161	11.32158	65 73797	67.48455	2.75	0.35738	0.00	
	(-1, -1, -1)	2,79814	6.14193	-9.63717	11.42796	-57.48995	66,85632	2.75	0.35738	0.00	(Imax
	(2.0.0)	3 23102	-4 16756	.0.38805	4 18559	5.31965	182 53851	3.18	0.3095	0.00	
	(2,0,0)	3,23102	4 16755	-0.38805	4 18559	5.31965	182 53851	3.18	0.3095	0.00	5 🕲
	(0.2.0)	3,23102	-4 16756	-0.38805	4 18559	5 31965	182 53851	3.18	0.3095	0.00	0 3 6 9 12 15
	(0, 2, 0)	3,23102	4.16756	-0.38805	4 18559	5.31965	182 53851	3.18	0.3095	0.00	
	(0, 0, 2)	3 23102	_4 16756	.0 38805	4 18550	5 31965	182 53851	3.18	0.3095	0.00	
	(0, 0, 2)	3,23102	4 16756	.0 38805	4 18559	5.31965	182 53851	3.18	0.3095	0.00	
	(2, 2, 0)	4 56935	10,21959	0.94507	10 2632	5 28348	74 44332	4.50	0.21885	0.00	Default Maximum Spacing : 16.789 [nm-1]
	(2,2,0)	4.56935	10,21959	0.94507	10.2632	5.28348	74.44332	4.50	0.21885	0.00	
	(2, 2, 0)	A 56035	10,21059	0.94507	10.2632	5.28348	74,44332	4.50	0.21885	0.00	Obligation (2012
	(2,2,0)	4.56035	10,21050	0.04507	10.2622	6.28348	74.44332	4.60	0.01885	0.00	(n,c)/number: 1243
	(2, 2, 0)	4.50935	10,21959	0.94507	10.2632	5.20340	74,44332	4.50	0.21885	0.00	
	(2, 0, 2)	4,00930	10.21909	0.94507	10.2032	5.26346	74,44332	4.00	0.21660	0.00	Atomic Form Factor
	(2, 0, 2)	4 56025	10.21959	0.94507	10.2032	0.40340	74,44332	4.50	0.21000	0.00	
	(2, 0, -2)	4,00930	10,21959	0.94507	10.2632	0.20340	74,44332	4.50	0.21865	0.00	DTSB EJK PRDW WK WKc. XRay JEM
_	(-2, 0, -2)	4.00935	10.21959	0.94507	10.2032	0.20340	74,44332	4.50	0.21000	0.00	
	(0, 2, 2)	4.00935	10.21959	0.94507	10.2632	5.28348	74,44332	4.50	0.21885	0.00	Relativistic correction
_	(0, -2, 2)	4.00930	10,21909	0.94507	10.2032	0.20340	74,44332	4.50	0.21665	0.00	
	(0, 2, -2)	4,56935	10,21959	0.94507	10.2632	5.28348	74,44332	4.50	0.21885	0.00	
_	(0, -2, -2)	4.56935	10.21959	0.94507	10.2632	5.28348	74,44332	4.50	0.21885	0.00	
	(3, 1, 1)	5.35804	3.04229	-5.25262	0.39189	-00.20100	119.53009	5.27	0.18004	0.00	
_	(3, +1, 1)	5.35804	2.41018	5.78773	0.27182	07.54113	121.81841	5.27	0.18004	0.00	
	(-3, 1, 1)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(-3, -1, 1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(3, 1, -1)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
_	(3, -1, -1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(-3, 1, -1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(-3, -1, -1)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(1, 3, 1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(1, -3, 1)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(-1, 3, 1)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(-1, -3, 1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(1, 3, -1)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(1, -3, -1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(-1, 3, -1)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(-1, -3, -1)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(1, 1, 3)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(1, -1, 3)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(-1, 1, 3)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(-1, -1, 3)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(1, 1, -3)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	
	(1, -1, -3)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(-1, 1, -3)	5.35804	3.64229	-5.25262	6.39189	-55.26165	119.53009	5.27	0.18664	0.00	
	(-1, -1, -3)	5.35804	2.41618	5.78773	6.27182	67.34113	121.81841	5.27	0.18664	0.00	

Figure 144: Table of ZnTe structure factors.

29.1 Tool buttons

The tool buttons allow to:

- \blacksquare : print the table.
- 📑 : save the table.
- \bullet \blacksquare : transfer the dialogue to the clipboard.
- \blacksquare : make a table with different maximum (hkl) indices.
- \mathbf{a} : reduce the table (Fig. 159).
- **L**: open electron powder pattern frame(Fig. 135).
- 🕲 : open rings pattern frame (Fig. 136).
- ¹⁰ : display a help file.

											10 here
	(h,X,I)	d*/nm	v,/v	v _i /v	Ampli / V	Phase / Deg	Ext / nm	Bragg / mikad	d/nm	Intens.	
_	(0, 0, 0)	0.000	21.70573	1.48463	21.75644	3.91282		0.00			
	(1, 1, 1)	2.79814	4.65215	10.32161	11.32158	65.73797	67,48455	2.75	0.35738	1000.00	0 3 6 9 12 15
	(2, 0, 0)	3.23102	-4,16/56	-0.38805	4.18009	5.31965	182.53851	3.18	0.3095	89.00	
	(2, 2, 0)	4.56935	10.21959	0.94507	10.2632	5.28348	74,44332	4.50	0.21885	755.00	k max.
	(3, 1, 1)	5.35804	3.04229	-5.25262	0.39189	-00.20100	119.53009	5.27	0.18004	499.00	
	(2, 2, 2)	5.59629	-2.35438	-0.34001	2.3788	8.21772	321.17924	5.51	0.17869	22.00	50
	(4, 0, 0)	6.46204	6.76917	0.79209	6.81535	6.67409	112.10262	6.36	0.15475	118.00	0 3 6 9 12 15
	(3, 3, 1)	7.04184	1.63206	4.08918	4.40284	68.24225	173.52797	6.93	0.14201	180.00	
	(4, 2, 0)	7.22478	-1.64745	-0.30134	1,67479	10.36562	456.18665	7.11	0.13841	25.00	I max.
	(4, 2, 2)	7.91434	5.08642	0.67912	5.13156	7.60489	148.8848	1.19	0.12635	218.00	
	(3, 3, 3)	8.39443	2.1225	-2.78984	3.50546	-52.73624	217.94836	8.26	0.11913	32.00	0 0 3 6 9 12 15
	(5, 1, 1)	8.39443	1.20656	3.15967	3.3822	03/03348	225.89075	8.20	0.11913	89.00	
	(4, 4, 0)	9.1387	4.02407	0.58808	4.06681	8.31444	187.86285	9.00	0.10942	59.00	
\$	(5, 3, 1)	9.55748	1.729	-2.22974	2.82156	-52.20906	270.77255	9.41	0.10463	109.00	
	(6, 0, 0)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	2.00	Default Maximum Spacing : 16.789 [nm-1]
	(4, 4, 2)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	8.00	
	(6, 2, 0)	10.21738	3.26927	0.51212	3.30914	8.90277	230.87428	10.06	0.09787	70.00	
	(5, 3, 3)	10.5936	0.72405	2.09328	2.21497	70.91985	344.92257	10.43	0.0944	30.00	(h,k,l) number : 53
	(6, 2, 2)	10.71607	-0.86402	-0.2181	0.89112	14.16695	857.33943	10.55	0.09332	5.00	
	(4, 4, 4)	11.19257	2.70064	0.44756	2.73748	9.40973	279.08479	11.02	0.08934	15.00	Atorik Form Factor
	(5, 5, 1)	11.53704	0.57301	1.74953	1.84098	71.86525	414.98805	11.36	0.08668	19:00	
5	(7, 1, 1)	11.53704	1.19833	-1.52327	1.93813	-51,80839	394.187	11.36	0.08568	21.00	DTSB EJK PRDW WK WKc. XRay JEMS
1	(6, 4, 0)	11.6496	-0.73653	-0.19703	0.76243	14.97646	1002.04269	11.47	0.08584	3.00	
1	(6, 4, 2)	12.08936	2.25769	0.3921	2.29148	9.85241	333.3997	11.90	0.08272	57.00	Relativistic correction
	(5, 5, 3)	12.40896	1.01101	-1.28578	1.63566	-51.822	467.07672	12.21	0.08059	14.00	
	(7, 3, 1)	12.40896	0.45722	1.47858	1.54766	72.81703	493.63302	12.21	0.08059	25.00	
	(8, 0, 0)	12.92407	1.90507	0.34411	1.9359	10.23878	394.63464	12.72	0.07738	5.00	
1	(7, 3, 3)	13.22351	0.85835	-1.09631	1.39236	-51.94099	548.68708	13.02	0.07562	10.00	
	(6, 4, 4)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00	
1	(8, 2, 0)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00	
2	(6, 6, 0)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	6.00	
	(8, 2, 2)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	13.00	
	(5, 5, 5)	13.99072	0.29631	1.08264	1.12245	74.69329	680.61854	13.77	0.07148	2.00	
	(7, 5, 1)	13.99072	0.73254	-0.94265	1.19382	-52.14897	639.92971	13.77	0.07148	13.00	
	(6, 6, 2)	14.08368	-0.49062	-0.14632	0.51198	16.60584	1492.17911	13.86	0.071	1.00	
1	(8, 4, 0)	14,44955	1.38662	0.26589	1,41188	10.85514	541.09119	14.22	0.06921	9.00	
3	(7, 5, 3)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	8.00	
	(9, 1, 1)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	4.00	
	(8, 4, 2)	14.80638	-0.43548	-0.13264	0.45524	16.94014	1678.14294	14.57	0.06754	2.00	
1	(6, 6, 4)	15.15482	1.19376	0.23396	1.21647	11.08847	628.00527	14.92	0.06599	6.00	
3	(9, 3, 1)	15,41097	0.54033	-0.7115	0.89342	-52.78593	855.08408	15.17	0.06489	7.00	
	(8, 4, 4)	15.82869	1.03301	0.20591	1.05333	11.27302	725.26436	15.58	0.06318	5.00	
	(9, 3, 3)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00	
	(7, 5, 5)	16.07411	0.46649	-0.62353	0.77872	-53.19783	981.02145	15.82	0.06221	2.00	
	(7, 7, 1)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00	
	(10, 0, 0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	0.00	
	(8, 6, 0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	1.00	
	(8, 6, 2)	16.47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	7.00	
	(10, 2, 0)	16,47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	3.00	
	(7,7,3)	16.71095	0.40391	-0.54912	0.68167	-53.66309	1120.67193	16.45	0.05984	2.00	
	(9, 5, 1)	16.71095	0.13115	0.62185	0.63552	78.0909	1202.04896	16.45	0.05984	3.00	
_		*******	A 44447	0.00030	0.000.00	17 17000	A244 A 4244	*****	AAFAFA	0.00	

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

27)=0.0	Image contrast	O Negative
	Diantou	J
	Real	Imaginary
	Amplitude	OPhase
	 Intensity 	 Diffractogram
	Intensity	
	Sum	0.9848662
	Controls Brightness / au	-Gamma / au
		300
	- 244	000
	- 144	-
	-	- 200
	- 44	
	J 5	-
	56	- 100
	156	
	-	-
		D-o
	-26	6.0
	Fine Live	Fine Live

Figure 146: Miscellany menu Load image frame.

30.1.2 Load super-cell

ŧ	Symbol	Wyckoff	x	y	z	Debye	Occupa	Absorpt	(x, y, z) shift
)	Pt		0.4347	0.1734	0.657	0.005	1.000	0.100	□ x + 1/2
1	Pt	_	0.4677	0.173	0.6812	0.005	1.000	0.100	□ y + 1/2
2	Pt		0.5008	0.1726	0.7054	0.005	1.000	0.100	□ z + 1/2
3	Pt	_	0.402	0.2061	0.6576	0.005	1.000	0.100	Slice thick / pm
1	Pt	_	0.4351	0.2057	0.6818	0.005	1.000	0.100	Slice thick. / htt
5	Pt	_	0.4681	0.2053	0.706	0.005	1.000	0.100	
3	Pt		0.5012	0.2049	0.7303	0.005	1.000	0.100	-
7	Pt		0.3694	0.2387	0.6582	0.005	1.000	0.100	- 0.8
3	Pt		0.4024	0.2383	0.6824	0.005	1.000	0.100	-
9	Pt	_	0.4355	0.2379	0.7067	0.005	1.000	0.100	- 0.6
10	Pt		0.4685	0.2375	0.7309	0.005	1.000	0.100	-
11	Pt	_	0.5016	0.2371	0.7551	0.005	1.000	0.100	- 0.4
12	Pt	_	0.3367	0.2714	0.6588	0.005	1.000	0.100	-
13	Pt	_	0.3698	0.271	0.683	0.005	1.000	0.100	- 0.2
14	Pt	_	0.4028	0.2706	0.7073	0.005	1.000	0.100	-
15	Pt	_	0.4359	0.2702	0.7315	0.005	1.000	0.100	" – 0
16	Pt	_	0.4689	0.2698	0.7557	0.005	1.000	0.100	1.0
17	Pt	_	0.502	0.2694	0.7799	0.005	1.000	0.100	

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

30.1.3 Make void

	Symbol	Werkoff	× .	v.	7	Dehve-Waller	Occupatory	Absorption	Chame	AFE	Unit cell duplication		
	Zn	1190001	0.000	0.000	0.000	0.01797	1,000	0.051	Def	0	Duplicate x	Duplicate y	Duplicate z
	Zn		0.500	0.500	0.000	0.01797	1.000	0.051	Def	0			
	Zn		0.000	0.500	0.500	0.01797	1.000	0.051	Def	0	- 16	- 15	
	Zn	a	0.500	0.000	0.500	0.01797	1.000	0.051	Def	0	- 10	- 25	- 20
	Te	3	0.250	0.250	0.250	0.01285	1.000	0.073	Def	0	- 17	- 17	- 17
	Te	3	0.750	0.750	0.250	0.01285	1.000	0.073	Def	0			
	Te	a	0.750	0.250	0.750	0.01285	1.000	0.073	Def	0		-9	-9
	Te	8	0.250	0.750	0.750	0.01285	1.000	0.073	Def	0	- T.	Τ.	Υ.
	Zn	a	1.000	0.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	2.000	0.000	0.000	0.01797	1.000	0.051	Def	0	6	6	6
	Zn	a	3.000	0.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	4.000	0.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	5.000	0.000	0.000	0.01797	1.000	0.051	Def	0	1014-004		
	Zn	8	1.500	0.500	0.000	0.01797	1.000	0.051	Def	0	Vod sze		
	Zn	8	4.500	0.500	0.000	0.01797	1.000	0.051	Def	0	- 5		
	Zn	8	5.500	0.500	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	1.500	0.000	0.500	0.01797	1.000	0.051	Def	0	- 4		
	Zn	a	4.500	0.000	0.500	0.01797	1.000	0.051	Def	0			
	Zn	a	5.500	0.000	0.500	0.01797	1.000	0.051	Def	0	- 3		
	Te	a	1.250	0.250	0.250	0.01285	1.000	0.073	Def	0			
	Te	a	4.250	0.250	0.250	0.01285	1.000	0.073	Def	0	- 2		
	Te	8	5.250	0.250	0.250	0.01285	1.000	0.073	Def	0	Q.		
	Te	a	5.750	0.750	0.250	0.01285	1.000	0.073	Def	0	- 1		
	Te	a	5.750	0.250	0.750	0.01285	1.000	0.073	Def	0			
	Zn	a	0.000	1.000	0.000	0.01797	1.000	0.051	Def	0	0		
	Zn	a	0.000	2.000	0.000	0.01797	1.000	0.051	Def	0	1.36		
	Zn	a	0.000	3.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	8	0.000	4.000	0.000	0.01797	1.000	0.051	Def	0	Fine Live		
	Zn	a	0.000	5.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.500	1.500	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.500	4.500	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.500	5.500	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.000	1.500	0.500	0.01797	1.000	0.051	Def	0			
	Zn	a	0.000	4.500	0.500	0.01797	1.000	0.051	Def	0			
	Zn	a	0.000	5.500	0.500	0.01797	1.000	0.051	Def	0			
	10	8	0.250	1,250	0.250	0.01285	1.000	0.073	Der	0			
	TO		0.250	4.250	0.250	0.01285	1.000	0.073	Def	0			
	10		0.250	5.250	0.250	0.01285	1.000	0.073	Der	0			
	10	3	0.750	5.750	0.250	0.01285	1.000	0.073	Der	0	_		
	10		0.250	5.750	0.750	0.01285	1.000	0.073	Der	0			
_	zn	3	1.000	1.000	0.000	0.01797	1.000	0.051	Def	0	_		
	20		1.000	5.000	0.000	0.01797	1.000	0.051	Der	0			
	2n Te		5.000	1.000	0.000	0.01797	1.000	0.051	Def	0			
	20		5.000	0.000	0.000	0.01797	1.000	0.051	Def	0	_		
	20		1.500	5.500	0.000	0.01797	1.000	0.051	Der	0	_		
	20		4.500	0.500	0.000	0.01797	1.000	0.051	Der	0			
	20	3	5.500	1.500	0.000	0.01797	1.000	0.051	Der	0	_		
	20	3	5.500	4.500	0.000	0.01797	1.000	0.051	Der	0			
	20	3	5.500	5.500	0.000	0.01797	1.000	0.051	Der	0	_		
	10		5.250	5.250	0.250	0.01285	1.000	0.073	Der	0			
	10		1.750	5.750	0.250	0.01285	1.000	0.073	Def	0			
	10	9	4.750	5.750	0.250	0.01285	1.000	0.073	Der	0			

Figure 148: Miscellany menu ${\bf Make~void}$ 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.

					Core Shell Con	Index						Core Shell Core-shell
e-shell lettice (4.50	9, 4.509, 4.923)				Core offer							
	Symbol	Wyckoff	x	У	z	Debye-Waller	Occupancy	Absorption	Charge	AFF		
	Au	a	0.36460412	0.45486804	0.458663415	0.005	1.000	0.034	Def	0		
	Au	a	0.36460412	0.45486804	0.541336585	0.005	1.000	0.034	Def	0	Slice	
	Au	а	0.36460412	0.54513196	0.458663415	0.005	1.000	0.034	Def	0		
	Au	a	0.36460412	0.54513196	0.541336585	0.005	1.000	0.034	Def	0	0.0	0.0
	Au	a	0.45486804	0.36460412	0.458663415	0.005	1.000	0.034	Def	0	O (04) [001]	O oxs [010] O oys [100]
	Au	a	0.45486804	0.36460412	0.541336585	0.005	1.000	0.034	Def	0	Sice thick. / nm	Sub-slices number
	Au	a	0.45486804	0.45486804	0.375990246	0.005	1.000	0.034	Def	0	1	
	Au	a	0.45486804	0.45486804	0.458663415	0.005	1.000	0.034	Def	0		- 120
	Au	a	0.45486804	0.45486804	0.541336585	0.005	1.000	0.034	Def	0	- 0.8	- 100
	Au	a	0.45486804	0.45486804	0.624009754	0.005	1.000	0.034	Def	0		
2	Au	a	0.45486804	0.54513196	0.375990246	0.005	1.000	0.034	Def	0	- 0.6	- 80
	Au	a	0.45486804	0.54513196	0.458663415	0.005	1.000	0.034	Def	0		
	AU	a	0.45486804	0.54513196	0.541336585	0.005	1.000	0.034	Def	0	-0.4	- 00
	AU		0.45486804	0.54513196	0.624009754	0.005	1,000	0.034	Der	0		- 40
	0.0		0.40486804	0.03039588	0.400663415	0.005	1.000	0.034	Def	0	- 0.2	
	AU	3	0.45486804	0.03539588	0.541336585	0.005	1,000	0.034	Der	0		1-20
	AU		0.54513196	0.30460412	0.400663415	0.005	1,000	0.034	Det	0	- 0	T - 0
	AU		0.54513196	0.35450412	0.541336585	0.005	1,000	0.034	Det	0	0.3767	10
0	AU	a	0.54513196	0.45485804	0.375990246	0.005	1,000	0.034	Der	0	0.3/3/	12
	Au	8	0.54513196	0,45486804	0,458063415	0.005	1,000	0.034	Def	0		
	AU	a	0.54513195	0.40486804	0.541330565	0.005	1,000	0.034	Def	0	Pine Live	
	~~		0.04013100	0.54540400	0.024009794	0.000	1,000	0.034	Det	0		
2	AU	a	0.54513195	0.54513190	0.375990246	0.005	1,000	0.034	Det	0		
3	~~		0.54513196	0.54513196	0,438063415	0.005	1.000	0.034	Del	0		
4	AU	a	0.54513196	0.54513196	0.541336565	0.005	1,000	0.034	Def	0		
0	AU	a	0.54513196	0.54513196	0.024009754	0.005	1,000	0.034	Det	0		
0 7	AU	a	0.54513195	0.63539568	0.458063415	0.005	1,000	0.034	Def	0		
•	Au		0.04013190	0.03039000	0.041330000	0.005	1,000	0.034	Def	0		
0	AU	a	0.03539588	0.45485804	0.408003415	0.005	1,000	0.034	Def	0		
9	AU		0.63539566	0.64512106	0.041330000	0.005	1,000	0.034	Def	0		
•	Au	3	0.63539588	0.54513190	0.641236685	0.005	1,000	0.034	Def	0		
	Au		0.40073608	0.40073408	0.458653415	0.005	1,000	0.034	Def	0		
1	Au		0.40973608	0.40973608	0.641336585	0.005	1,000	0.034	Def	0		
4	Au		0.40973608	0.500	0.458663415	0.005	1,000	0.034	Def	0		
5	Au		0.40973608	0.500	0.541336585	0.005	1,000	0.034	Def	0		
6	Au		0.40973608	0.59026392	0.458663415	0.005	1,000	0.034	Def	0		
7	Au		0.40973608	0.59026392	0.541336585	0.005	1.000	0.034	Def	0		
8	Au		0.500	0.40973508	0.458663415	0.005	1,000	0.034	Def	0		
9	Au		0.500	0.40973608	0.541336585	0.005	1.000	0.034	Def	0		
10	Au		0.500	0.500	0.375990246	0.005	1.000	0.034	Def	0		
1	Au		0.500	0.500	0.458653415	0.005	1.000	0.034	Def	0		
2	Au	a	0.500	0.500	0.541336585	0.005	1.000	0.034	Def	0		
3	Au		0.500	0.500	0.624009754	0.005	1.000	0.034	Def	0		
4	Au	a	0.500	0.59026392	0.458663415	0.005	1.000	0.034	Def	0		
5	Au		0.500	0.59026392	0.541336585	0.005	1.000	0.034	Def	0		
6	Au		0.59026392	0.40973608	0.458663415	0.005	1.000	0.034	Def	0		
7	Au		0.59026392	0.40973608	0.541336585	0.005	1.000	0.034	Def	0		
8	Au		0.59026392	0.500	0.458663415	0.005	1.000	0.034	Def	0		
9	Au	8	0.59026392	0.500	0.541336585	0.005	1.000	0.034	Def	0		
0	Au	a	0.59026392	0.59026392	0.458663415	0.005	1.000	0.034	Def	0		
	A.,		0.50026302	0.50026102	0.541336585	0.005	1.000	0.034	Daf	0		

Figure 149: Miscellany menu To core-shell frame.



(c) Core-shell particle view.



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

Sumbol	Wheekoff	1	[w		Debus-Waller	Occupancy	Absorption	Charge	AFE			
Zn	a	0.000	0.000	0.000	0.01797	1.000	0.051	Def	0	Duplicate x	Duplicate y	Duplicate
Zn	a	0.0625	0.0625	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.000	0.0625	0.0625	0.01797	1.000	0.051	Def	0	-	· ·	-
Zn	a	0.0625	0.000	0.0625	0.01797	1.000	0.051	Def	0	- 41	- 41	
Te	a	0.03125	0.03125	0.03125	0.01285	1.000	0.073	Def	0	- 33	- 33	
Te	a	0.09375	0.09375	0.03125	0.01285	1.000	0.073	Def	0	- 26	- 26	
Те	a	0.09375	0.03125	0.09375	0.01285	1.000	0.073	Def	0			
Te	a	0.03125	0.09375	0.09375	0.01285	1.000	0.073	Def	0	- 17	- 17	-
Zn	a	0.125	0.000	0.000	0.01797	1.000	0.051	Def	0		1	11 1.
Zn	a	0.250	0.000	0.000	0.01797	1.000	0.051	Def	0	Y-*	- 1 Y.*	- Y-
Zn	a	0.375	0.000	0.000	0.01797	1.000	0.051	Def	0	1 - 1	1-1	
Zn	a	0.500	0.000	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.625	0.000	0.000	0.01797	1.000	0.051	Def	0	8	8	8
Zn	a	0.750	0.000	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.875	0.000	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.1875	0.0625	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.3125	0.0625	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.4375	0.0625	0.000	0.01797	1.000	0.051	Def	0	Slice		
Zn	a	0.5625	0.0625	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.6875	0.0625	0.000	0.01797	1.000	0.051	Def	0			
Zn	8	0.8125	0.0625	0.000	0.01797	1.000	0.051	Def	0	🖸 Oxy (C	01] Oxz [010]	Oyz [100]
Zn	a	0.9375	0.0625	0.000	0.01797	1.000	0.051	Def	0	Sire thick /	nm	on number
Zn	a	0.125	0.0625	0.0625	0.01797	1.000	0.051	Def	0	Caco unce. 1	000-98	Jes manazer
Zn	a	0.250	0.0625	0.0625	0.01797	1.000	0.051	Def	0	-1		- 120
Zn	a	0.375	0.0625	0.0625	0.01797	1.000	0.051	Def	0	-		
Zn	a	0.500	0.0625	0.0625	0.01797	1.000	0.051	Def	0	- 0.1	°	- 100
Zn	a	0.625	0.0625	0.0625	0.01797	1.000	0.051	Def	0			- 80
Zn	а	0.750	0.0625	0.0625	0.01797	1.000	0.051	Def	0	Q.		
Zn	a	0.875	0.0625	0.0625	0.01797	1.000	0.051	Def	0	- 0.4	٤ - L	
Zn	а	0.1875	0.000	0.0625	0.01797	1.000	0.051	Def	0	-		- 40
Zn	a	0.3125	0.000	0.0625	0.01797	1.000	0.051	Def	0	- 0.1	2	- 20
Zn	a	0.4375	0.000	0.0625	0.01797	1.000	0.051	Def	0	-		
Zn	a	0.5625	0.000	0.0625	0.01797	1.000	0.051	Def	0	' - 0		- 0
Zn	a	0.6875	0.000	0.0625	0.01797	1.000	0.051	Def	0	0.55	0.2	
Zn	a	0.8125	0.000	0.0625	0.01797	1.000	0.051	Def	0	0.00	102	0
Zn	a	0.9375	0.000	0.0625	0.01797	1.000	0.051	Def	0			
Te	a	0.15625	0.03125	0.03125	0.01285	1.000	0.073	Def	0	Fine I	live	
Te	a	0.28125	0.03125	0.03125	0.01285	1.000	0.073	Def	0			
Te	0	0.40625	0.03125	0.03125	0.01285	1.000	0.073	Def	0			
Te	8	0.53125	0.03125	0.03125	0.01285	1.000	0.073	Def	0			
Te	0	0.65625	0.03125	0.03125	0.01285	1.000	0.073	Def	0	Show	spherical	
Te		0.78125	0.03125	0.03125	0.01285	1.000	0.073	Def	0			
Te	0	0.90625	0.03125	0.03125	0.01285	1.000	0.073	Def	0			
10		0.0002.0	0.0012.0	0.0012.0	0.01200	1.000	0.070	0.1	-			

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

30.1.6 To precipitate

					Precipitate Matrix	Model					Precip	itate Matrix Model
te precip	tato lattice (5.0658,	5.0658, 5.0658)	6.	1	1-	1	1.0	(Les.	1.00 (a)		
	Zo	уускоп	X 0.317468728	y 0.429156243	Z 0.439156243	Debye-waller	1 000	Absorption 0.051	Charge	AFF		
	Zn	0	0.317468728	0.439156243	0.560843757	0.01797	1.000	0.051	Def	0	Slice	
	Zn	3	0.317468728	0.560843757	0.439156243	0.01797	1,000	0.051	Def	0		
	Zn	3	0.317468728	0.560843757	0.560843757	0.01797	1,000	0.051	Def	0		
	Zn		0.439156243	0.317468728	0.439156243	0.01797	1,000	0.051	Def	0	Oxy [001]	Oxz [010] Oyz [100]
	Zn	a	0.439156243	0.317468728	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.439156243	0.439156243	0.317468728	0.01797	1.000	0.051	Def	0	Silce thick. / nm	Sub-slices number
	Zn	a	0.439156243	0.439156243	0.439156243	0.01797	1.000	0.051	Def	0	- 1	L
	Zn	a	0.439156243	0.439156243	0.560843757	0.01797	1.000	0.051	Def	0	-	- 120
	Zn	a	0.439156243	0.439156243	0.682531272	0.01797	1.000	0.051	Def	0	- 0.8	- 100
	Zn	a	0.439156243	0.560843757	0.317468728	0.01797	1.000	0.051	Def	0	· · · ·	- 80
	Zn	a	0.439156243	0.560843757	0.439156243	0.01797	1.000	0.051	Def	0	- 0.6	-
	Zn	a	0.439156243	0.560843757	0.560843757	0.01797	1.000	0.051	Def	0	-04	- 60
	Zn	a	0.439156243	0.560843757	0.682531272	0.01797	1.000	0.051	Def	0	- 0.4	- 40
	Zn	a	0.439156243	0.682531272	0.439156243	0.01797	1.000	0.051	Def	0	- 0.2	
	Zn	a	0.439156243	0.682531272	0.560843757	0.01797	1.000	0.051	Def	0	-	- 20
	Zn	a	0.560843757	0.317468728	0.439156243	0.01797	1.000	0.051	Def	0	- o	D-0
	Zn	a	0.560843757	0.317468728	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.560843757	0.439156243	0.317468728	0.01797	1.000	0.051	Def	0	0.619	3
	Zn	a	0.560843757	0.439156243	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.560843757	0.439156243	0.560843757	0.01797	1.000	0.051	Def	0	Fine Live	
	Zn	a	0.560843757	0.439156243	0.682531272	0.01797	1.000	0.051	Def	0		
	Zn	a	0.560843757	0.560843757	0.317468728	0.01797	1.000	0.051	Def	0		
	Zn	a	0.560843757	0.560843757	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.560843757	0.560843757	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.560843757	0.560843757	0.682531272	0.01797	1.000	0.051	Def	0		
	Zn	a	0.560843757	0.682531272	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.560843757	0.682531272	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.682531272	0.439156243	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.682531272	0.439156243	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.682531272	0.560843757	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.682531272	0.560843757	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.378312485	0.378312485	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	а	0.378312485	0.378312485	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	а	0.378312485	0.500	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.378312485	0.500	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.378312485	0.621687515	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.378312485	0.621687515	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	а	0.500	0.378312485	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.500	0.378312485	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.500	0.500	0.317468728	0.01797	1.000	0.051	Def	0		
	Zn	a	0.500	0.500	0.439156243	0.01797	1.000	0.051	Def	0		
	Zn	a	0.500	0.500	0.560843757	0.01797	1.000	0.051	Def	0		
	Zn	a	0.500	0.500	0.682531272	0.01797	1.000	0.051	Def	0		

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



(a) Precipitate 3D-view.



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



(b) 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

Symbol	Wyskoff	x	Y.	z	Debye-Waller	Occupancy	Absorption	Charge	AFF			
Zn	a	0.000	0.000	0.000	0.01797	1.000	0.051	Def	0	Duplcate x	Duplicate y	Ouplic
Zn		0.083333333	0.083333333	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.000	0.083333333	0.083333333	0.01797	1.000	0.051	Def	0	- 16	- 16	
Zn	a	0.083333333	0.000	0.083333333	0.01797	1.000	0.051	Def	0	1 10	- 40	
Te	a	0.041666667	0.041666667	0.041666667	0.01285	1.000	0.073	Def	0	- 17	- 17	
Te	a	0.125	0.125	0.041666667	0.01285	1.000	0.073	Def	0			
Te	a	0.125	0.041666667	0.125	0.01285	1.000	0.073	Def	0	- 9	- 9	
Te		0.041666667	0.125	0.125	0.01285	1.000	0.073	Def	0		11 1.	
Zn		0.166666667	0.000	0.000	0.01797	1.000	0.051	Def	0	- 1.01	0.1	
Zn	8	0.333333333	0.000	0.000	0.01797	1.000	0.051	Def	0		1	1
Zn		0.500	0.000	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.666666667	0.000	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.833333333	0.000	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.250	0.083333333	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.416666667	0.083333333	0.000	0.01797	1.000	0.051	Def	0	Slice		
Zn	a	0.583333333	0.083333333	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.750	0.083333333	0.000	0.01797	1.000	0.051	Def	0			
Zn	a	0.916666667	0.083333333	0.000	0.01797	1.000	0.051	Def	0	Oxy (001	i] 🔿 Oxz (010) 🖸 O	yz [100]
Zn	a	0.166666667	0.083333333	0.083333333	0.01797	1.000	0.051	Def	0	Stee Birk / a	- Sub-star	
Zn	a	0.333333333	0.083333333	0.083333333	0.01797	1.000	0.051	Def	0	0000 1104.71	000-800	is mornoler
Zn		0.500	0.083333333	0.083333333	0.01797	1.000	0.051	Def	0	-1		- 120
Zn	a	0.666666667	0.083333333	0.083333333	0.01797	1.000	0.051	Def	0			
Zn		0.833333333	0.083333333	0.083333333	0.01797	1.000	0.051	Def	0	- 0.8		- 100
Zn		0.250	0.000	0.083333333	0.01797	1.000	0.051	Def	0			
Zn		0.416666667	0.000	0.083333333	0.01797	1.000	0.051	Def	0	- 0.6		
Zn	8	0.583333333	0.000	0.083333333	0.01797	1.000	0.051	Def	0			- 60
Zn		0.750	0.000	0.083333333	0.01797	1.000	0.051	Def	0	- 0.4		
Zn	8	0.916666667	0.000	0.083333333	0.01797	1.000	0.051	Def	0			- 40
Te		0.208333333	0.041666667	0.041666667	0.01285	1.000	0.073	Def	0	-0.2		- 20
Te		0.375	0.041666667	0.041666667	0.01285	1.000	0.073	Def	0			
Te		0.541666667	0.041666667	0.041666667	0.01285	1.000	0.073	Def	0	- 0		- 0
Te		0.708333333	0.041666667	0.041666667	0.01285	1.000	0.073	Def	0	0.20	13	18
 Te		0.875	0.041666667	0.041666667	0.01285	1.000	0.073	Def	0			
Te		0.291666667	0.125	0.041666667	0.01285	1.000	0.073	Def	0	Fine L	ve	
Te		0.458333333	0.125	0.041666667	0.01285	1,000	0.073	Def	0			
Te	8	0.625	0.125	0.041666667	0.01285	1.000	0.073	Def	0			
Te	a	0.791666667	0.125	0.041666667	0.01285	1.000	0.073	Def	0			
Te		0.958333333	0.125	0.041666667	0.01285	1.000	0.073	Def	0			
Te	a	0.291666667	0.041666667	0.125	0.01285	1.000	0.073	Def	0			
Te		0.458333333	0.041666667	0.125	0.01285	1.000	0.073	Def	0			
Te	a	0.625	0.041666667	0.125	0.01285	1.000	0.073	Def	0			
Te	a	0.791666667	0.041666667	0.125	0.01285	1.000	0.073	Def	0			
Te	a	0.958333333	0.041666667	0.125	0.01285	1.000	0.073	Def	0			
Te	8	0.208333333	0.125	0.125	0.01285	1.000	0.073	Def	0			
Te		0.375	0.125	0.125	0.01285	1.000	0.073	Def	0			
Te		0.541666667	0.125	0.125	0.01285	1.000	0.073	Def	0			
Te		0.708333333	0.125	0.125	0.01285	1.000	0.073	Def	0			
 Te		0.875	0.125	0.125	0.01285	1.000	0.073	Def	0			
Zo		0.000	0.166666667	0.000	0.01797	1,000	0.051	Def	0			
Zn		0.000	0.3333333333	0.000	0.01797	1 000	0.051	Def	0			
Zn		0.000	0.500	0.000	0.01797	1,000	0.051	Def	0			
 4.0		0.000	0.000	0.000	0.01707	1.000	0.001					

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



(a) Table of slices.



(b) 3D-view of a slice.



30.1.8 To triclinic

	Symbol	Wyckoff	x	y .	z	Debye-Waller	Occupancy	Absorption	Charge	AFF			
	Zn	a	0.958333334	0.041666667	0.000	0.01797	1.000	0.051	Def	0	Duplic	ation /Oxyz rotatio	[uvw] rotation
	Zn	a	0.958333334	0.000	0.083333333	0.01797	1.000	0.051	Def	0	Destinate a	Development of	Destinates
	Te	a	0.979166667	0.020833334	0.041666667	0.01285	1.000	0.073	Def	0	Dupicase x	Oupscase y	Ouplicase 2
	Te	a	0.9375	0.0625	0.041666667	0.01285	1.000	0.073	Def	0			
	Te	a	0.979166667	0.0625	0.125	0.01285	1.000	0.073	Def	0	- 25	- 25	- 25
	Te	a	0.9375	0.020833334	0.125	0.01285	1.000	0.073	Def	0			
	Zn	8	0.958333334	0.125	0.000	0.01797	1.000	0.051	Def	0	- 17	- 17	- 17
	Zn	a	0.958333334	0.208333334	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.958333334	0.291666667	0.000	0.01797	1.000	0.051	Def	0	- 9	- 9	- 9
	Zn	8	0.958333334	0.375	0.000	0.01797	1.000	0.051	Def	0	5.1	5-1	51
	Zn	a	0.958333334	0.458333333	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.958333334	0.083333334	0.083333333	0.01797	1.000	0.051	Def	0	2	2	1
	Zn	a	0.958333334	0.166666667	0.083333333	0.01797	1.000	0.051	Def	0			
	Zn	a	0.958333334	0.250	0.083333333	0.01797	1.000	0.051	Def	0			
	Zn	a	0.958333334	0.333333334	0.083333333	0.01797	1.000	0.051	Def	0	- Botate r	- Rotate v	Rotate z
	Zn	a	0.958333334	0.416666667	0.083333333	0.01797	1.000	0.051	Def	0	Notate X	- and y	
	Te	a	0.979166667	0.104166667	0.041666667	0.01285	1.000	0.073	Def	0	- 360	- 360	- 360
	Te	a	0.979166667	0.1875	0.041666667	0.01285	1.000	0.073	Def	0	- 270	- 270	- 270
	Te	a	0.979166667	0.270833334	0.041666667	0.01285	1.000	0.073	Def	0			
	Te	a	0.979166667	0.354166667	0.041666667	0.01285	1.000	0.073	Def	0	- 180	- 180	- 180
	Te	a	0.979166667	0.4375	0.041666667	0.01285	1.000	0.073	Def	0			
	Te	a	0.9375	0.145833334	0.041666667	0.01285	1.000	0.073	Def	0	- 90	- 90	 90
	Te	8	0.9375	0.229166667	0.041666667	0.01285	1.000	0.073	Def	0	50	50	- 0
	Te	8	0.9375	0.3125	0.041666667	0.01285	1.000	0.073	Def	0			
	Te	a	0.9375	0.395833334	0.041666667	0.01285	1.000	0.073	Def	0	0	0	90
	Te	a	0.9375	0.479166667	0.041666667	0.01285	1.000	0.073	Def	0			
	Te	a	0.979166667	0.145833334	0.125	0.01285	1.000	0.073	Def	0			
	Te	a	0.979166667	0.229166667	0.125	0.01285	1.000	0.073	Def	0			
	Te	8	0.979166667	0.3125	0.125	0.01285	1.000	0.073	Def	0			
	Te	a	0.979166667	0.395833334	0.125	0.01285	1.000	0.073	Def	0			
	Te	a	0.979166667	0.479166667	0.125	0.01285	1.000	0.073	Def	0			
	Te	a	0.9375	0.104166667	0.125	0.01285	1.000	0.073	Def	0			
	Te	a	0.9375	0.1875	0.125	0.01285	1.000	0.073	Def	0			
	Te	a	0.9375	0.270833334	0.125	0.01285	1.000	0.073	Def	0			
	Te	a	0.9375	0.354166667	0.125	0.01285	1.000	0.073	Def	0			
	Te	a	0.9375	0.4375	0.125	0.01285	1.000	0.073	Def	0			
	Zn	a	0.916666667	0.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.833333334	0.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.750	0.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.666666667	0.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.583333334	0.000	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.875	0.041666667	0.000	0.01797	1.000	0.051	Def	0			
	Zn	8	0.791666667	0.041666667	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.708333334	0.041666667	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.625	0.041666667	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.541666667	0.041666667	0.000	0.01797	1.000	0.051	Def	0			
	Zn	a	0.875	0.000	0.083333333	0.01797	1.000	0.051	Def	0			
	Zn	а	0.791666667	0.000	0.083333333	0.01797	1.000	0.051	Def	0			
	Zn	a	0.708333334	0.000	0.083333333	0.01797	1.000	0.051	Def	0			
	Zn	8	0.625	0.000	0.083333333	0.01797	1.000	0.051	Def	0			
	Zn	a	0.541666667	0.000	0.083333333	0.01797	1.000	0.051	Def	0			
	Zn	a	0.916666667	0.041666667	0.083333333	0.01797	1.000	0.051	Def	0			
_	Zo		0.8333333334	0.041666667	0.0833333333	0.01797	1.000	0.051	Def	0			

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.
- \blacksquare : transfer the frame to the clipboard.
- \cong : load a CBED image.
- \blacksquare : move the Center of the Laue Circle (CLC) down.
- 1 : move the CLC up.
- 🗲 : move the CLC left.
- \Rightarrow : move the CLC right.
- \blacksquare : make a table with different maximum (hkl) indices.
- \mathbf{a} : reduce the table (Fig. 159).

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

	0.60	a cost	N 1N	N. / N	Amoli /M	Obase / Dec	Ext (em	Report (mRad	diam	Interes	[6] chmax
-	(0,0,0)	0.000	21 70573	1,48463	21.75644	3.91282	EAL/IIII	0.00	0711	mans.	
	(5, 5, 5)	2 70814	465315	10.22161	11.22159	65 73707	67 10155	2.75	0.25739	1000.00	5 😋
	(2.0.0)	3,23102	A 16756	-0.38805	A 18550	6.91065	182 53851	2.10	0.3095	89.00	0 3 6 9 12 15
2	(2, 2, 0)	4 56035	10 21050	0.04607	10.2632	6 28348	74.44932	4.60	0.0000	765.00	
	(2, 2, 0)	5 35804	3.64220	.6.25262	6.30180	.65.26165	110 53000	5.27	0.18664	400.00	k max.
	(0, 7, 1)	6.60620	2.05429	0.24001	0.37105	9.01770	221 17024	6.61	0.17940	22.00	
	(4, 0, 0)	6.46204	6 76017	0.79209	6.91525	6.67400	112 10262	6.26	0.17009	119.00	5 0 3 5 9 12 15
	(4, 0, 0)	7.04184	1.03000	4 08018	4.40084	68.04005	172 52707	6.03	0.10470	100.00	
	(3, 3, 1)	7.04104	1.63206	4.00010	1.07420	10.24223	113.02797	2.11	0.19201	25.00	1 mm
	(4, 2, 0)	7.01476	E 08640	0.00104	6 10160	7.00480	140 0040	7.10	0.10041	23.00	1000
	(0, 2, 2)	9.30443	0.00042	2.72084	0.13100	62 73624	217.04836	9.26	0.12030	210.00	5.0
	(3, 3, 3)	0.33443	1.1223	2.10204	3.00040	-02.7 3024	217.04030	0.20	0.11913	32.00	0 3 6 9 12 15
	(0, 1, 1)	0.39443	1.20000	3.15907	3.3622	09,09990	220.09070	0.20	0.11913	69.00	
	(4, 4, 0)	9.1387	4.02407	0.56506	4.00081	8.31444	187.80280	9.00	0.10942	59.00	
	(5, 3, 1)	9.00746	1.729	-2.22914	2.82100	-02.20900	210.11255	3.41	0.10463	109.00	
	(6, 0, 0)	9.69305	-1.03353	-0.24197	1.06147	13.1/67	/19./5409	9.54	0.10317	2.00	Default Maximum Spacing : 16.789 [nm-1]
	(4, 4, 2)	9.69305	-1.03353	-0.24197	1.06147	13.1767	719.75409	9.54	0.10317	8.00	
	(0, 2, 0)	10,21738	3.20927	0.51212	3.30914	8.90277	230.87428	10.06	0.09787	70.00	
	(5, 3, 3)	10.5936	0.72405	2.09328	2.21497	70.91985	344.92257	10.43	0.0944	30.00	(h,k,l) number : 53
	(6, 2, 2)	10.71607	-0.86402	-0.2181	0.89112	14.16695	857.33943	10.55	0.09332	5.00	
	(4, 4, 4)	11.19257	2.70064	0.44756	2.73748	9.40973	279.08479	11.02	0.08934	15.00	Abarik Form Factor
	(5, 5, 1)	11.53704	0.57301	1.74953	1.84098	71.86525	414.98805	11.36	0.08668	19.00	
	(7, 1, 1)	11.53704	1.19833	-1.52327	1.93813	-51,80839	394.187	11.36	0.08568	21.00	DTSB EJK PRDW WK WKc. XRay JEN
	(6, 4, 0)	11.6496	-0.73653	-0.19703	0.76243	14.97646	1002.04269	11.47	0.08584	3.00	
	(6, 4, 2)	12.08936	2.25769	0.3921	2.29148	9.85241	333.3997	11.90	0.08272	57.00	Relativistic correction
	(5, 5, 3)	12.40896	1.01101	-1.28578	1.63566	-51.822	467.07672	12.21	0.08059	14.00	
	(7, 3, 1)	12.40896	0.45722	1.47858	1.54766	72.81703	493.63302	12.21	0.08059	25.00	
	(8, 0, 0)	12.92407	1.90507	0.34411	1.9359	10.23878	394.63464	12.72	0.07738	5.00	
	(7, 3, 3)	13.22351	0.85835	-1.09631	1.39236	-51.94099	548.68708	13.02	0.07562	10.00	
	(6, 4, 4)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00	
	(8, 2, 0)	13.32183	-0.55657	-0.16145	0.57951	16.17662	1318.29015	13.11	0.07506	2.00	
	(6, 6, 0)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	6.00	
	(8, 2, 2)	13.70805	1.61995	0.30235	1.64793	10.57223	463.5908	13.49	0.07295	13.00	
	(5, 5, 5)	13.99072	0.29631	1.08264	1.12245	74.69329	680.61854	13.77	0.07148	2.00	
	(7, 5, 1)	13.99072	0.73254	-0.94265	1.19382	-52.14897	639.92971	13.77	0.07148	13.00	
	(6, 6, 2)	14.08368	-0.49062	-0.14632	0.51198	16.60584	1492.17911	13.86	0.071	1.00	
	(8, 4, 0)	14,44955	1.38662	0.26589	1,41188	10.85514	541.09119	14.22	0.06921	9.00	
	(7, 5, 3)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	8.00	
	(9, 1, 1)	14.71799	0.24024	0.93554	0.96589	75.59819	790.93139	14.49	0.06794	4.00	
	(8, 4, 2)	14.80638	-0.43548	-0.13264	0.45524	16.94014	1678.14294	14.57	0.06754	2.00	
	(6, 6, 4)	15.15482	1,19376	0.23396	1,21647	11.08847	628.00527	14.92	0.06599	6.00	
	(9, 3, 1)	15,41097	0.54033	-0.7115	0.89342	-52.78593	855.08408	15.17	0.06489	7.00	
	(8, 4, 4)	15.82869	1.03301	0.20591	1.05333	11.27302	725.26436	15.58	0.06318	5.00	
	(9, 3, 3)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00	
	(7, 5, 5)	16.07411	0.46649	-0.62353	0.77872	-53.19783	981.02145	15.82	0.06221	2.00	
	(7, 7, 1)	16.07411	0.15985	0.70945	0.72723	77.30266	1050.47524	15.82	0.06221	2.00	
	(10.0.0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	0.00	
	(8.6.0)	16.15509	-0.34862	-0.10902	0.36527	17.36495	2091.45493	15.90	0.0619	1.00	
	(8.6.2)	16.47502	0.89802	0.18123	0.91612	11.40944	833 87518	16.22	0.0607	7.00	
	(10, 2, 0)	16.47502	0.89802	0.18123	0.91612	11.40944	833.87518	16.22	0.0607	3.00	
	(7.7.3)	16 71095	0.40391	-0.54912	0.68167	.53.66309	1120 67193	16.45	0.05984	2.00	
	(9.5.1)	16 71095	0.13115	0.62185	0.63552	78,0909	1202.04896	16.45	0.05984	100	
	(0, 0, 1)	10.71095	0.10110	0.04100	0.003002	10.0303	14/04/04/09/0	10.40	0.00304	10.000	

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

32 Perspective



Figure 160: ZnTe perspective view.

32.1 Popup menu

Print drawing Save drawing Transfer to clipboard

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. Calculate powder pattern Export to Mathematica Reset Save structure Start movie Stop movie

Figure 161: 3-D view popup menu.

32.2 Tool buttons

The tool buttons allow to:

- \blacksquare : print the table.
- 📑 : save the table.
- 🖺 : transfer the frame to the clipboard.
- 🖻 : open the **Specimen** dialogue (Fig. 84a).
- **L**: 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.



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).



(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 Black & White figure (165a) or to look at (hkl) planes (Fig. 165b).



(a) Zn colour and (b) Te colour and (c) Define the bond- (d) Resolution of the size. si

ing of ZnTe.

Start movie Stop movie



Atoms Direction	Display Duplicate View					
3-D view	Cut Movie Plane					
ut origin / nm	Cut thickness / nm					
- 5	- 5					
- 3	- 4					
· .						
	- 3					
P1	- 2					
3	- 1					
· .	· · · · ·					
5	- 0					
Fine	Fine					
-0.5	0.45					

Atoms Direction Display Duplicate 3-D view Cut Movie Plane



- (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).

spheres and bonds.

Figure 164: Atoms and Display Tabs.



(a) B & W ZnTe model.

(b) ZnTe (111) plane.



33 Indexing SAED patterns



Figure 166: Indexing SAED patterns.

33.1 Tool buttons

The tool buttons allow to:

- \blacksquare : print the image.
- 📑 : save the image.
- 🖺 : transfer the frame to the clipboard.
- 🗳 : open an image.
- = : process image.
- $\mathbf{\mathbf{y}}$: start indexing process.
- \bullet \blacksquare : show diffractogram (when an HRTEM image has been loaded).
- 🕄 : magnify part of image.
- $\stackrel{\frown}{=}$: tabulate the image.
- 😕 : open keeper dialogue (Fig. 90).
- 🧖 : display a help file.

33.2 Tabs



Align Crystals Crystals Align Crystal itename Align Crystal itena

(b) Table of the crystal files selected for

(a) Rotation of the spot indexing mask.



(c) Mask showing the spots selected for indexing.



(d) Controls of the microscope parameters.

Figure 167: Controls and tabs of SAED patterns indexing.

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Refort Image Horizontal Indexing options Extended search Indexing likelihood 0.2 0.4 0.5 0.6 0.7 0.8 0.9 1.0	Background	d 🗌 Show mask 🗹 Snap to maxima
Indexing options Extended search I tat quadrant solution 3 spots indexing Indexing likelihood 0.2 0.4 0.5 0.6 0.7 0.8 0.9 0 1.0	Refectimens	
Indexing options Extended search Ist quadrant solution 3 spots indexing Indexing likelihood 0.2 0.4 0.5 0.6 0.7 0.8 0.9 0 1.0	Horizontal	Vertical
Extended search Ist quadrant solution 3 spots indexing Indexing likelihood 0.2 0.4 0.5 0.6 0.7 0.8 0.9 1.0	Indexing options	
Indexing likelihood	Extended search	✓ 1st quadrant solution 3 spots indexing
0.2 0.4 0.5 0.6 0.7 0.8 0.9 1.0	Indexing likelihood	
	0.2 0.4 0.5	0.6 0.7 0.8 0.9 0 1.0

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

alibration Cam. leng	th Beam conv. M	ask Scale	Zoom
aling			
Jnits		Scale size	
⊖ mm	19.69044	- 100	
🗿 1/nm	10.00000	- 80	
O degree	1.12803	- 60	
mrad	19.68790	- 40	
pixel size (µm)	98.45222	- 20	
pixel size [1/µm]	50.00000	Τ-0	
	Scale	10.0	
		Fine Live	
Order spot 0	Order spot 1	Order	spot 2
			_
- 9	- 9		- 9
-	-		-
- 7	- 7		- 7
-	-		-
- 5	- 5		- 5
	-		-
- 3	- 3		- 3
-			-
" — 1	- 1		>1

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

Actions	noograme optione i	
Binarize	Colorize	Equalize
Rot. average	SVD	
Brightness		
<u>.</u>	2.1	
Contrast		
Gamma		
	2 - 1	

(b) Image processing tab.



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

Figure 168: Controls and tabs of SAED patterns indexing.

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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 (\mathfrak{R} .)

(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 Bright and Dark 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:

- \blacksquare : print the selected ADF image tab.
- \blacksquare : save the selected ADF image tab.
- 🖺 : transfer the ADF frame to the clipboard.
- \blacksquare : display the interpolated ADF image and allows tabulating the selected ADF image.
- 上 : 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.

 \bullet $\ensuremath{\textcircled{0}}$: 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).

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

Iteration Multislice Options Sampling Scanning Signa

wĸ

PRDW

Atomic Form Fa

1

			Re	set			
o Analytic		O Direct			O Fourier		
Pixel size of	high resolutio	n images / nm					
0.002	0.003	0.004		0.005	0.006	C	0.007
0.008	0.009	0.010		0.020	0.030	C	0.040
O(Δz) rozen lattic Bicubic	Ο (Δ z ²) Enable		Temperat	ure [K]	· I	
Configuratio	ns number						

(b) Controls the potential generation method (Analytic 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.

1))
-1))
m-1])
nm-1])
))
· ·

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



O WKc. DTSB EJK JEMS Channels HAADF Bright-field Save Movies Nano-diffraction Single unit cell parent crysta [0,0,1] (default) 2 Parent not yet defined BF/DF/SD/HAADF images Stack index Stack Show progress 0 4 8 12

(c) Selects Atomic Form Factors source, allows Bright, Dark, Sector or HAADF image calculation and when checkbox **Save** is selected saves all the calculated images.



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



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



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



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



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



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.

³⁶The 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

- \blacksquare : print either the probe position or probe shape image.
- F : 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 Magnetic noise and vibration (Fig. 180c).
- **Microscope** : to set the aperture diameter, accelerating voltage and virtual source size (Fig. 180d).

		Slider	s Table		
C ₀ (Co W ₀₀) [mm]	1.0		$\mathbf{C}_{(0)} \left(\left. \mathbf{C}_{(0)} \right \mathbf{W}_{(0)} \right) \left[mm \right]$	5.0	
C ₀₁ (1)W ₁₁ (m)	0.0	0.0	$C_{52}(65_{5} W_{62})[mm]$	0.0	0.0
C ₁₀ (Z W ₂₀)[nm]	5.8		$C_{54}(6R_g W_{54}) mm]$	0.0	0.0
$\mathbf{G}_{12}(\mathbf{A}_{1} \mathbf{W}_{22}) \mathbf{v}\mathbf{v} $	0.0	0.0	$\mathbf{G}_{gg}\left(\mathbf{A}_{g} \mid \mathbf{W}_{gg}\right)\left[mm\right]$	0.0	0.0
C ₂₁ (38 ₂ W ₃₁) (nm)	0.0	0.0	$\mathbf{G}_{g,1}\left(\mathbf{7B}_{g} \mid \mathbf{W}_{g,1}\right)\left[mm\right]$	0.0	0.0
$G_{23}(A_2 W_{33}) m $	0.0	0.0	$\mathbf{G}_{\mathbf{g}_3}\left(T\mathbf{D}_{\mathbf{g}} \mid \mathbf{W}_{\mathbf{g}_3}\right)\left[mm\right]$	0.0	0.0
C ₂₀ (C ₃ W ₄₀)(mm)	-0.03		$\mathbf{G}_{ab}\left(\mathbf{TF}_{a} \mid \mathbf{W}_{rb}\right)\left(mm\right)$	0.0	0.0
$C_{32}^{}(48_{3} W_{62}) [an]$	0.0	0.0	$\mathbf{G}_{g\gamma}\left(\mathbf{A}_{g}\left(\mathbf{W}_{\gamma\gamma}\right) mm\right)$	0.0	0.0
$\mathbf{G}_{24}\left(\mathbf{A}_{2}\left \mathbf{W}_{64}\right\rangle\left \mathbf{J}\mathbf{H}\right $	0.0	0.0	$\mathbf{G}_{\mathrm{PO}}\left(\mathbf{G}_{\mathrm{y}} \mathbf{W}_{\mathrm{BO}}\right)\left[\mathbf{x}\right]$	0.0	
$C_{41}(58_4 W_{51})[\mu m]$	0.0	0.0	$\mathbf{C}_{p_2}(88_p \mathbf{W}_{g_2})[[n]$	0.0	0.0
$C_{45}(SD_4 W_{53})[\mu m]$	0.0	0.0	$C_{74}(8R_{y} W_{04}) n $	0.0	0.0
$\mathbf{C}_{45}\left(\mathbf{A}_{4} \mathbf{W}_{55}\right)[\mu \pi]$	0.0	0.0	$C_{\gamma_0}(8G_y \mid W_{00})(n)$	0.0	0.0

(a) Aberrations table. 3fold 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) Thermal Magnetic 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).

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