# ADF Imager

P. Stadelmann jems-swiss Chemin Rouge 15 CH-1805 Jongny Switzerland info@jems-swiss.ch

December 3, 2020

# Contents

1	Intr	oduction 3
<b>2</b>	Moo	dels 6
	2.1	Graphene
	2.2	III-V semiconductors
3	Con	trols 14
	3.1	Iteration tab
	3.2	Multislice tab
	3.3	Options tab
	3.4	Scanning tab
	3.5	Signal tab
4	Ima	ge tabs 25
	4.1	Bright-field image tab
	4.2	Dark-field image tab
	4.3	Sector images tab
	4.4	Sectors image tab
	4.5	Model slices tab
	4.6	Projected potential tab
	4.7	Absorption potential tab

	4.8 Fresnel propagator tab	34
	4.9 Phase-object tab	36
	4.10 Power spectrum tab	37
	4.11 Bright-field detector tab	38
	4.12 Dark-field detector tab	39
	4.13 Sectors detector tab	40
	4.14 Wave-function tab	41
<b>5</b>	Probe imager dialogue	42
	5.1 Scan area and probe position	43
6	Setting the bright-, dark-field and sectors detectors	45
U		10
7	Doing a bright- or dark-field and sectors image calculation	47
7 8	Doing a bright- or dark-field and sectors image calculation Example: GaAs [110]	47 49
7 8 9	Doing a bright- or dark-field and sectors image calculation Example: GaAs [110] Notes	47 49 53
7 8 9	Doing a bright- or dark-field and sectors image calculation         Example: GaAs [110]         Notes         9.1       Note 1: Debye-Waller temperature factor	47 49 53 53
7 8 9	Doing a bright- or dark-field and sectors image calculation         Example: GaAs [110]         Notes         9.1 Note 1: Debye-Waller temperature factor	47 49 53 53 54
7 8 9	Doing a bright- or dark-field and sectors image calculation Example: GaAs [110] Notes 9.1 Note 1: Debye-Waller temperature factor	<b>47</b> <b>49</b> <b>53</b> 53 54 54
7 8 9	Doing a bright- or dark-field and sectors image calculation Example: GaAs [110] Notes 9.1 Note 1: Debye-Waller temperature factor	<b>47</b> <b>49</b> <b>53</b> 53 54 54 54

# 1 Introduction

ADFImager dialogue (Fig. 1) is used to calculate STEM bright-ield (BF), dark-field (DF) and sector-bright- or sector-dark-field (SE) images<sup>1</sup>.



Figure 1: STEM images, annular dark-field, bright-field images or sector-brightor -dark-field images are calculated using the ADFImager dialogue.

The controls and calculated images are grouped in 2 tabs. The model crystal is described as slices in the left tab (**Iteration**, ...), the generated BF, DF or SE images are displayed in the right tab (*BF*, *DF SE*, *images*, *model*, ..., *detectors*, *wave-function*).

The tool buttons of Fig. 2 allow to:

1. Save the ADFImager dialogue.

 $<sup>^1\</sup>mathrm{jems}$  version 4.3906u2016 or later.



Figure 2: Tool buttons of the ADF imager dialogue.

- 2. Transfer the ADFImager dialogue to the clipboard (for documenting the calculations).
- 3. Print the ADFImager dialogue.
- 4. Tabulate the bright- and dark-field images or thickness series (stack) of BF/DF images.
- 5. Adjust the bright- and dark-field detectors radii.
- 6. Select a microscope and set the probe aberrations, i.e. defocus, astigmatism. Aberrations up to order 8 can be accounted for.
- 7. Select specimen related parameters.
- 8. Display the optical transfer function, probe shape and Ronchigram.
- 9. Display the ADFImager dialogue help.

The calculations are initialized, started and stopped using the buttons of Fig. 3. The **Initialize** button (1) generates the projected potential of all the slices at once as well as the phase-object function (PO). The Fresnel propagator (FP) of all the slices of the model are initialized when needed during the calculations. Calculation time is saved when all the slices have the same thickness. The **Start** and **Stop** buttons starts and stops the ADF calculation respectively.

		_
Initialize	Start	Stor

Figure 3: Initialize, Start and Stop buttons. Initialize button (button 1) should be pushed after setting the ADF image calculations parameters.

Note that a popup menu is attached to every drawing or image. Popup menus are displayed as usual (mouse right-click or by a mouse double click). On a touch

screen have the finger stays longer on the control. Popup menus allow to print, save or send the drawing or image to the clipboard.

# 2 Models

#### 2.1 Graphene

One of the models that are employed in this document is a **graphene** sheet where one carbon atom has been replaced by a nitrogen atom. With this model calculations are performed within minutes (Fig. 4). The graphene model is made of atoms placed at (x, y, z) coordinates in an orthogonal box of sides a, b, c with  $0 \le x, y, z \le 1$ . Note that the model is projected along the Oz direction ([0,0,1] parallel to  $\vec{c}$ . It is best to have a tetragonal model, i.e. with a = b, since this allows a faster display of the generated images and power spectra.



Figure 4: Graphene model with labelled atoms. Labels are obtained using the popup menu attached to the projection. Popup menus are shown when the mouse is positioned on the drawing or table and a double click is issued.

Thicker crystal models should be prepared as series of slices. This is easily achieved

using tools provided by the **Miscellany** menu. Electrons are traveling from top the slice (somename\_0000.txt) to the bottom slice (somename\_nnnn.txt). The slices thickness does not have to be identical<sup>2</sup>.

#### 2.2 III-V semiconductors

The calculation of [110] bright-field, dark-field or sector images of III-V semiconductors (AlAs, AlP, AlSb, GaAs, GaP, GaSb, InAs, InP, InSb and ZnTe) requires to transform the cubic unit cell (space-group  $F\bar{4}3m$ ) into an orthorhombic unit cell of c axis || to the cubic [001]. The procedure is as follow (the example uses ZnTe):

- 1. Open the ZnTe model (Fig. 5). Verify the atom coordinates, occupancy and Debye-Waller temperature factor.
- 2. In menu *Crystal* select menu item *Make orthogonal* (Fig.8). Note that the orthogonal unit cell can be pretty large and also that orthogonality can't always be achieved perfectly (there is a tolerance of 0.2 degree).
- 3. After selecting the [110] direction, close the specimen dialog (Done). The right tab of the dialog will then show the orthogonal unit cell and its geometrical relationship with the ZnTe unit cell (Fig. 9). Note that the new cell [uvw] directions and (hkl) indices are given with respect to its own metrics. The space-group is the new cell is set to P1.
- 4. Using 3-D display, it is easy to see that the new unit cell is doubled in the [001] direction (Fig.10). In this particular case, it would be possible to keep only a half unit cell (menu *Miscellany* menu item *To slices*).
- 5. The generation of super-cells is made possible by several menu items grouped in the *Miscellany* menu. Since the new orthogonal unit cell must be cut in thinner sub-slices in order to perform BF, ADF or SE image simulations, the dialog attached to the *To slices* menu item is activated (Fig. 12). This dialog allows one to duplicate a cell in  $[100]_x, [010]_y or [001]_z$  directions and to cut it into thinner sub-slices parallel to either Ox, Oy or Oz.
- 6. For ADF image simulation it is better to generate approximately square super-cells. This is achieved here by duplicating the cell 5 times along Ox and 7 times along Oy (Fig.13), a, b, c have length 4.377, 4.333 and 0.875 nm respectively.

<sup>&</sup>lt;sup>2</sup>Though a single slice thickness requires less computer memory.

- 7. The cell is finally sliced in 4 sub-slices perpendicular to Oz using the popup menu attached to the table. A slice thickness of of 0.2 nm is appropriate. After slicing and saving the sub-slices (give the sub-slices a meaning full name, for example ZnTe110) close the *To slices* dialog. The subslices are named  $ZnTe110_{-}0000.txt$ , ..., ZnTe110\_0003.txt.
- 8. Finally open subslice ZnTe110\_0000.txt (Fig. 14).



Figure 5: ZnTe model. Te atom at (0,0,0) Figure 6: Make orthogonal generates orthogand Zn at  $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ . onal units cell with c axis  $\parallel$  to any [uvw] direction the selected crystal.



Figure 7: Make orthogonal dialog. The left Figure 8: A [uvw] direction is selected using tab shows the original unit cell, the right tab the specimen dialog (toolbuton 1, Fig.7). will show the orthogonal unit cell after select-

ing a [uvw] direction. By default the [001] direction is selected (i.e. left and right tabs show the same structure.



Figure 9: The orthogonal unit cell has  $[001] \parallel$  Figure 10: 3-D perspective view of the or- $[\bar{1}\bar{1}0]_{ZnTe}$ ,  $[010] \parallel [001]_{ZnTe}$  and  $[001] \parallel$  thogonal cell. Ox, Oy, Oz axes given by red,  $[110]_{ZnTe}$ . Its unit cell volume is twice the green, blue arrows. Note that the cell is douvolume of ZnTe. bled in the [001] direction (blue).



Figure 11: After closing the *Make orthogonal* Figure 12: Super-cells are generated and dialog a [001] projection is shown as well as sliced using menu *Miscellany*, menu item *To* a table of the atoms coordinates. *slices*.

00			toSlicesBo	x::ZnTe::5 * 7	* 1 unit cell(s	)::560 atoms::4	.3769913 x 4.333 x	0.8753982 nm^3	
3									
#	Symbol	Wyckoff	x	y	z	Debye-Wall	er Occupation	Unit cell duplication	
)	Zn	a	0.750	0.500	0.750	0.01797	1.000	Duplicate x Duplicate y	Duplicate z
l	Zn	۵	0.250	0.500	0.750	0.01797	1.000	L- L-	ſ -
2	Te	a	0.500	0.250	0.750	0.01285	1.000	- 29 - 29	- 29
3	Te	۵	0.000	0.250	0.750	0.01285	1.000	- 25 - 25	- 25
1	Zn	a	0.500	0.000	0.500	0.01797	1.000		
5	Zn	۵	0.000	0.000	0.500	0.01797	1.000	- 21 - 21	- 21
5	Te	a	0.750	0.750	0.500	0.01285	1.000	- 17 - 17	- 17
7	Te	۵	0.250	0.750	0.500	0.01285	1.000	- 13 - 13	- 13
3	Zn	a	0.250	0.500	0.250	0.01797	1.000		
•	Zn	۵	0.750	0.500	0.250	0.01797	1.000	-9 -9	- 9
0	Te	a	0.000	0.250	0.250	0.01285	1.000	- 5 - 5	- 5
1	Te	a	0.500	0.250	0.250	0.01285	1.000		1
2	Zn	a	0.000	0.000	0.000	0.01797	1.000		
3	Zn	a	0.500	0.000	0.000	0.01797	1.000	5 7	1
4	Te	a	0.250	0.750	0.000	0.01285	1.000		
5	Te	۵	0.750	0.750	0.000	0.01285	1.000		
6	Zn	a	1.750	0.500	0.750	0.01797	1.000		
7	Zn	a	2.750	0.500	0.750	0.01797	Print table	Sub-slices	
в	Zn	a	3.750	0.500	0.750	0.01797	Courtable	💽 💿 Oxy [001] 🔅 Oxz [010	0] Oyz [100]
9	Zn	۵	4.750	0.500	0.750	0.01797	Save table	Slice thick. / nmSu	ib-slices number
0	Zn	a	1.250	0.500	0.750	0.01797	Transfer to clipboard	0 - 1	
1	Zn	۵	2.250	0.500	0.750	0.01797	1.000		- 120
2	Zn	a	3.250	0.500	0.750	0.01797	Slice x	- 08	
3	Zn	۵	4.250	0.500	0.750	0.01797	Slice y	-	- 100
4	Te	a	1.500	0.250	0.750	0.01285	Slice z	- 06	- 80
5	Te	۵	2.500	0.250	0.750	0.01285	1.000	0.0	-
6	Te	a	3.500	0.250	0.750	0.01285	1.000	- 04	- 60
7	Te	۵	4.500	0.250	0.750	0.01285	1.000	0.4	- 40
8	Te	a	1.000	0.250	0.750	0.01285	1.000		-
9	Te	۵	2.000	0.250	0.750	0.01285	1.000	- 0.2	- 20
0	Te	a	3.000	0.250	0.750	0.01285	1.000		
1	Te	۵	4.000	0.250	0.750	0.01285	1.000		
2	Zn	a	1.500	0.000	0.500	0.01797	1.000	Fine 0.2188	4
3	Zn	۵	2.500	0.000	0.500	0.01797	1.000		
4	Zn	٥	3.500	0.000	0.500	0.01797	1.000		
5	Zn	۵	4.500	0.000	0.500	0.01797	1.000	Options	
6	Zn	a	1.000	0.000	0.500	0.01797	1.000	Show slices	
7	Zn	۵	2.000	0.000	0.500	0.01797	1.000		
8	Zn	a	3.000	0.000	0.500	0.01797	1.000		
9	Zn	۵	4.000	0.000	0.500	0.01797	1.000		
0	Te	a	1.750	0.750	0.500	0.01285	1.000		
1	Te	۵	2.750	0.750	0.500	0.01285	1.000		
2	Te	٥	3.750	0.750	0.500	0.01285	1.000		
3	Te	۵	4.750	0.750	0.500	0.01285	1.000		
4	Te	٥	1.250	0.750	0.500	0.01285	1.000		
5	Te	a	2,250	0.750	0.500	0.01285	1 000		

Figure 13: The orthogonal unit cell is duplicated 5 times in Ox direction (a) and 7 times in Oy direction (b). The new lattice parameters show that the super-cell is nearly tetragonal (when lattice parameter a and b are almost equal, all the images shown during the ADF image calculation will have their proper geometry (some are not interpolated before they are displayed in order to speed up simulations).



Figure 14: The original ZnTe folder now contains the ZnTe cubic unit cell, 4 super-cells (subslices) and the whole unsliced super-cell (ZnTe110\_slices.txt).

0	0 (	)									jer	ms∷4	1.363	B1U2	015														
F	ile	Crystal	Drawing	Imaging	Indexing	Meas	uring	Para	meter	rs	Wind	wob	Mi	scelle	any	De	velop	omen	t										He
	~		<b>B</b>	ADF i	mager	^A					٦ſ					1													
				Bloch	wave	^B			-		JU	•	<b>1</b>	JIL	888	Ľ			-										
P	Atom(:	s) in the u	nit cell	Howie	-Whelan	^н		3	-D vier	w																			
	#	Atom	Wyckoff	HRST	EM imager	^s																							
	0	Te	۵	HRTE	M imager	^T )	C		ΙГ																				
	1	Te	۵	Load	in inager		C																						
	2	Zn	۵	Aultic	0.0357143	~	C				•		•		•	×.		×.		×.					•	×.	•	- I	
	3	Zn	۵	Murris	sice	(M)	C		I T		· ·		×.		×.		· ·		×.		×.		×.				×.		
	4	Zn	٥	Proces	ssing	TP )																							
1	5	∠n Z-	٥	0.800	0.750	0.000	C													•		•		•		•			
	0	Zn Zn	٥	0.800	0.60/1429	0.000	C			-	•		•	-	•		•	×	•		•		•		•		•		
	/ 0	Zn	a	0.800	0.221/204	0.000	C		ľ				-								Ĩ		Ĩ						
	0	Zn	a	0.800	0.1795714	0.000	c																						
	7 10	Zn	a	0.600	0.8028571	0.000	ć																						
11	11	Zn	a	0.600	0.750	0.000	c								•	×.			•	×.	•		•		•	×.		- T	
	12	Zn	0	0.600	0.6071429	0.000	č		ΙT		· ·		· ·		· ·		×.		· ·		×		×		· ·		×.		
	13	Zn	a	0.600	0.4642857	0.000	c																						
	14	Zn	a	0.600	0.3214286	0.000	c																						
	15	Zn	۵	0.600	0.1785714	0.000	c				•		•		•		•	×.		· ·	•				•	Ŭ	•	Ť	
	16	Te	۵	0.350	0.0714286	0.000	с		ΙT		· ·		· ·		· ·		· ·		-		· ·				· ·		×.		
	17	Te	۵	0.550	0.0714286	0.000	C																						
	18	Te	۵	0.750	0.0714286	0.000	C																						
	19	Te	۵	0.950	0.0714286	0.000	C				•				•		•		•	×.	•				•			- I	
	20	Te	۵	0.250	0.0714286	0.000	C		ΙT		-		-		· ·		-		· ·		×		×		· ·		×.		
	21	Te	۵	0.450	0.0714286	0.000	C																						
	22	Te	۵	0.650	0.0714286	0.000	C			-																		•	
	23	Te	۵	0.850	0.0714286	0.000	C				-		-		-		-		•						•		•	- I	
	24	Zn	۵	0.300	0.0357143	0.000	C		ľ		-		-		-		-												
	25	Zn	۵	0.500	0.0357143	0.000	C																						
	26	Zn	۵	0.700	0.0357143	0.000	C																						
	27	Zn	۵	0.900	0.0357143	0.000	C				-		-		-		-				•						•	-	
	28	Zn	٥	0.200	0.0357143	0.000	C		ľ				-		-		Zr	۱Te	110	_00	000	):[	0,0	D, 1	<u> </u>		-		
	Status																												
	java V	M::Free m	emory = 4415	194928, av	ailable memor	y = 44302	233600	), percer	t used	d = 0																			1:24:33 PM

Figure 15: The ADFImager dialogue is found in the *Imaging* menu.

# 3 Controls

#### 3.1 Iteration tab

The buttons of the **Iteration** tab (Fig. ??) allow to control the stack of slices describing the model<sup>3</sup>. Slice numbered  $somename_0000.txt$  is the top slice of the stack. Buttons 1 to 6:

- 1. Load one slice of the model.
- 2. Load a series of slices (numbered *somename\_0000.txt*, *somename\_0001.txt*, ...., *somename\_9999.txt*) <sup>4</sup>.
- 3. Suppress the slice that is selected from the stack.
- 4. Suppress all slices.
- 5. Save the series of slices.
- 6. Display a 3-D view of the model.

The total specimen thickness. i.e. the cumulated thicknesses of all the slices is displayed (Fig. 16). The maximum number of slices is 10'000. Note also that a **popup menu** is attached to the table of slices that allows to duplicate the stack. It is also possible to remove or add single super-cells in order to select a particular total crystal thickness.

 $<sup>^3 \</sup>rm Only$  slices in jems .txt format are accepted.

 $<sup>^4\</sup>mathrm{A}$  maximum of 10'000 slices is considered.



(c) Popup menu to duplicate the stack

(d) Stack with 512 super-cells

Figure 16: Iteration tab and stack of super-cells. Buttons 1: loads a single super-cell, 2: loads series of super-cells, 3: suppresses a one super-cell, 4: suppresses all the super-cells, 5: saves a list of the super-cells, 6: displays a 3-D model of stack.



Figure 17: 3-D view of the model reconstructed using the super-cells.

#### 3.2 Multislice tab

The controls of the multislice tab are shown in Fig. 18. The <u>Reset</u> button resets the calculation of the phase-object function of all the slices.

The controls are grouped in 5 boxes that allow to:

- 1. Select the method employed to generate the projected potential of the slice. The Fourier method generates the potential in Fourier space. It is the most precise, but also the slower. The Analytic method uses an analytic form of the projected potential of the atoms at their (x, y) position, it is selected by default and is slower than the direct one. The Direct method generates the slice projected potential by patching the projected potential of the atoms at their (x, y) position in the slice. It is the fastest method and less precise one (see note 9.2). It can result in square patterns in the ADF images of thick crystals.
- 2. Define the sample size. The sample size is directly related to the maximum scattering angle (given in the **tool tip text**. The maximum scattering sets the default outer radius of the annular dark-field detector<sup>5</sup>. When  $(N_x, N_y)$  samples are used, the maximum scattering angle is:

$$q_{max} = Min\left(\frac{N_x}{2a}, \frac{N_y}{2b}\right)$$

In order to cancel aliasing errors due to convolution the Fresnel propagator is band limited to  $\frac{2}{3}q_{max}$ .

- 3. Define the multislice precision  $O(\Delta z)$  or  $O(\Delta z^2)$  and to take absorption into account. Absorption is better introduced when using Wieckenmeir-Kohl atomic scattering factors (WKc) of the Options tab.
- 4. Define the potential or image interpolation method and enable the lattice vibration at a selected temperature. The Debye-Waller temperature factor is adjusted according to the temperature value (linear approximation). Uncorrelated (Einstein model) atomic vibrations model is used (frozen lattice, see note 9.1).
- 5. Repeat the whole calculation using a new configuration of atoms (frozen lattice). 5 configurations are often sufficient to obtain significant BF, ADF or SE images.

 $<sup>^5\</sup>mathrm{The}$  tool tip text of any control is displayed when the pointer (or mouse) rests 2 seconds on the control



Figure 18: Multislice tab. The **Reset** button erases the pre-calculated slice potential arrays of the whole stack of slices.

#### 3.3 Options tab

The controls of the **Options** tab (Fig. 19) are grouped in 6 boxes. Box number:

- 1. Select the source of the atomic form factors. It is, in principle, best to use the *Weickenmeier-Kohl* tabulation (WK or WKc) since it doesn't describe the atomic form factor as a sum of gaussian functions and introduces absorption using the Debye-Waller temperature factor (see note 9.2).
- 2. The ADFImager allows to specify 4 different Bright-field, Dark-field or Sectors detectors at once. The different channels (Bright-field, Dark-field or Sectors) are selectable (and not need to be all selected) and when calculating images for more than one configuration (Frozen lattice), the images can be saved automatically (Save<sup>6</sup>
- 3. Select a calculation method<sup>7</sup>.
- 4. Select the unit cell crystal that has been duplicated to generate the supercells and the [uvw] orientation with respect to it. In this example GaAs and zone axis [110] are specified in order to have the diffraction patterns drawn when selecting the detectors acquisition angles with the ZnTe cubic structure not the super-cells.
- 5. When the model is made of several slices, the BF, DF and SE images after each slice are saved as a stack of images. The BF/DF/SD progress checkbox allows to follow the progress of the calculations<sup>8</sup>.
- 6. Display the BF, and SD detectors outer and inner-outer radii.

#### 3.4 Scanning tab

The controls of the scanning tab (Fig. 19) are grouped in 6 boxes:

1. Allow to introduce masks that attenuate aliasing and sampling artefacts introduced by the discrete nature of the multislice calculation (see note 9.5).

<sup>&</sup>lt;sup>6</sup>The different channels are saved in different folders that are named using the scheme **ConfnBFm** where **n** is the configuration number and **m** the detector number.

<sup>&</sup>lt;sup>7</sup>Only the Frozen lattice method is available in jems version 4.

<sup>&</sup>lt;sup>8</sup>Images can be displayed after a given percentage of the scan has been performed. The percentage is selected in the **Scanning** tab.

Atomic Form Fa	ictor				
	$\bigcirc$	$\bigcirc$	$\bigcirc$	•	
	EJK	PRDW	WK	WKc.	
Signals being ac	quired				
• Frozen lat	ttice				
Channels					
Bright-fie	eld 🗸	Dark-field	Sector	rs	Save
Single unit cell p	parent crystal				
	Parent n	ot yet defin		[0,0,1]	
_					
Options			-Sta	ck index	
				)	
	BF/DF/S	5D progress			
BF, ADF & Sect	ors detectors				
BF1 ou SD in	ter detector rac ner detector rac	dius:: 10.0 [mrac dius:: 10.0 [mrac	1] (3.99 [nm-1])		
SD ou	ter detector rac	dius:: 60.0 [mrad	d] (23.92 [nm-1])	1	
ADF1 a	outer detector r	adius:: 150.0 [m <sup>-1</sup>	rad] (59.75 [nm-	.1])	
BFi (2 ADFi (	<=i<= 4) = BF1 + ( 2 <=i<= 4) = ADF	(i - 1) 20.0 [mra 1 + (i - 1) 20.0 [i	d] mradl		
BF/AD	F/SD detectors	center::(0.000,	0.000, 0.000)		

Figure 19: Options tab. The BF,DF or SD detectors radii are provided in box 5. These radii can be adjusted when the calculation is running. There is a fixed selectable radius increment for the BF and DF detectors.

- 2. Define the size of the multislice calculation. The different **Radiobuttons** are enabled according to the pixel size selected in the **Multislice** tab.
- 3. Define the size of the scanned area. It is usually better to start a new calculation using a small scan area size and a large **Scan step size**. The calculation will be faster since not all scan points are taken into account.
- 4. Allow to mask some artefacts of the multislice calculation<sup>9</sup>. The artefacts are imaged using a large *Power spectrum logarithm scale*. When masked the DF detector area is reduced <sup>10</sup>. These artefacts are of several possible origins (Fig.21:
  - (a) Too coarse super-cells sampling, the projected potential displays discontinuities.
  - (b) too coarse multislice size, aliasing effects start to be important. Increase the multislice size or introduce a mask and/or cross-mask.
  - (c) Use the Direct method to generate the projected potential of the slices.
  - (d) Accumulation of rounding errors during the multislice calculations. Note that they only are appearant when a very large logarithm scaling factor is employed to display the power spectrum and the intensity on the detectors. These artefacts only appear for thick crystal.
- 5. change the rate of refreshing the BF, DF or SD images.

#### 3.5 Signal tab

The **Signal** tab controls the BF, DF or SD signals intensity and change the brightness, contrast and gamma of the BF and DF images (Fig. 22). The last set of *radiobuttons* changes the multiplication factor (**a**) that is introduced when power spectrum images are displayed using a logarithm scale:

displayed intensity =  $log [1 + a \times signal intensity]$ 

It is equivalent to increase the signal gain by a factor of  $10^n$ .

The pixels value of the BF and DF images do not use a logarithm scale. They are given by:

<sup>&</sup>lt;sup>9</sup>These artefacts are of very small amplitude, usually  $10^2$  to  $10^6$  smaller than inelastic scattering intensity for very thin models. For models made of very light atoms, they can be larger. They are made more visible when the inner radius of the DF detector is large

<sup>&</sup>lt;sup>10</sup>The reduction is displayed in the jems console.



Figure 20: Scanning tab.

Figure 21: ADF artefacts.

• Bright-field (BF):

$$BF_{pixel value} = BF_{signal integrated on BF detector} \times BF_{gain}$$

• Dark-field (DF):

$$DF_{pixel value} = DF_{signal integrated on DF detector} \times DF_{gain}$$

• Sector detector (SD): The four sectors have the same gain.

$$SD_{pixel\,value} = SD_{signal\,integrated\,on\,Sd\,sector} \times SD_{gain}$$

For a 100 pA incident probe intensity, the DF signal intensity will be  $100 pA \times \frac{1}{DF_{gain}}$ .

Image brightness, contrast and  $\gamma$  correction are modified using Brightness, Contrast, Contrast, Gamma. This is possible only when the simulation is finished. Changing the signal gain will introduce bright or dark lines in the images.

	Histogra	am / Sigr		Signal			
		,		,			
The second se							
Brichtner				2000	Gamma	]	
Brightnes:	s	(	Contrast x 10	0000	Gamma		
Brightnes: Bright field	is d gain	•	Contrast x 10	0000	Gamma	•	
Brightnes: Bright field ⊙ 10 <sup>0</sup>	d gain	0 10 <sup>2</sup>	Contrast x 10 0 10 <sup>3</sup>	0000 0 10 <sup>4</sup>	Gamma	0 10 <sup>6</sup>	

Figure 22: The BF, DF and SD signal intensity is provided by integrating the power spectrum intensity over the BF, DF or SD detectors. Finally the integrated values are multiplied by the BF gain (default is 1), DF gain (default is  $10^9$ ) or SD gain (default is  $10^3$ ) respectively. The incident probe intensity is initialised to 1.



Figure 23: The BF channel (BF1,..., BF4) Figure 24: The DF channel (DF1,..., DF4) can be selected during the simulation and the can be selected during the simulation and the intensity is displayed in the corresponding re- intensity is displayed in the corresponding result tab. sult tab.



Figure 25: The signal intensity of any one of Figure 26: Images obtained using the sector the 4 channels SE1,..., SE4 can be selected detector  $S_1$ . Sectors images can be added or and displayed in the corresponding panel. subtracted. When the calculation ends these channels

can be added and/or subtracted in order to produce differential contrast images.

# 4 Image tabs

#### 4.1 Bright-field image tab

The scan of bright-field, dark-field or SD images is performed twice (Fig. 27). The first one starts at pixel (x = 0, y = 0) and continues at pixel (2, 0), i.e. even columns first, while the second one starts at (1, 0) and continues at (3, 0), i.e. odd columns second. In this way BF, DF or SD images are displayed almost immediately. In order to obtain faster complete calculations it is indeed necessary to set the **Display rate** to 100 % or to uncheck the **BF/DF progress** of the **Options** tab.



Figure 27: Bright-field image tab.

When using a small **Scan area size**, the first scan position is (x = 0, y = 0) and the next is  $(n \times 2, 0)$  where n is the **Scan step size**. Calculated images are smaller by a factor n, but can be tabulated and displayed interpolated to a

dimension given by  $(Scan area size \times Step size)$  (Fig. 28 and 29)<sup>11</sup>.



Figure 28: Interpolated gray scale bright- Figure 29: Interpolated coloured bright-field image  $(512 \times 512)$ . image  $(512 \times 512)$ .

Interpolation produces images of size  $(scanSize_x \times scanStep_x, scanSize_y \times scanStep_y)$ .

 $<sup>^{11}\</sup>text{Use tool button 4 to tabulate BF,}$  DF or SD images.

## 4.2 Dark-field image tab

The calculation of the dark-field images is performed in parallel to the bright-field images  $^{12}$  (Fig. 30).

slice size 28 x 128 256 x 256 512 x 512 1024 x 1024 2048 x 2048 size 4 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024	
ares size 4 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024	
trep size. ○ ○ ○ ○ ○ Z 4 8 16	
mask size. 2 4 6 8 10 12 14 16 18 20	
y rate [% done] • • • • • • 2 5 10 20 50 100	

Figure 30: Dark-field image tab displays the DF image when a given percent of the calculation has been performed (*Display rate*).

The DF image is tabulated, using tool 4 (Fig. 2) and displayed interpolated as shown in Figs. 31 and 32.

 $<sup>^{12}</sup>$  Use tool button 4 to tabulate BF and DF images.



Figure 31: Interpolated gray scale dark-field Figure 32: Interpolated coloured dark-field image  $(512 \times 512)$ . Note that the N atom contrast.

#### 4.3 Sector images tab

The calculation of the 4 sectors images is performed in parallel to the bright-, dark-field images<sup>13</sup> (Fig. 33). During the calculations the sector that is being displayed is selected in the **Signal tab**.

After completing the simulations, the different sectors images  $(S_1, ..., S_4)$  can be added or subtracted using the 7 buttons at the bottom of this image tab. For example  $S_1 + S_2 + S_3 + S_4$  will add the images of the 4 sectors (it will then be either a BF or DF image).

<sup>&</sup>lt;sup>13</sup>Use tool button 4 to tabulate BF, DF or SD images.

Bright-field image	Dark-field image	Sector image	Projection
S <sub>1</sub> +S <sub>2</sub> +S <sub>3</sub> +S <sub>4</sub>	S <sub>1</sub> +S <sub>2</sub> -S <sub>3</sub> -S <sub>4</sub> S <sub>1</sub> -S	5 <sub>2</sub> + 5 <sub>3</sub> - 5 <sub>4</sub> -5 <sub>1</sub> + 5	<sub>2</sub> - 5 <sub>3</sub> + 5 <sub>4</sub>
S <sub>1</sub> +S <sub>2</sub> +S <sub>3</sub> +S <sub>4</sub>	$S_1 + S_2 - S_3 - S_4$ $S_1 - S_4$	$5_2 + 5_3 - 5_4$ $-5_1 + 5_2$	<sub>2</sub> - S <sub>3</sub> + S <sub>4</sub>
$S_{1} + S_{2} + S_{3} + S_{4}$ -S_{1} - S_{2} + S_{3} + S_{4}	$S_1 + S_2 - S_3 - S_4$ $S_1 - S_2 - S_3 + S_4$ $-S_1 + S_2$	$S_2 + S_3 - S_4$ $-S_1 + S_5_2 + S_3 - S_4$	2 - S3 + S4

Figure 33: Sector image tab displays the Sector image when a given percent of the calculation has been performed (*Display rate*).

#### 4.4 Sectors image tab

The sector detector is divided in 4 quadrants  $S_1$  (top right),  $S_2$  (top left),  $S_3$  (bottom left) and  $S_4$  (bottom right). Their intensity content can be added and/or subtracted in order to obtain differential phase contrast images (Fig.34).



(c) Detector  $S_3$ 







Figure 35: Channels sum and DPC image.

#### 4.5 Model slices tab

Any slice when selected can be displayed in this tab (Fig. 36). The atoms displacement are not shown on the model drawing, but on the projected potential images and, during the calculations, on the phase-object images.

/ Stop calculation	F imaging ADF CBED
Initialize Start Stop	Crystal potential stack calculation done. Ready to start multislice calculation:Elapsed time : 3 [s]::173
Iteration Multislice Options Scanning Signal	Projection Projected potential Absorption potential Fresnel propagator
tomic Form Factor       DTSB     EJK     PRDW     WK     WKc.     XRay       nage calculation method	
ptions  F4 ADF detectors  BF out of the tector radius: 12.000 [mrad] BF detector radius: 12.000 [mrad] DF iner detector radius: 129.000 [mrad] DF detector radius: 149.000 [mrad] DF detector r	

Figure 36: Model's slices tab.

# 4.6 Projected potential tab

The projected potential of the selected slice is displayed in this tab (Fig. 37).

isflice masks Crass Phase object Probe isflice size 28 x 128 256 x 256 512 x 512 1024 x 1024 2048 x 2048 area size 64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 isflice size 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		Multislice masks         Cress       Phase object         Multislice size         128 x 128       256 x 256         5con area size         64 x 64       128 x 128         2       4         1       2         2       4         8       10         1       2         4       8         1       2         4       8         1       1         2       4         8       10         1       1         2       4         8       10         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1       1         1 <t< th=""><th>Alultislice mesks         Cress       Phase object         Multislice size         Nultislice size         128 x 128       256 x 256         5con area size         64 x 64       122 x 128         26 x 04       0         1       2         2       4         0       2         2       4         1       2         2       5         1       2         2       5         1       2         2       5         1       2         2       5         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         4       0         5       &lt;</th><th>Walitelice modes         Crease       Phase object       Probe         Walitelice modes       O       O       O         128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         Scone area size       O       O       O       O       O       O       O         64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024       1024 x 1024         Scone step size       O       O       O       O       O       O       O         1       2       4       6       8       10       12       14       16       18       20         0       2       4       6       8       10       12       14       16       18       20         1       2       5       10       20       50       100       0</th><th>Initialize masks         Initialize masks</th><th>Intellec models         Cross       Phase object         Phase object       Probe         Itilice size       Itilice size         128 x 128       256 x 256       512 x 512         128 x 128       256 x 256       512 x 512       1024 x 1024         on orea size       Itilice size       Itilice size         1       2       4       8       10         1       2       4       8       10         1       2       4       8       10         1       2       4       8       10         1       2       4       8       10         1       2       5       10       20       50         1       2       5       10       20       50         1       2       5       10       20       50       100</th><th>Higher marks         Cross       Phase object       Probe         Higher size.       Image: Constraint of the size of the si</th><th>2x marke         2x marke         2x marke         2x first         x 128         256 x 256         512         x 128         2x first         x 128         256 x 256         512         x 128         2 4         8 10         2 4         8 10         2 4         8 10         2 4         8 10         2 5         0 0         2 5         10 0         2 5         10 0         10</th><th>Multislice masks       Cross     Phase object       Multislice size       128 x 128     256 x 256       5con ones size       64 x 64     128 x 128       5con step size       1     2       4     8       1     2       4     8       16     2</th><th></th></t<>	Alultislice mesks         Cress       Phase object         Multislice size         Nultislice size         128 x 128       256 x 256         5con area size         64 x 64       122 x 128         26 x 04       0         1       2         2       4         0       2         2       4         1       2         2       5         1       2         2       5         1       2         2       5         1       2         2       5         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         3       0         4       0         5       <	Walitelice modes         Crease       Phase object       Probe         Walitelice modes       O       O       O         128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         Scone area size       O       O       O       O       O       O       O         64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024       1024 x 1024         Scone step size       O       O       O       O       O       O       O         1       2       4       6       8       10       12       14       16       18       20         0       2       4       6       8       10       12       14       16       18       20         1       2       5       10       20       50       100       0	Initialize masks	Intellec models         Cross       Phase object         Phase object       Probe         Itilice size       Itilice size         128 x 128       256 x 256       512 x 512         128 x 128       256 x 256       512 x 512       1024 x 1024         on orea size       Itilice size       Itilice size         1       2       4       8       10         1       2       4       8       10         1       2       4       8       10         1       2       4       8       10         1       2       4       8       10         1       2       5       10       20       50         1       2       5       10       20       50         1       2       5       10       20       50       100	Higher marks         Cross       Phase object       Probe         Higher size.       Image: Constraint of the size of the si	2x marke         2x marke         2x marke         2x first         x 128         256 x 256         512         x 128         2x first         x 128         256 x 256         512         x 128         2 4         8 10         2 4         8 10         2 4         8 10         2 4         8 10         2 5         0 0         2 5         10 0         2 5         10 0         10	Multislice masks       Cross     Phase object       Multislice size       128 x 128     256 x 256       5con ones size       64 x 64     128 x 128       5con step size       1     2       4     8       1     2       4     8       16     2	
isiloe size isiloe size izex 128 256 x 256 512 x 512 1024 x 1024 2048 x 2048 isree size 64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 isree size 0 2 4 8 16		Multislice size     •     •       128 x 128     256 x 256     512 x 512     1024 x 1024       Scen area size     •     •       64 x 64     128 x 128     256 x 256     512 x 512       1     2     4     8       1     2     4     8       1     2     4     8       10     2     4     6     10       128 x 128     10     12     14     16       1     2     4     8     10	Multislice size       O         128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         -Scon orea size       O       O       O       O       O       O         -Scon step size       O<	128       128       128       256       256       122       1024       1	128       1	128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         on orea size:       •       •       •       •         64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         an step size:       •       •       •       •         0 2 4 6 8       10       12       14       16       18       20         ploy rote [% done]       •       •       •       •       •       •         1       2       5       10       20       50       100	Islice size     Islice size       128 x 128     256 x 256     512 x 512     1024 x 1024       10 cross size     Image: Size size size size     Image: Size size size size size size size size s	xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx	Multislice size     O       128 × 128     256 × 256       50cm area size       64 × 64       128 × 128       256 × 256       512 × 512       1       2       4       8       1       2       4       8       16	
28 x 128 256 x 256 512 x 512 1024 x 1024 2048 x 2048 area size 64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 (step size 0 2 4 8 16		Scon area size       0       0       0         64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         5con area size       0       0       0       0         64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         5con area size       0       0       0       0       0         0       2       4       8       16         1       2       4       8       16         0       2       4       6       8       10         1       2       4       8       16         1       2       4       8       16         1       2       4       8       16         1       2       4       8       16         10       2       4       6       8       10         10       12       14       16       18       20         10       12       14       16       18       20	Scon area size       O       O         64 x 64       128 x 128       256 x 256       512 x 512         1       2       4       8       10         -Crosts mask size       O       O       O         0       2       4       6       10         -Display rate [% dows]       O       O       O         1       2       5       10       20         -Display rate [% dows]       O       O       100	128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         Son orea size	128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         an area size       -       -       -       -       -         64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         an area size       -       -       -       -       -       -       -         1       2       4       8       16       -       -       -       -         11       2       4       8       16       -       -       -       -       -       -         128 x 128       10       12       14       16       18       20       -	128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         an area size.       64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         an area size.       0       0       0       0       0       0         1       2       4       8       10         2       4       6       8       10       12       14       16       18       20         play rate [%. date]       0       0       0       0       1       2       5       10       20       50       100	128 x 128       25 x 256       512 x 512       1024 x 1024       2048 x 2048         1 2 4 18       26 x 256       512 x 512       1024 x 1024         1 2 4 8 16       0       0       0         1 2 4 6 8 10 12 14 16 18 20       0       0         1 2 5 10 20 50 100       0       0	x 128 256 x 256 512 x 512 1024 x 1024 2048 x 2048 a size c 64 128 x 128 256 x 256 12 x 512 1024 x 1024 p size 2 4 8 16 ask size 0 2 4 6 8 10 12 14 16 18 20 arts (5, done) 2 5 10 20 50 100	128 x 128       256 x 256       512 x 512       1024 x 1024       2048 x 2048         Scon orne size       64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         Scon step size       0       0       0       0       0         1       2       4       8       16         -       1       2       4       8       16	886
ores size 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		Scon ares size       0       0       0         64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         Scon step size       0       0       0       0         1       2       4       8       10         Cress mark size       0       0       0       0         0       2       4       6       8       10         Display rate [% done]       0       0       0       0	Scan area size 64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 Scan step size Crass mask size 0 0 0 2 4 6 8 10 12 14 16 18 20 Display rate [% dans] 0 0 0 0 0 0 0 0 0 0 0 0 1 2 5 0 0 0 0 0 0	Scan area size         64 × 64       128 × 128       256 × 256       512 × 512       1024 × 1024         Scan area size       0       0       0       0       0         1       2       4       8       15         Cress mask size       0       0       0       0       0         0       2       4       6       8       10         1       2       4       6       8       10         0       2       4       6       8       10         1       2       5       10       20       50       100	an area B122 64 x 64 128 x 128 256 512 x 512 1024 x 1024 an artep 5122 1 2 4 8 10 2 4 6 8 10 12 4 16 18 20 play rate [% dona] 1 2 5 10 20 50 100	an area size 64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 an step size 1 2 4 8 10 1 2 4 6 8 10 12 14 16 18 20 play rate [% dons] 2 5 10 20 50 100	n area size. • • • • • • • • • • • • • • • • • • •	as size c 64 128 x 128 256 x 256 512 x 512 1024 x 1024 p size 2 4 8 15 ask size. 2 4 6 8 10 12 14 16 18 20 refre [% done] 2 5 10 20 50 100	Scen area size 64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 Scen step size 0 0 0 0 0 1 2 4 8 10 Crease mask size	000
64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 step size 2 4 8 16		64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         Scan step size:       0       0       0       0       0         Cross mark size:       0       0       0       0       0       0         Display rate [% done]       0       12       14       16       18       20	64x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         "Scan step size"       0       0       0       0         1       2       4       8       10         -Cross mask size       0       0       0       0         0       2       4       6       10       12         Display rate [% daws]       0       0       0       10	64 x 64       128 x 128       256 x 256       512 x 512       1024 x 1024         Scon step size       0 <th>64 × 64 128 × 128 256 × 256 512 × 512 1024 × 1024 an attep size 0 2 4 6 8 10 12 14 16 18 20 ploy rate [X done] 1 2 5 10 20 50 100</th> <th>64 × 64 128 × 128 256 × 256 512 × 512 1024 × 1024 an step size 1 2 4 8 16 ass mask size 0 2 4 6 8 10 12 14 16 18 20 play rate [% done] 1 2 5 10 20 50 100</th> <th>64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 ns tep size 0 2 4 6 8 10 12 14 16 18 20 signer te [% done] 1 2 5 10 20 50 100</th> <th>c 64       128 x 128       256 x 256       512 x 512       1024 x 1024         p size       2       4       8       10         z 4       6       8       10       12       14       16       18       20         stds size      </th> <th>64 x 64         128 x 128         256 x 256         512 x 512         1024 x 1024           Scen step size         •</th> <th></th>	64 × 64 128 × 128 256 × 256 512 × 512 1024 × 1024 an attep size 0 2 4 6 8 10 12 14 16 18 20 ploy rate [X done] 1 2 5 10 20 50 100	64 × 64 128 × 128 256 × 256 512 × 512 1024 × 1024 an step size 1 2 4 8 16 ass mask size 0 2 4 6 8 10 12 14 16 18 20 play rate [% done] 1 2 5 10 20 50 100	64 x 64 128 x 128 256 x 256 512 x 512 1024 x 1024 ns tep size 0 2 4 6 8 10 12 14 16 18 20 signer te [% done] 1 2 5 10 20 50 100	c 64       128 x 128       256 x 256       512 x 512       1024 x 1024         p size       2       4       8       10         z 4       6       8       10       12       14       16       18       20         stds size	64 x 64         128 x 128         256 x 256         512 x 512         1024 x 1024           Scen step size         •	
(step size		Scon step size         Image: Construct of the size         Image: Constr	Sconstep size         O         O         O           1         2         4         8         10           Crosts mask size         0         0         0         0         0           0         2         4         6         10         12         14         16         18         20           Display rate [% dows]         0         0         0         0         0         0         10	Scon step size       0     0       1     2       4     8       0     0       0	an step size. 1 2 4 8 10 ses mask size. 0 2 4 6 8 10 12 14 16 18 20 ploy rate [% done] 1 2 5 10 20 50 100	an step size. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	n strep size 1 2 4 8 16 ss mark size 0 2 4 6 8 10 12 14 16 18 20 slop rote [% done] 2 5 10 20 50 100	p size 2 4 8 10 atk size or 2 5 10 20 50 100	O         O         O           1         2         4         8         16	2000
		1     2     4     8     10       Cress mark size     0     0     0     0     0       0     2     4     6     8     10     12     14     16     18     20       Display rate [% done]	1     2     4     8     16       -Cross mask size	1     2     4     8     15       Cress mask size     0     0     0     0     0       0     2     4     6     8     10       1     2     5     10     12     14     16       0     1     2     5     10     20     50	1     2     4     8     10       ass mask size     0     0     0     0     0       0     2     4     6     8     10       12     4     6     12     14     16       18     20     20     50     0       1     2     5     10     20     50	1     2     4     8     10       sss mask size     0     0     0     0     0       0     2     4     6     8     10       ploy rate [% done]     0     0     0     0       1     2     5     10     20     50	1     2     4     8     10       ss mark size	2     4     8     15       ask size.     0     0     0     0       2     4     6     8     10       2     4     6     18     20       otte [% done]     0     0     0       2     5     10     20     50     100	1 2 4 8 10	<u> eee</u>
	***********	Cress mask size         0	Crosts mask size         0	Creas mask size 0 2 4 6 8 10 12 14 16 18 20 Disploy rate [% done] 1 2 5 10 20 50 100	ass mask size         a	ess marks size 0 2 4 6 8 10 12 14 16 18 20 ploy rate [% dona] 2 5 10 20 50 100	as mark size 0 2 4 6 8 10 12 14 16 18 20 slov rate [% done] 2 5 10 20 50 100	aik dize         2       4       6       8       10       12       14       16       18       20         aik dize	Cross mask size	***
s mask size		O         2         4         6         8         10         12         14         16         18         20           Display rate [% done]	0 2 4 6 8 10 12 14 16 18 20 Display rate [% date] 0 0 0 0 0 0 0 1 2 5 10 20 50 100	0     2     4     6     8     10     12     14     16     18     20       Display rate [% done]	0 2 4 6 8 10 12 14 16 18 20 ploy cate [% done] 0 0 0 0 0 0 0 0 1 2 5 10 20 50 100	0     2     4     6     8     10     12     14     16     18     20       ploy rate [%. done]	0     2     4     6     8     10     12     14     16     18     20       3loy rate (% done)	2       4       6       8       10       12       14       16       18       20         wate [% done]		666
2 4 6 8 10 12 14 16 18 20	————————————————————————————————————	Display rate [% done]	Display rate [% done]	Display rate [% done] O O O O O O 1 2 5 10 20 50 100	ploy rate [% done] 0 0 0 0 0 0 1 2 5 10 20 50 100 	ploy rate [% done]	bloy rate [% done] 0 0 0 0 0 0 1 2 5 10 20 50 100 		0 2 4 6 8 10 12 14 16 18 20	***
iay rate [% done]				1 2 5 10 20 50 100					Disploy rate [% done]	666
2 E 10 20 E0 100	the second se	1 2 5 10 20 50 100							1 2 5 10 20 50 100	2000
2 5 10 20 50 100										and and and a

Figure 37: Projected potential tab.

## 4.7 Absorption potential tab

The absorption potential takes into account inelastic scattering events of plasmon or core origin (Fig. 38). It is best calculated using Weickenmeier-Kohl method (see 9.2). Absorption  $\mu_{TDS}$  should not be included (though there are always some electrons scattered outside the detectors).

rt / Stop calculation		
Initialize Start Stop	Crystal potential stack calcu	lation done. Ready to start multislice calculation:Elapsed time : 3 [s]::173
Iteration Multislice Options Scanning Signal	< Absorption potential	Fresnel propagator Phase object Power spectrum
Atomic Form Factor DISB EJK PRDW WK WKC, XRey		
-Image calculation method		
Frezen lattice     Tshizuka     Wang		
Parent not yet defin. [0.0.1]		
Options Stack index		
Image stack BF/DF progress		
-BF & ADF detectors BF outer detector radius::12.000 [mrad] BF detector conter at (0.000, 0.000, 0.000) DF inner detector radius::149.000 [mrad] DF outer detector radius::149.000 [mrad] DF detector conter at (0.000, 0.000)		

Figure 38: Absorption potential tab.

#### 4.8 Fresnel propagator tab

This tab shows the Fourier transform of Fresnel propagator (Fig. 39)  $FP(x, y; \Delta_z)$  used by multislice method ( $\overline{FP}(u, v; \Delta z)$ ). When the  $O(\Delta z)$  approximation is selected, a multislice iteration cycle is performed as:

$$\Psi(x, y; z + \Delta z) = FP(x, y; \Delta z) \otimes (PO(x, y, \Delta z) \times \Psi(x, y; z))$$

When the  $O(\Delta z^2)$  approximation is selected, a multislice iteration cycle is performed as:

$$\Psi(x,y;z+\Delta z) = FP(x,y;\frac{\Delta z}{2}) \otimes \left[PO(x,y,\Delta z) \times \left(FP(x,y;\frac{\Delta z}{2}) \otimes \Psi(x,y;z)\right)\right]$$

The convolution  $FP\otimes$  is performed using a direct Fourier transform, a multiplication and an inverse Fourier transform. The  $O(\Delta z^2)$  requires twice the number of Fourier transforms of the  $O(\Delta z)$ .

Note that a small crystal tilt can be introduced ( $\approx 1-2$  degrees) can be introduced using the specimen dialogue (tilting the Ewald sphere).



Figure 39: Fresnel propagator tab. The Fresnel propagator,  $FP(x, y, \Delta z)$ , is shown as as  $\overline{FP}(u, v; \Delta z)$ .

## 4.9 Phase-object tab

The phase-object  $(PO(x, y, \Delta z))$  is only displayed during the multislice iterations (real part on the left and imaginary part on the right, Fig. 40).



Figure 40: Phase-object tab. The phase-object,  $PO(x, y, \Delta_z)$  is shown here multiplied by a mask.

#### 4.10 Power spectrum tab

The power spectrum (PS(u, v)) of the wave-function,  $\Psi(x - x_o, y - y_o)$ , at a given scan position  $(x_o, y_o)$  is shown in this tab (Fig. 41. The intensity can be premultiplied by a *Power spectrum logarithm scale* (see **Signal** tab).



Figure 41: Power spectrum tab shows the logarithm of the whole power spectrum (PS(u, v)).

The logarithm of the whole power spectrum, PS(u, v), can be premultiplied by a scaling factor in order to enhance the intensity of high spatial frequency reflections.

# 4.11 Bright-field detector tab

The signal collected by the **BF detector** is displayed in this tab (Fig 42).

Multislice masks Cross		<b>⊘</b> Phase object	,	<b>⊘</b> Probe		
Multislice size O 128 × 128 a	0 256 x 256	• 512 × 512	0 1024 × 102	O 24 2048 x		
Scan area size O 64 x 64 1	• 128 × 128	0 256 × 256	0 512 x 512	0 1024 x 1	024	
Scan step size O 1	0 2	• 4	0			
Cross mask size	6	0 8 10	• • 12 14	• • 16 18	0 20	•
Display rate [% done O 1 2	e] 0 5	0 10	0 20	0 50	0 100	

Figure 42: Bright-field detector tab. Portion of PS(u, v) collected by the BF detector.

## 4.12 Dark-field detector tab

The signal collected by the **DF detector** is displayed in this tab as the logarithm of its intensity (Fig. 43). It can be premultiplied by a large factor in order to better display the inelastically scattering intensity.

Iterat	on   Multisl	lice   Opti	ions Sco	inning S	signal	Bright-field detector     Dark-field detector     Wave-func
Cross		☑ Phase object	t	<b>⊘</b> Probe		
Multislice size 0 128 × 128	O 256 x 256	• 512 × 512	0 1024 × 10	0 24 2048 x		
Scan area size 0 64 x 64	• 128 × 128	 256 × 256	0 512 × 512	0 1024 x 1	1024	
Scan step size O 1	0 2	• 4	0	) 3		
Cross mask size O 2	• • 4 6	0 0 8 10	• • 12 14	• • 16 18	0 20	
Display rate [% O 1 2	done] O 5	0 10	0 20	0 50	0 100	

Figure 43: Dark-field detector tab. Portion of  $PS(\boldsymbol{u},\boldsymbol{v})$  collected by the DF detector.

#### 4.13 Sectors detector tab

The imaginary part wave-function,  $\Psi(x, y)$ , is shown in this tab (Fig. 44).



Figure 44: Sectors detectors tab. The sectors detector inner- and outer- radii are defined by the outer-radius of  $BF_1$  and the inner-radius of  $ADf_1$ . The inner-radius can be larger than the outer-radius of  $BF_1$  and smaller than the inner-radius of  $ADf_1$ .

# 4.14 Wave-function tab

The imaginary part wave-function,  $\Psi(x, y)$ , is shown in this tab (Fig. 45).

Iteration Multislice Options Scanning Signal	Bright field detector	ark field detector Wavefunction
ADF signal control Bright field Dark field		
Histogram O Signal	0	۲
Brightness Contrest x 10000 Gamma		
Bright field gain. 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		
Power spectrum logarithm scale.		

Figure 45: Wave-function tab. Imaginary part of  $\Psi(x, y)$  at the bottom of the last slice of the model.

# 5 Probe imager dialogue

After complete initialisation, the **Start** button is enabled and the calculation can be started. The **Probe imager dialogue** will popup (Fig. 46). This dialogue allows to define the scan area position (when smaller than the phase-object size) and the probe shape. The probe shape depends on defocus, virtual objective aperture size (or convergence defined by  $C_2/C_3$ ) and source size. Aberrations up to order 8 can be introduced (i.e. C78, A7 or W88). The aperture size can be displayed as  $[nm^-1]$  or [mrad] (see note 9.4).

	[	
Oth order 1st order 2nd order 3rd order	C <sub>c</sub> ( Cc   W <sub>00</sub> ) [mm] 2.0	(Probe position Probe Shape)
Amplitude	C <sub>01</sub> (I   W <sub>11</sub> ) [nm] 0.0 0.0	
-W00: Cc	$c_{10} (z   w_{20}) [nm] = -5.8$	
	$c_{12} (A_1   W_{22}) [rm] = 0.0$	
	C <sub>21</sub> (3B <sub>2</sub>   W <sub>31</sub> ) [rm] 0.0 0.0	
	$C_{23} (A_2   W_{33}) [nm] 0.0 0.0$	
	C <sub>30</sub> ( C <sub>3</sub>   W <sub>40</sub> ) [mm] _−0.03	
	C <sub>32</sub> (45 <sub>3</sub>   W <sub>42</sub> ) [µm] 0.0 0.0	
	C <sub>34</sub> ( A <sub>3</sub>   W <sub>44</sub> ) [µm] 0.0 0.0	
	C <sub>41</sub> (58 <sub>4</sub>   W <sub>51</sub> ) [µm] 0.0 0.0	
	C <sub>43</sub> (5D <sub>4</sub>   W <sub>53</sub> ) [µm] 0.0 0.0	************************************
	C <sub>45</sub> ( A <sub>4</sub>   W <sub>55</sub> ) [µm] 0.0 0.0	• • • • • • • • • • • • • • • • • • •
	C <sub>50</sub> ( C <sub>5</sub>   W <sub>60</sub> ) [mm] 5,0	A state of a state
	C <sub>52</sub> (65 <sub>5</sub>   W <sub>62</sub> ) [mm] 0.0 0.0	Construction and the transmission of transmission of the transmission of transmission of the transmissi
	C <sub>54</sub> (6R <sub>5</sub>   W <sub>64</sub> ) [mm] 0.0 0.0	A statute to the test statute to the test statute
	C <sub>56</sub> ( A <sub>5</sub>   W <sub>66</sub> ) [mm] 0.0 0.0	and the second second second second second
	C <sub>61</sub> (78 <sub>6</sub>   W <sub>71</sub> ) [mm] 0,0 0.0	**************************************
	C <sub>63</sub> (7D <sub>6</sub>   W <sub>73</sub> ) [mm] 0.0 0.0	
	C <sub>65</sub> (7F <sub>6</sub>   W <sub>75</sub> ) [mm] 0.0 0.0	
	C <sub>67</sub> ( A <sub>6</sub>   W <sub>77</sub> ) [mm] 0.0 0.0	Set
	C <sub>70</sub> (C <sub>7</sub>   W <sub>80</sub> ) [m] 0.0	
	C <sub>72</sub> (85 <sub>7</sub>   W <sub>82</sub> ) [m] 0.0 0.0	
	C <sub>74</sub> (8R <sub>7</sub>   W <sub>84</sub> ) [m] 0.0 0.0	
	C <sub>76</sub> (8G <sub>7</sub>   W <sub>86</sub> ) [m] 0.0 0.0	
	C <sub>78</sub> (A <sub>7</sub>   W <sub>88</sub> ) [m] 0.0 0.0	
Formula		

Figure 46: Probe imager dialogue. The scan area (square) and probe position are selected using the pointing device, i.e. usually mouse.

#### 5.1 Scan area and probe position

The probe is shown at the centre of the scan area (Fig. 47). It is moved using the pointer or the mouse. The probe shape (Fig. 48 and 49) is adjusted using the controls of the probe imager dialogue left tab.



Figure 47: Scan area and probe position.



Figure 48: Probe shape with dimension circles.



Figure 49: Probe shape 3-D.

The probe size is adjusted using the defocus, the **Aperture diam.** and the **Source size** controls.**Coherent** and **Envelope** illumination approximation can

be selected respectively. The aperture radius and source size controls are found in the **Microscope** tab (Fig. 50). Note that most of the sliders have a popup menu that allows to set its *Minimum*, *Maximum* or *Default* value. The popup menus of the **Aperture diam.** (and **Beam half conv.**) sliders allow to change the unit from [mrad] to  $[nm^{-1}]$  or from  $[nm^{-1}]$  to [mrad].



Figure 50: Adjusting the probe size.

# 6 Setting the bright-, dark-field and sectors detectors

Before selecting the bright-field and dark-field detectors size (equivalent to adjusting the diffraction camera length), it is suggested to define the "Single unit cell parent crystal", and the [u, v, w] observation direction equivalent to the model [0, 0, 1] observation direction. For graphene, the **graphite** unit cell and [0, 0, 1]observation direction are selected (Fig. 51). The Bright-field controls adjust the camera length used to display the SAED pattern and the outer-radius of the BF detector (Fig. 52).



Figure 51: Parent crystal settings: graphite Figure 52: Detectors selector: bright-field unit cell and [0,0,1] observation direction. detector tab allows to adjust the diffraction camera length and the bright-field detector angle ([mrad]).

The inner- and outer-radii of the dark-field detector are adjusted similarly using the **Dark-field** tab (Fig. 53). When the parent crystal is defined, the reflections of the first-order Laue zone are easily identified and a DF detector inner-radius

can be adjusted in order to avoid them  $^{14}$  (Fig. 54). BF and DF sizes can be adjusted during the calculations.



Figure 53: Dark-field detector selection using Figure 54: Inner- and outer-radii of 86 and inner- and outer-radii ([mrad]). 150 ([mrad]) are necessary to avoid first-order Laue zone reflections.

<sup>&</sup>lt;sup>14</sup>Note that a graphene sheet doesn't generate first order reflections.



Figure 55: Sectors detector selection using Figure 56: Sectors detector can be made very large by decreasing the BF detector outer-radius and increasing the DF detector inner-

radius.

# 7 Doing a bright- or dark-field and sectors image calculation

In order to perform BF, DF and SE images calculations do the following:

- 1. Prepare the model and slice it into slices not thicker than  $\approx 0.2$  nm.
- 2. Start jems and load slice *somename\_0000.txt*.
- 3. Start the ADF imager dialogue and load the series of slices from *some*-name\_0001.txt.
- 4. Set the ADF calculations parameters using the controls in tabs **Multislice** to **Signal**.
- 5. Push the <u>Initialize</u> button to initialise the phase-object, Fresnel propagator stacks.
- 6. Push the Start button when enabled. The Stop button aborts the calculation.

The detectors sizes (either in mrad or  $nm^{-1}$  units and their common center, shown as (hkl) indices of the ZOLZ, are displayed on the option tabs where  $BF_i$  are the bright-field detectors 1 to 4,  $ADF_i$  are the dark-field detectors 1 to 4 and SD the sectors detector.

```
BF1 outer detector radius:: 25.0 [mrad] (9.97 [nm-1])
SD inner detector radius:: 25.9 [mrad] (10.33 [nm-1])
SD outer detector radius:: 60.0 [mrad] (23.92 [nm-1])
ADF1 inner detector radius:: 60.0 [mrad] (23.92 [nm-1])
ADF1 outer detector radius:: 117.4 [mrad] (46.78 [nm-1])
BFi (2 <=i<= 4) = BF1 + (i - 1) 5.0 [mrad]
ADFi (2 <=i<= 4) = ADF1 + (i - 1) 10.0 [mrad]
BF/ADF/SD detectors center::(0.000, 0.000, 0.000)</pre>
```

You might have to introduce the **Cross** mask in order to cancel weak multislice artefacts (see note 9.5). Assuming an isotropic radial distribution of intensity on the **Dark field** detector, the intensity collected by this detector is reduced by a factor that is display in the console together with the area of the BF and DF detectors (as a fraction of the power spectrum area).

Without the **Cross** mask:

BF detector area [a.u.] = 0.0036172867 DF detector area [a.u.] = 0.06423378

Without a **Cross** mask of 23 pixels width that cancels most of the multislice artefacts:

BF detector area [a.u.] = 0.0036172867DF detector area [a.u.] = 0.06423378DF detector + cross wire area [a.u.] = 0.056114197

# 8 Example: GaAs [110]

Figures 57 and 58 show the stack of slices and the 3-D model for calculating BF and DF images (GaAs [110]). The GaAs model is prepared using **Make orthogonal** (**Crystal**). The GaAs [110] unit cell is then duplicated using **To triclinic** (menu **Miscellany**) and finally sliced in 4 slices of  $\approx 0.2$  nm thick slices using **To slices** (menu **Miscellany**).

Super-cells		
s	Specimen thickness	:::6.3945637 [nm]
Name	Iteration	File/Class
GaAsSlices_0000	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0001	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0002	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0003	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0000	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0001	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0002	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0003	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0000	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0001	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0002	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0003	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0000	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0001	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0002	1	/Users/pierrestadelmann/Deskta
GaAsSlices_0003	1	/Users/pierrestadelmann/Deskta
Generalizer 0000	1	/Liener/ninenactedalmonn/Dackta
	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	
H N		🔶 📑 🗾

Figure 57: GaAs [110] stack of slices (8 × Figure 58: Stack of slices shown as a 3-D 4 slices). Total model thickness is  $8 \times 0.79 =$ model. 6.3 nm.

Figs. 59 and 60 show BF and DF images stacks. Fig. 64 shows a profile plot across the Ga and As atoms position. Only 2 atomic configurations have been used for this  $512 \times 512$  multislice calculation, scan size of  $64 \times 64$ , 32 slices (calculation time is  $\approx 1$  hour, Intel i7, iMac).

BF and DF images using a  $256 \times 256$  calculation, performed in  $\approx 10$  minutes, are shown in Figs. 62 and 63. It is advised to start with calculations of small sizes and to increase their size when absolutely needed (i.e. for quantitative purposes).

Doing 512x512 simulations takes much more computer time (several hours or days). The next figures show some dark-field images of GaAs [110] and different dark-field detector sizes. It should noted that the detector outer-radius must not be larger than 2/3 of the maximum spatial frequency imposed by the anti-aliasing that depends on the multislice calculation size. Also since the ADF images is

ê 🗟 🗋 📗 🚺 🗮 🖉 💈	8 😭 📋 📕 📕 🖉 🚳
Stack intex	Strack controls

Figure 59: GaAs [110], BF image stack Figure 60: GaAs [110], DF image stack  $(512 \times 512 \text{ multislice calculation})$ , BF detec-  $(512 \times 512 \text{ multislice calculation})$ , DF detector radius 10 mrad. tor inner- and outer-radius 60 - 185 mrad.



Figure 61: Intensity profile across Ga and As atoms ( $512 \times 512$  multislice calculation).



Figure 62: GaAs BF ( $256 \times 256$  multislice cal-Figure 63: GaAs BF ( $256 \times 256$  multislice calculation). Note that scan area is not identical culation). Note that scan area is not identical to previous BF image (Fig. 59). to previous DF image (Fig. 60).



Figure 64: Intensity profile across Ga and As atoms ( $256 \times 256$  multislice calculation). Note that the qualitative agreement is fair for  $6 \times shorter$  calculation time.

using single precision floating point numbers the accumulation of rounding errors finally makes the errors of large image spatial frequencies as large as the TDS signal. This effect can be observed on the images Fig. ??fig:ADFDetector1 to ??fig:ADFDetector4 where the GaAs crystal thickness is 51 nm (256 slices of 0.2 nm). Possible solutions would be to do 1024x1024 multislice calculation or to perform simulation using double precision floating point numbers. Note also that Kikuchi lines are visible on the power spectrum image that is only calculated with a single atomic configuration (Fig.66(a)).



(a) ADF detector inner- and outer radius: 60, 150 mrad.



(b) ADF detector inner- and outer radius: 75, 165 mrad



(c) ADF detector inner- and outer radius:90, 180 mrad (too large for thicknesses larger than 35 nm



(d) ADF detector inner- and outer radius: 105, 195 mrad (too large for thicknesses larger than 25 nm

Figure 65: Image artefacts introduced by large outer-radius ADF detector (150 to 195).



(a) Power spectrum (1 atomic configuration) 55 nm thick GaAs.



(b) ADF detector inner- and outer radius: 60, 150 mrad

Figure 66: Rounding or aliasing errors are accumulating perpendicularly to the GaAs dumbells (GaAs [110]).

#### 9 Notes

#### 9.1 Note 1: Debye-Waller temperature factor

The Debye-Waller temperature factor  $M_k$  is given by  $M_k = 8\pi^2 < u^2 >_k$ , where  $\langle u^2 \rangle_k$  is the mean-square vibrational amplitude of atom k in the unit cell. In the Debye model for lattice vibrations, a linear dispersion relationship is assumed and the excitation spectrum is parameterized using the Debye-temperature  $\theta_D$ :

$$< u^2 >= \frac{3h^2}{4\pi^2 m_k \theta_D} \left(\frac{1}{4} + \frac{T^2}{\theta_D^2} \int_0^{T/\theta_D} \frac{x}{e^x - 1}\right) dx$$

where  $m_k$  is the mass of atom k.

Using the harmonic approximation for the vibration of the atoms, the temperature dependance of  $\langle u^2 \rangle$  is given by:

$$\langle u^2 \rangle = \frac{\hbar}{2m} \int_0^{\omega_m} \coth\left(\frac{\hbar\omega}{2k_BT}\right) \frac{g(w)}{w} d\omega$$

where  $g(\omega)$  is the normalized phonon density of states and  $w_m$  the maximum phonon frequency. Using either the Debye- or the Einstein model for lattice vibration, it is found that for high temperatures  $\langle u^2 \rangle$  is a linear function of temperature.

#### 9.2 Note 2: calculation of the atomic scattering amplitude

The atomic scattering amplitude for electrons  $f^B(g)$  has been given in analytical form by Weickenmeier and Kohl<sup>15</sup>:

$$f^{B}(s) = \frac{1}{s^{2}} \sum_{i=1}^{6} A_{i} \left[ 1 - e^{-B_{i}s^{2}} \right] \qquad \qquad s = g/4\pi$$

where the  $A_i$  and  $B_i$  are tabulated for atomic number 1 to 92. Options  $WK_c$  also includes core absorption.

The projected potential is computed in 3 possible ways:

- 1. Analytic The projected potential of an atom is described by an analytic function of its (x, y) position.
- 2. Direct The atom potential is calculated, integrated over z and patched at its (x, y) position.
- 3. *Fourier* The Fourier transform of the projected potential is computed and then inverse Fourier transform. It is the most accurate method, but also the slowest.

#### 9.3 Note 3: absorption coefficient $\mu_{TDS}$

$$\mu_{TDS} = \frac{1}{k_0^2 \Omega_0} \sum_a \int d\sigma(\tau) \left| f_a^B(\tau) \right|^2 \left( 1 - e^{-2Wa(\tau)} \right)$$

where  $k_0$  is the incident wave vector.  $\Omega_0$  the volume of an atom and  $e^{-W_a(\tau)}$  the Debye-Waller factor of atom a. The surface integral is taken from the inner edge of the dark-field detector to infinity. This formulation allows to calculate the TDS intensity falling on the dark-field detector within K. Ishizuka approximation.

#### 9.4 Note 4: popup menu attached to slider controls

A popup menu is attached to most sliders. It is displayed as all popup menus are, i.e. with a right button click or a double click when the mouse or pointer is placed

<sup>&</sup>lt;sup>15</sup>A. Weickenmeier and H. Kohl. Computation of Absorptive Form Factors for High-Energy Electron Diffraction. Acta Cryst. A47:590-597, 1991.

on the slider handle (Figs. 67 and 68). Slider of Fig. 68 allows to switch between [mrad] and  $[nm^{-1}]$  units.





Figure 67: Standard slider popup menu.

Figure 68: Popup menu allowing to switch from [mrad] to  $[nm^{-1}]$  unit (here [mrad] are selected).

#### 9.5 Note 5: sampling artefacts

Though all the calculations are performed in double precision, due to the discrete nature of the multislice method, calculation artefacts could appear centred as weak intensity bands centred at spatial frequency (0, 0) and distributed in the  $O_u$ (horizontal) or  $O_v$  (vertical) directions. These artefacts are visible when a high DF signal gain is set.

The intensity falling on the DF detector is show in Fig. 69. The  $df_{signal}$  gain  $(df_{gain})$ , defined in the **Signal** tab, is 10<sup>9</sup> and a logarithm scale is used to display the intensity:

$$log \left[1 + df_{gain} \times df_{signal}\right]$$

In Fig. 70 the intensity is shown as:

$$log \left[1 + 10^6 \times df_{gain} \times df_{signal}\right]$$



Figure 69: DF detector, dark-field signal gain Figure 70: DF detector, dark-field signal gain is  $10^9$ , logarithm scale = 1. is  $10^9$ , logarithm scale =  $10^9$ . The combined df signal gain is  $10^{15}$ , i.e. matching the double precision error  $(2^{-53} = 1.11 \times 10^{-16})$ . i.e. a  $10^{15} df_{gain}$  makes the sampling artefacts visible. The  $10^6$  factor is selected at the bottom of the **Signal** tab.

The calculation artefacts can be eliminated (and quantified) by placing a cross mask in front of the DF-detector (Fig. 71 and 72). The width of the cross bars is adjusted by using a set of radio buttons.



Figure 71: A cross placed in front of the DF Figure 72: The width of the cross bars selecdetector masks the artefacts. The minimum width is 3 pixels.