#### Image Simulation Laboratory Notes

CCEM Summer School on Electron Microscopy at McMaster University June 5 - 9, 2017

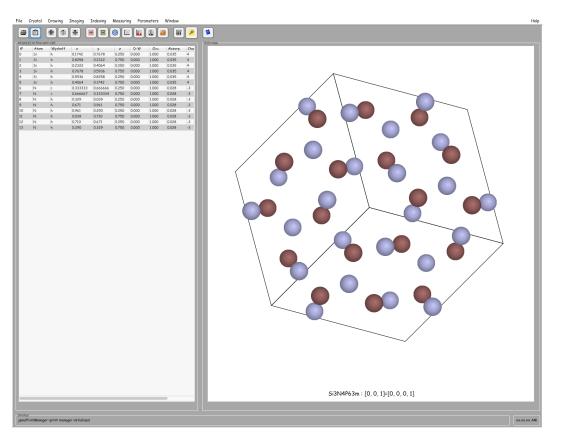
> Pierre Stadelmann JEMS-SAAS CH-3906 Saas-Fee Switzerland

> > May 15, 2019

# Starting jems

Start jems student version<sup>1</sup> with this icon:

that you see on the desktop. jems main window will open:



Main jems window, Si atoms position (left panel) and [001] projection of one unit cell (right) of Si crystal structure.

<sup>&</sup>lt;sup>1</sup>http://www.jems-saas.ch

#### jems MenuBar: part 1

File Crystal Drawing Imaging Indexing Measuring Parameters Window Miscellany jems MenuBar.

0	0			
File	Crystal	ng	١ı	
Ne	w from clip	board	^N	
Pag	je setup		^Z	
Pri	nt		^P	
Se	ect		^A	
Exi	t -		^E	

File menu: to select a crystal structure.

Crystal	Drawing	Imaging
Atom		^A
Calcule	ator	^c
Make	^o	
Struct	ture factor	^v
Syster	n	•
Transf	^т	
Zone	^Z	

Crystal menu: to define crystal structures.

Drawing	Imaging	Indexir
Diffract	ion	^D
Image	3D	^ı
Perspe	ctive	^P
Recipro	cal space	^ <sub>R</sub>
Stereo	gram 0.200	^s
Thon d	iagram 500	^н
Transfe	r function	^T
X-Ray	powder line	^x

Drawing menu: to draw crystal structures, diffraction patterns.

Imaging	Indexing	Mea
ADF		^ <u>A</u>
Blochw	ave	^B
Howie-\	Whelan	^н
HRSTE	M imager	^s
HRTEM	imager	^т
Load		ः )∙ः
Multislic	e 0.500	^м
Process	sing	^P
0.750		0.250.

Imaging menu: to perform Blochwave or multislice calculations.

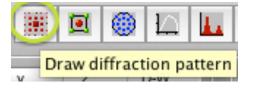
### jems MenuBar: part 2

			Miscellany
Imaging Indexing Mea			Load image Load super-cell
ADF ^A Blochwave ^B Howie-Whelan ^H HRSTEM imager ^S	No accessional Descentes	Parameters Window	Make void Thon diagram
HRTEM imager ^T Load Multislice ^M Processing ^P	Measuring Parameter Camera MTF Goniometer Thickness	Microscope ^M Preferences ^P Specimen ^X	To core-shell To particle To slices To triclinic
Indexing menu: to inde diffraction patterns.	x Measuring menu: to measure camera MTF, specimen thickness.	Parameters menu: to configure jems, define microscope or specimen properties.	Miscellany menu: to loa or create super-cells.

Menu items that are frequently used are repeated in the ToolBar:



Note that a tool tip text is attached to any jems tool or control. For example:



to load

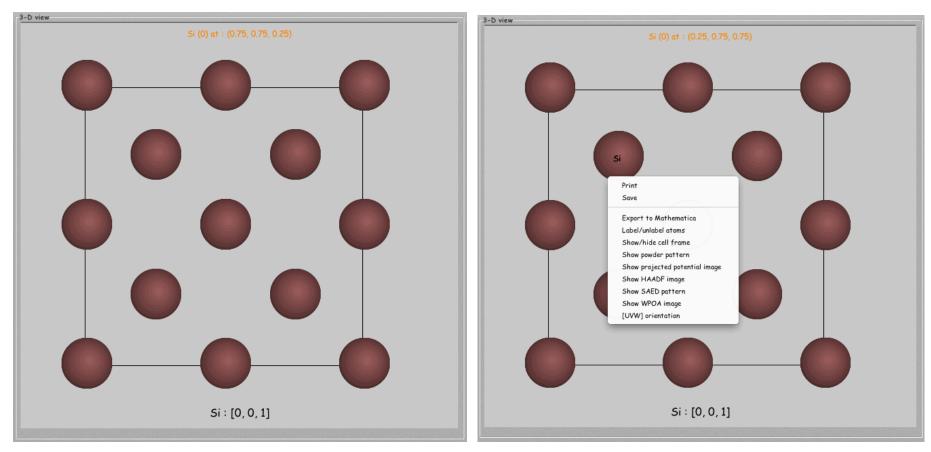
#### Main window left panel

#	Atom	Wyckoff	x	У	z	D-W	Occ.	Absorp.	Charge	AFF
0	Si	٥	0,000	0,000	0,000	0.0049	1,000	0.029	Def	0
1	Si	۵	0.250	0.250	0.250	0,0049	1,000	0.029	Def	0
2	Si	a	0.500	0.500	0,000	0.0049	1,000	0.029	Def	0
3	Si	۵	0,000	0.500	0.500	0.0049	1,000	0.029	Def	0
4	Si	٥	0.500	0,000	0.500	0.0049	1,000	0.029	Def	0
5	Si	۵	0.750	0.750	0.250	0.0049	1,000	0.029	Def	0
6	Si	٥	0.250	0.750	0.750	0.0049	1,000	0.029	Def	0
7	Si	۵	0.750	0.250	0.750	0,0049	1,000	0.029	Def	0

The left panel displays a tabular list of the silicon atoms.

With the alternate non-centric F d -3 m space group the Si structure contains 8 atoms. Only the atom at Wyckoff position a, (x, y, z) = (0, 0, 0), must defined. All the other atom positions are generated by the symmetry operations of the space-group.

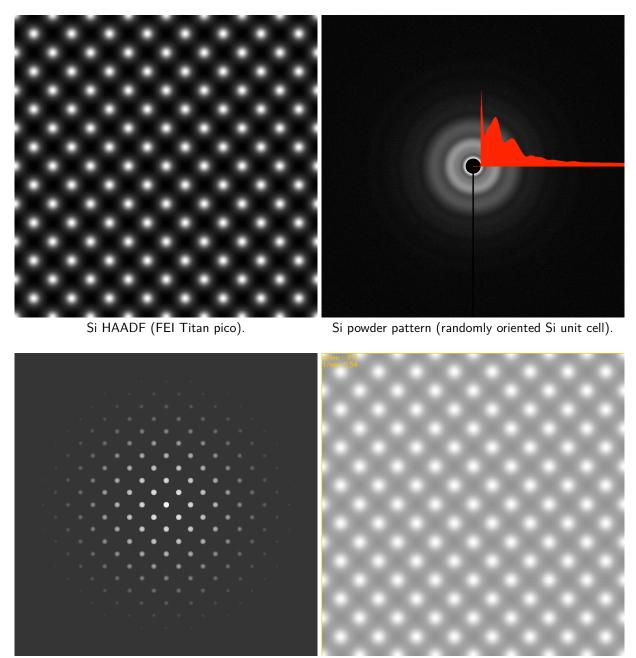
- 0: atom sequence number.
- Si: atom symbol.
- ► a: Wyckoff position.
- 0.000: x coordinate [0, 1]
- 0.000: y coordinate [0, 1]
- 0.000: z coordinate [0, 1]
- ▶ 0.0049: Debye-Waller temperature factor [nm<sup>2</sup>]
- 1.000: site occupancy [0, 1[.
- 0.029: absorption coefficient.
- Def: charge.
- O: Atomic Form Factor source (Doyle-Turner or Smith-Burge).



The right panel shows a projection of a silicon unit cell. Note that all atoms of the FCC Bravais lattice are shown. A mouse click on an atom position labels the atom and a right mouse click displays a popup menu (Ctrl-mouse click on Mac OSX). Note that a popup menu is attached to many drawings and tables. The popup menu of the right panel allows to:

- Print: generates a pdf printout of the drawing.
- Save: generates an image of the drawing (using the format defined in the Preferences).
- Export to Mathematica: exports the structure as a Mathematica notebook.
- ► Show/hide cell frame: displays or hides the cell frame.
- Show powder pattern: uses Debye formula to display a powder pattern.
- Show HAADF image: displays a HAADF image (projected potential convoluted with the OTF).
- Show SAED pattern: displays a kinematical diffraction pattern (1 unit cell thick crystal).
- Show WPOA image: displays a HRTEM image using the Weak Phase Object Approximation (1 unit cell thick crystal).
- ► [*UVW*] orientation: changes the zone axis.

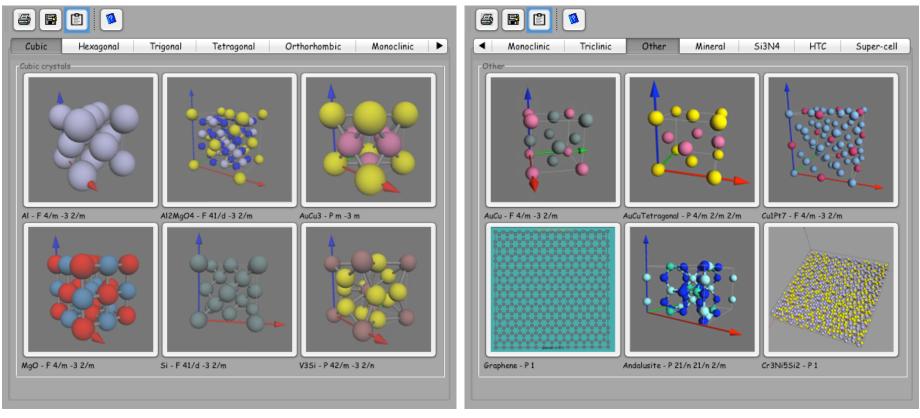
#### Popup menus items



Si [001] kinematical selected area diffraction pattern.

Si HRTEM image (WPOA) approximation.

jems student editions offers 72 selectable crystal structures. They are available in tabs Cubic, Hexagonal, ...of *Select crystal dialogue*.



6 different *Cubic* crystals can be selected.

6 different Other crystals.

#### Displaying structures using openGL

Image stripe / montage       Maximum aberrations order         Show stripe       Show montage         • 4       5       6       7       8         Lowest beam amplitude considered for imaging       • 10-8       10-7       10-6       10-5       10-4       10-3       10-2         Maximum dimension of GUI panels       Maximum dimension of reduced images       • 256       512       • 768       1024       • 1536         Maximum mage dimension       • 256       • 384       • 512       • 640       • 768       896       • 1024       • 2048       • 4096         Maximum mage dimension       • 256       • 384       • 512       • 640       • 768       896       • 1024       • 2048       • 4096         Maximum map dimension       • 512       • 640       • 768       896       • 1024       • 2048       • 4096         Maximum map dimension       • 0005       • 0001       • 0002       • 003       • 0.04       • 0.05         Resize loaded images       • method       • 1000       • 0002       • 0.003       • 0.04       • 0.05         Resize loaded images       • Interpolate       • Subsample       • Bilinear       • Bicubic         Power spectrum       • As is       • Inte	lany
<ul> <li>0 10-8</li> <li>0 10-7</li> <li>0 10-6</li> <li>0 10-5</li> <li>10-4</li> <li>10-3</li> <li>10-2</li> </ul> Maximum dimension of cUI panels <ul> <li>512</li> <li>640</li> <li>768</li> <li>1024</li> <li>1536</li> </ul> Maximum mage dimension <ul> <li>256</li> <li>384</li> <li>512</li> <li>640</li> <li>768</li> <li>896</li> <li>1024</li> <li>2048</li> <li>4096</li> <li>8192</li> <li>16384</li> </ul> Maximum mage dimension <ul> <li>512</li> <li>640</li> <li>768</li> <li>896</li> <li>1024</li> <li>2048</li> <li>4096</li> <li>8192</li> <li>16384</li> </ul> Pixel size of high resolution images / nm <ul> <li>0.0005</li> <li>0.001</li> <li>0.002</li> <li>0.005</li> <li>0.01</li> <li>0.02</li> <li>0.03</li> <li>0.04</li> <li>0.05</li> </ul> Power spectrum <ul> <li>Power spectrum log scale</li> <li>0.01</li> <li>0.1</li> <li>1</li> <li>10</li> <li>100</li> </ul> Java 3D <ul> <li>Holography tab</li> </ul> Check atom site occupancy	
• 512       640       768       1024       1536         Maximum image dimension       256       384       512       640       768       896       1024       2048       4096         Maximum map dimension       512       640       768       896       1024       2048       4096         Maximum map dimension       512       640       768       896       1024       2048       4096         Pixel size of high resolution images / nm       00005       0.001       0.002       0.003       0.04       0.05         Resize loaded images       0.001       0.002       0.005       0.01       0.02       0.03       0.04       0.05         Power spectrum       Potential interpolation       Bilinear       Bilinear       Bilinear       Bilinear         Power spectrum       Power spectrum log scale       0.01       0.1       1       10       1000         Java 3D       Holography tab       Check atom site occupancy	
<ul> <li>256 384 512 640 768 896 1024 2048 4096</li> <li>Maximum map dimension</li> <li>512 640 768 896 1024 2048 4096 8192 16384</li> <li>Pixel size of high resolution images / nm</li> <li>0.0005 0.001 0.002 0.005 0.01 0.02 0.03 0.04 0.05</li> <li>Resize loaded images</li> <li>As is Therpolate Subsample</li> <li>Power spectrum</li> <li>Bilinear Bicubic</li> <li>Power spectrum</li> <li>Linear scale Ligarithm scale</li> <li>Power spectrum</li> <li>0.01 0.1 0.1 0.1 0.00 1000</li> <li>Java 3D</li> </ul>	
<ul> <li>512  640  768  896  1024  2048  4096  8192  16384</li> <li>Pixel size of high resolution images / nm</li> <li>0,0005  0.001  0.002  0.005  0.01  0.02  0.03  0.04  0.05</li> <li>Resize loaded images</li> <li>As is  Interpolate  Subsample</li> <li>Potential interpolation</li> <li>Bilinear  Bicubic</li> </ul>	
<ul> <li>0.0005 0.001 0.002 0.005 0.01 0.02 0.03 0.04 0.05</li> <li>Resize loaded images         <ul> <li>As is</li> <li>Interpolate</li> <li>Subsample</li> </ul> </li> <li>Power spectrum         <ul> <li>Linear scale</li> <li>Logarithm scale</li> <li>Power spectrum log scale</li> <li>0.01 0.1 0 1 0 100 1000</li> </ul> </li> <li>Java 3D</li> </ul>	
<ul> <li>As is</li> <li>Interpolate</li> <li>Subsample</li> <li>Bilinear</li> <li>Bicubic</li> <li>Power spectrum</li> <li>Linear scale</li> <li>Logarithm scale</li> <li>O.01</li> <li>O.1</li> <li>I</li> <li>IO</li> <li>IOO</li> <li>IOO<!--</td--><td></td></li></ul>	
O Linear scale <ul> <li>Logarithm scale</li> <li>O.01</li> <li>O.1</li> <li>O</li> <lio< li=""> <li>O</li> <lio< li=""></lio<></lio<></ul>	
O Linear scale O Logarithm scale O 0.01 O 0.1 O 1 O 100 O 1000 Java 3D Holography tab Check atom site occupancy	
uve these preferences ?	

Cross the Save check box in order to save your preferences.

The preferences dialogue allows to set many jems parameters. Parameters are organised by tabs. The Imaging tab contains defaults for image calculations. In order to display structures or images using openGL, enable the Java 3D check box.

### Today's HRTEM image simulation lab

We have already seen how to load or define a crystal structure. I suggest to select the Si crystal structure. With this structure we will learn how to:

- Display the structure with openGL.
- Make a table of structure factors, a powder line plot and how to compare it with X-ray or neutron plots.
- Calculate SAED kinematical and dynamical electron diffraction patterns:
  - with HOLZ lines.
  - with Kikuchi lines.
- HRTEM image simulation:
  - Multislice approach.
  - Blochwave approach.
- Measuring CCD MTF.
- CBED and LACBED.

We will finally learn how to define a super-cell and use it to perform HRTEM image simulation. More information is available in jems ../pdfFiles folder.

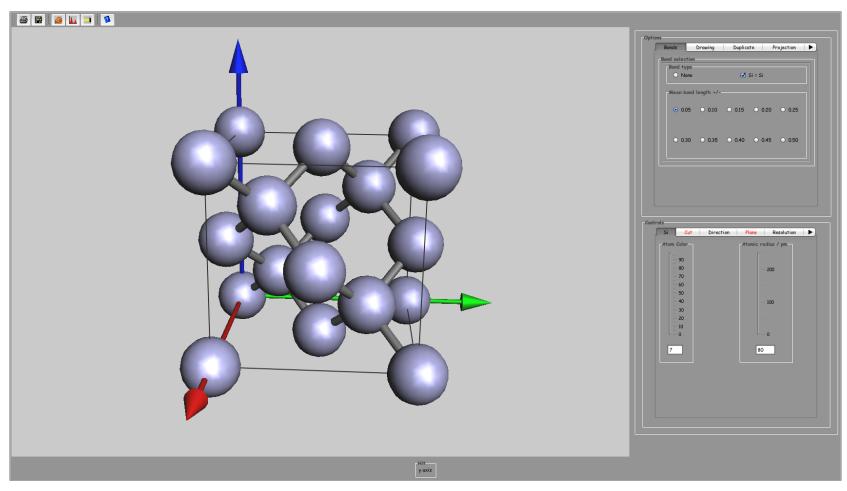
#### Documentation folder

Documentation	CalculationsImages.pdf
📘 jemsLinux64.zip	CDDistribution.pdf
🚹 jemsMacOSX.mpkg.pkg.zip	ConfigurationAndSetup.pdf
jemsWindows7.zip	InstallationInstructions.pdf
jemsWindowsXP.zip	jemsInstallation.pdf
	JemsLicenseCode.pdf
	License.pdf
	MacOSXLicense.pdf
	🕷 Manual.pdf
	Multislice.pdf
	PrecessionElffraction.pdf
	QCBED.pdf
	ReadImage.pdf
	SAEDIndexing.pdf
	Simulation.pdf
	TEMImageSimulation.pdf
	TEMImageSisingJEMS.pdf
	WeberIndices.pdf

Documentation folder contains .pdf files explaining how to perform simulations using jems.

# OpenGL display

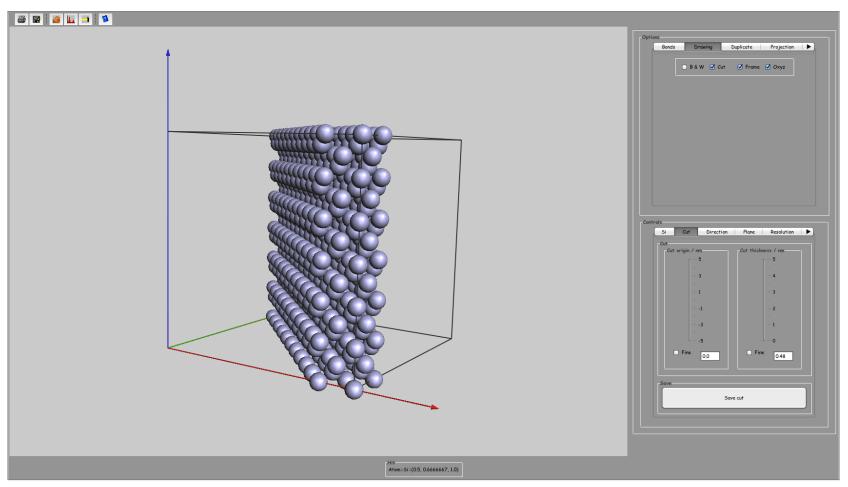
Use **Drawing**  $\implies$  **Perspective** (or the associated tool button) to display the Si structure in 3-D.



One can change the atom color, size or add bonds, cut the unit cell by parallel (hkl) planes, etc. One can also duplicate the unit cell in order to generate larger unit cells.

### Duplicated cell and cut

Select tab Duplicate, and x, y, z duplications 6, 6, 6. Then push the little hammer tool button.



Under tab Drawing select X cut and use tab Plane to select the (hkl) plane and tab cut to cut the structure.

#### Table of structure factors

Use **Crystal**  $\implies$  **Structure factor** to generate a table of structure factors. The table provides the (complex) structure factor, spacing between (hkl) planes, Bragg angle and other useful information.

68	- 9						
#	(h,k,l)	d* / nm-1	Vr / V	Vi / V	Ampli / V	Phase / Deg	Ext. / nm
)	(0, 0, 0)	0.000	22.08305	0.64041	22.09233	1.66111	
	(1, 1, 1)	3.18925	5.91545	6.2688	8.61919	46.66111	88.64305
2	(1, -1, 1)	3.18925	6.2688	-5.91545	8.61919	-43.33889	88.64305
3	(-1, 1, 1)	3.18925	6.2688	-5.91545	8.61919	-43.33889	88.64305
4	(-1, -1, 1)	3.18925	5.91545	6.2688	8.61919	46.66111	88.64305
5	(1, 1, -1)	3.18925	6.2688	-5.91545	8.61919	-43.33889	88.64305
5	(1, -1, -1)	3.18925	5.91545	6.2688	8.61919	46.66111	88.64305
7	(-1, 1, -1)	3.18925	5.91545	6.2688	8.61919	46.66111	88.64305
8	(-1, -1, -1)	3.18925	6.2688	-5.91545	8.61919	-43.33889	88.64305
7	(2, 0, 0)	3.68263	0.000	0.000	0.000	0.000	0.000
.0	(-2, 0, 0)	3.68263	0.000	0.000	0.000	0.000	0.000
11	(0, 2, 0)	3.68263	0,000	0.000	0.000	0.000	0.000
12	(0, -2, 0)	3.68263	0.000	0.000	0.000	0.000	0.000
13	(0, 0, 2)	3.68263	0.000	0.000	0.000	0.000	0.000
14	(0, 0, -2)	3.68263	0.000	0.000	0.000	0.000	0.000
15	(2, 2, 0)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
16	(2, -2, 0)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
17	(-2, 2, 0)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
18	(-2, -2, 0)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
19	(2, 0, 2)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
20	(-2, 0, 2)	5,20803	6.8708	0.19925	6.87369	1.66111	111.15209
21	(2, 0, -2)	5,20803	6.8708	0.19925	6.87369	1.66111	111.15209
22	(-2, 0, -2)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
23	(0, 2, 2)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
24	(0, -2, 2)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
25	(0, 2, -2)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
26	(0, -2, -2)	5.20803	6.8708	0.19925	6.87369	1.66111	111.15209
27	(3, 1, 1)	6.10695	2.80514	-2.64703	3.85688	-43.33889	198.09282
28	(3, -1, 1)	6.10695	2.64703	2.80514	3.85688	46.66111	198.09282
29	(-3, 1, 1)	6.10695	2.64703	2.80514	3.85688	46.66111	198.09282
30	(-3, -1, 1)	6.10695	2.80514	-2.64703	3.85688	-43.33889	198.09282
31	(3, 1, -1)	6.10695	2.64703	2.80514	3.85688	46.66111	198.09282
32	(3, -1, -1)	6.10695	2.80514	-2.64703	3.85688	-43.33889	198.09282
33	(-3, 1, -1)	6.10695	2.80514	-2.64703	3.85688	-43.33889	198.09282
34	(-3, -1, -1)	6.10695	2.64703	2.80514	3.85688	46.66111	198.09282
35	(1, 3, 1)	6.10695	2.80514	-2.64703	3.85688	-43.33889	198.09282
24	(4, 5, 4)	( 10/05	2 ( 4702	0.00514	3.05(00	4/ //111	100.00000

#### Use Reduce icon to generate the multiplicity of the reflections.

#### Tool buttons icons structure factors dialogue

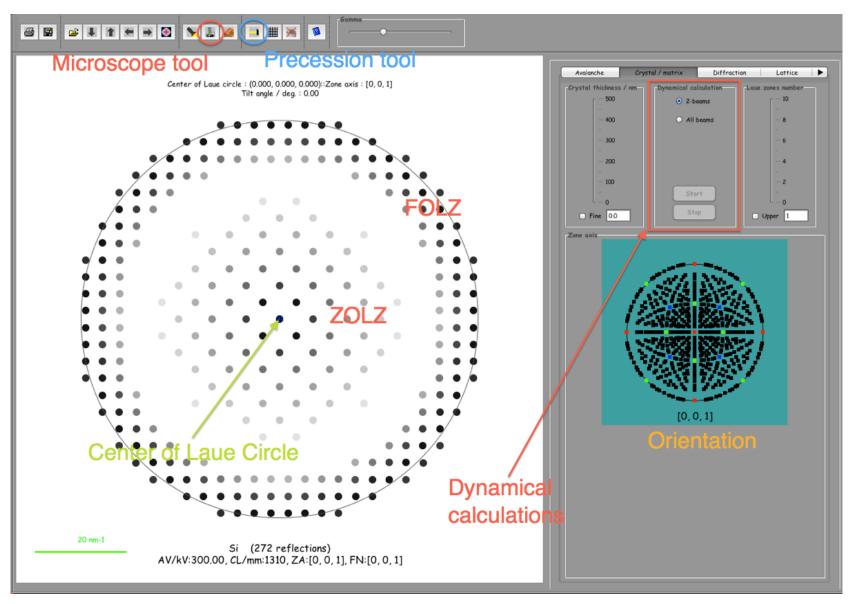


# Multiplicity

8	8 🖃 😣		1											
#	(h,k,l)	d* / nm-1	Vr / V	Vi / V	Ampli / V	Phase / Deg	Ext. / nm							
1	(0, 0, 0)	0.000	22,04901	0.7416	22.06148	1.92636								
8	(1, 1, 1)	3.18925	5.99687	6.2183	8.63885	46.03851	88.44134						,	
12	(2, 2, 0)	5.20803	6.8288	0.159	6.83066	1,33383	111.85234	h ma	1×.	5		3 6 9	12 15	
24	(3, 1, 1)	6.10695	2,78815	-2.64629	3.84403	-43.50469	198.75513				_	5 0 9	12 15	
6	(4, 0, 0)	7.36526	4.08513	0.12377	4.08701	1.73543	186.93735			_	-			$\sim$
24	(3, 3, 1)	8.02611	1.72516	1.84124	2.52317	46.86418	302.79852	k ma	18.	5 .				•
24	(4, 2, 2)	9.02057	2.95358	0.10605	2.95549	2.05641	258.50374				0	369	12 15	
8	(3, 3, 3)	9.56776	1.39135	-1.29023	1.89751	-42.8403	402.63353							
24	(5, 1, 1)	9.56776	1.29023	1.39135	1.89751	47.1597	402.63353						,	
12	(4, 4, 0)	10.41605	2,32818	0.0941	2.33009	2.31451	327.88263	l ma	ux,	5		3 6 9	12 15	•
48	(5, 3, 1)	10.89337	1.1245	-1.03409	1.5277	-42.60172	500.09381						12 15	
24	(6, 2, 0)	11.6455	1.9251	0.0849	1.92697	2.52507	396.46994							
24	(5, 3, 3)	12,07431	0.86275	0.94465	1.27933	47.59441	597.1713	Default	maximum spac	ing : 15.946 [nn	n-11			
8	(4, 4, 4)	12.75701	1.63906	0.07731	1.64088	2,70042	465.5881	Conduit	marman space		,			
24	(5, 5, 1)	13.14962	0.73832	0.81308	1.09828	47.75898	695.60967							
24	(7, 1, 1)	13.14962	0.81308	-0.73832	1.09828	-42,24102	695.60967							
48	(6, 4, 2)	13.77914	1,42274	0.07081	1.4245	2.84928	536.30451							
24	(5, 5, 3)	14,14341	0,71141	-0.64281	0.95881	-42,10044	796.78354		_					
18	(7, 3, 1)	14,14341	0.64281	0.71141	0.95881	47.89956	796.78354			(h,k,l	) number : 2	5		
5	(8, 0, 0)	14,73052	1.25182	0.06511	1.25351	2.97759	609.45083							
24	(7, 3, 3)	15.07182	0.62978	-0.56663	0.84717	-41.97871	901.76804							
2	(6, 6, 0)	15.62408	1.11251	0.06005	1.11413	3.08944	685.68855	Atomic Form						
24	(8, 2, 2)	15.62408	1.11251	0.06005	1.11413	3.08944	685.68855	•	•	•	0	۲	0	
3	(5, 5, 5)	15.94626	0.50415	0.56243	0.75531	48.12776	1011.43011	DTSB	EJK	PRDW	WK	WKc.	XRay	
18	(7, 5, 1)	15.94626	0.56243	-0.50415	0.75531	-41.87224	1011.43011	🗹 Relativ	istic correction	<ul> <li>Atomic</li> </ul>				
		Multip	licity											

Kinematically forbidden reflections are not tabulated (for example (2,0,0) structure factor is null but the reflection is observed dynamically).

#### SAED kinematical diffraction

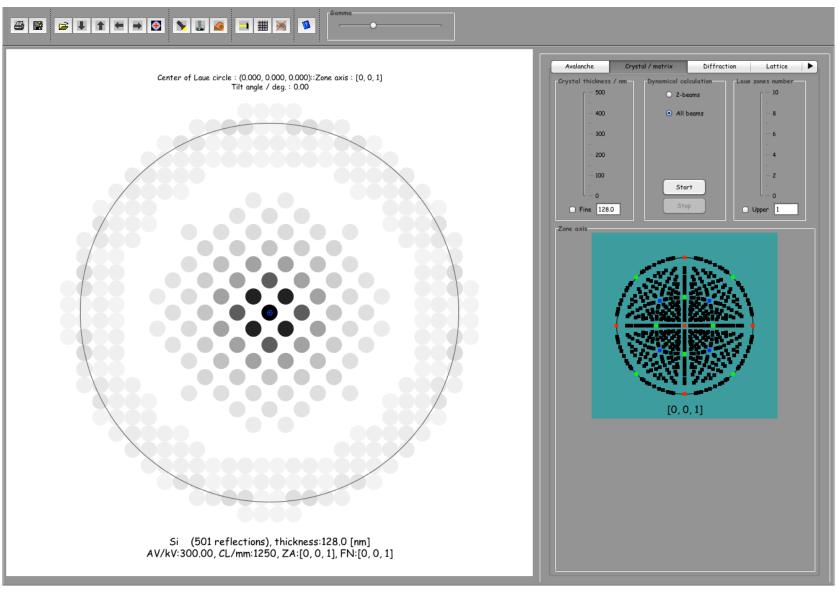


ZOLZ and FOLZ intensities are scaled independently.

Use check box X LZ colours of tab Options to define the same scale for all Laue zone reflections. Tab Options allows to add Kikuchi lines, HOLZ lines, colors, etc to the plot.

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## SAED dynamical diffraction



**Dynamical SAED** 

Dynamical SAED pattern are calculated using the Blochwave approach. Select tab Crystal/Matrix, radio button  $\odot$  All beams and Start. Change the crystal thickness using the thickness slider.

Two methods:

- Image calculations using Blochwave approach.
  - 1. Best for crystal of small unit cell.
  - 2. Easy calculations for low symmetry [uvw] directions.
  - 3. High order Laue zone effects simple to introduce.
- Image calculations using Multislice approach (Physical optics & periodic continuation).
  - 1. Best for crystal of large unit cell or for defects imaged in high symmetry orientation (i.e. [001]).
  - 2. May require a unit cell transformation to slice crystal  $\perp$  [uvw].
  - 3. Slices must be of the order of 50  $\lambda$ .

 $\mathsf{Imaging} \Longrightarrow \mathsf{Blochwave}$ 

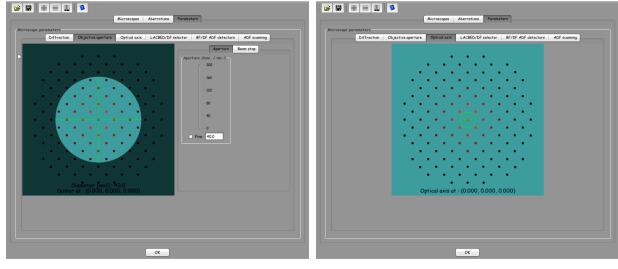
**Imaging**  $\implies$  **Multislice** : how to calculate a map of HRTEM images?

#### Select the microscope: **Parameters** $\implies$ **Microscope**

Reverges Aberrations Parameters	Image:
Microscopes Abernations Parameters	Microscopes Abernations Parameters
◀ Jeol 2100F Cs Jeol 3010 Jeol 4000 EX Topcon 0028 Titan 80-300	Oth order 1st order
FEI Titan 80-300 Cs corrected	$C_c (Cc   W_{00}) [mm] 2.0$
● 50 kV ● 100 kV ● 150 kV ● 200 kV ● 250 kV ● 300 kV	Amplitude C <sub>01</sub> ( I   W <sub>11</sub> ) [nm] 0.0 0.0
Acc. volt. / kV 300.000 0 312.5 625 937.5 1250 • ++	W00: Cc
	$C_{12} (A_1   W_{22}) [nm] = 0.0$
Cc / mm 2000	C <sub>21</sub> (3B <sub>2</sub>   W <sub>31</sub> ) [rm] 0.0 0.0
0 2 4 6 8 10	C <sub>23</sub> ( A <sub>2</sub>   W <sub>33</sub> ) [rm] 0.0 0.0
Cs/mm -0030	C <sub>30</sub> (C <sub>3</sub>   W <sub>40</sub> ) [mm] -0.03
-2 0 2 4 6 8	C <sub>32</sub> (45 <sub>3</sub>   W <sub>42</sub> ) [µm] 0.0 0.0
C5 / mm 5.00	C <sub>34</sub> (A <sub>3</sub>  W <sub>44</sub> )[µm] 0.0 0.0
C5 / mm 5.00	31. 3 44 5 . 00
Defocus / nm -9.42	
	Reset
Ener.spread / eV 0.60 0 1 2 3 4 5	
Lens stability / ppm 1.00 0 4 8 12 16 20	
Voltage stability / ppm 1.00 0 4 8 12 16 20	
ОК	OK
-h	

Select a microscope. When not available, edit a new one +

Aberrations: order selected using **Parameters**  $\implies$  **Preferences**.



Objective aperture diameter  $\geq$  information transfer.

Optical axis can be moved to simulated dark field images.

# Open the multislice dialogue: $Imaging \implies Multislice$

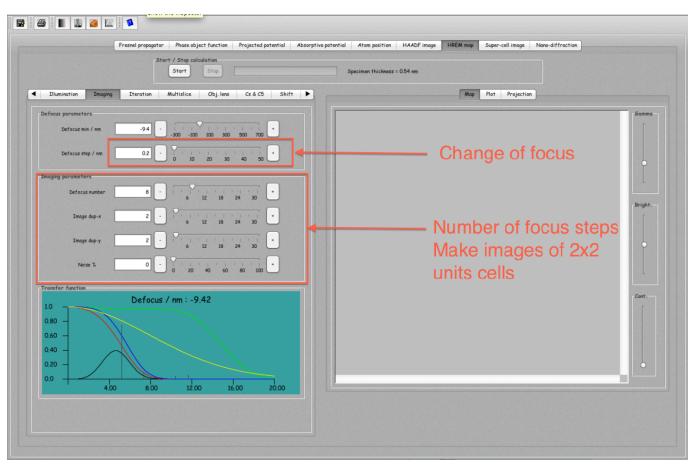
	Fresnel propagator       Phase object function       Projected potential       Absorptive potential       Atom position       HAADF image       HREM map       Super-cell image       Nano-diffraction         Start       Stop       Specimen thickness = 0.54 nm       Specimen thickness = 0.54 nm       Specimen thickness = 0.54 nm							
Illumination Im	noging Iteration Multislice Obj.lens Cs & C5 Shift	Map Plot Projection						
Illumination model O Coherent	⊙ O Envelope TCC	Gen						
Half-conv. / mrad - 100 - 80 - 60 - 40 - 20 - 20 - 0 Fine 1.0 Transfer function	Defocus spread / nm - 50 - 40 - 30 - 20 - 10 - 10 - 50 - 20 - 20 - 50 - 40 - 30 - 20 - 50 - 40 - 30 - 50 - 40 - 30 - 50 - 40 - 30 - 50 - 40 - 50 - 40 - 50 - 40 - 50 - 5	Image formation						
1.0 0.80 - 0.60 - 0.40 - 0.20 - 0.0	Defocus / nm : -9.41 4.00 8.00 12.00 16.00 20.00							

HRTEM image calculation by multislice approach.

The HRTEM map tab is augomatically selected.

Select  $\odot$  Envelope in order to introduce effects of partial spatial and temporal coherence.

# Select the Imaging tab

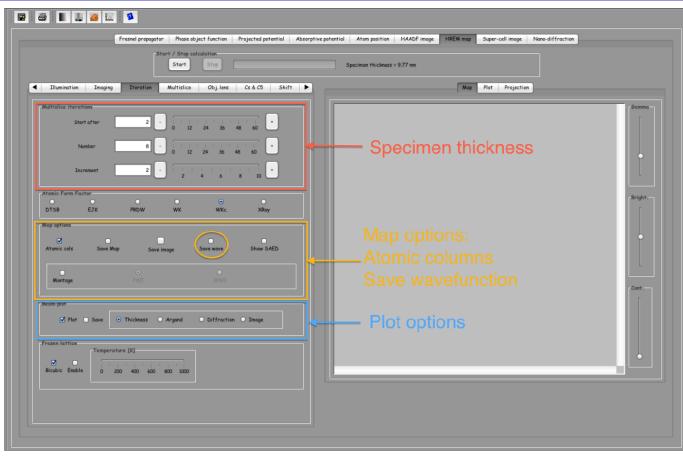


HRTEM image calculation by multislice approach.

Imaging tab sets:

- 1. The defocus between two images of a defocus series and the defocus of the first image (defocus increases).
- 2. The defocus series size.
- 3. The image duplication.

#### Select the Iteration tab

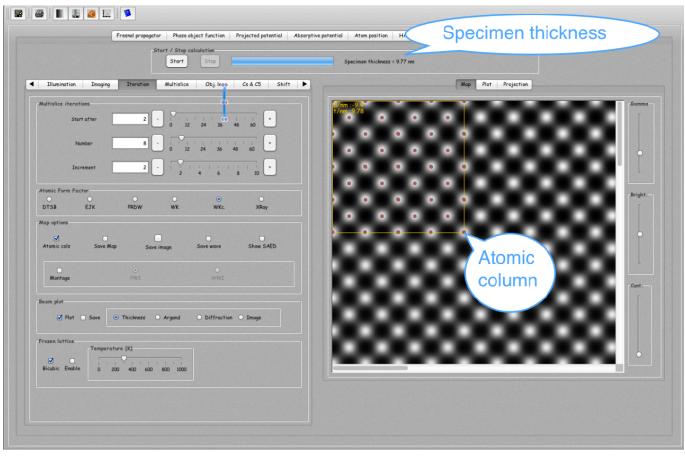


HRTEM image calculation by multislice approach.

Iteration tab sets:

- 1. The minimum thickness of the specimen (Start after).
- 2. The number of thickness steps.
- 3. The thickness between two defocus series images.
- 4. The total specimen thickness is displayed.

# Push Start

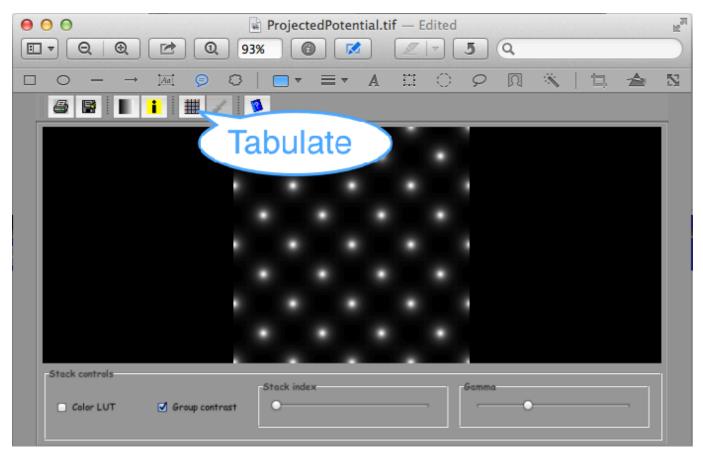




Notice that:

- 1. X Atomic cols generates cursor mask showing the position of the atomic columns.
- 2. X Plot generates plots of beam amplitude and phase as a function of specimen thickness.

#### Projected potential

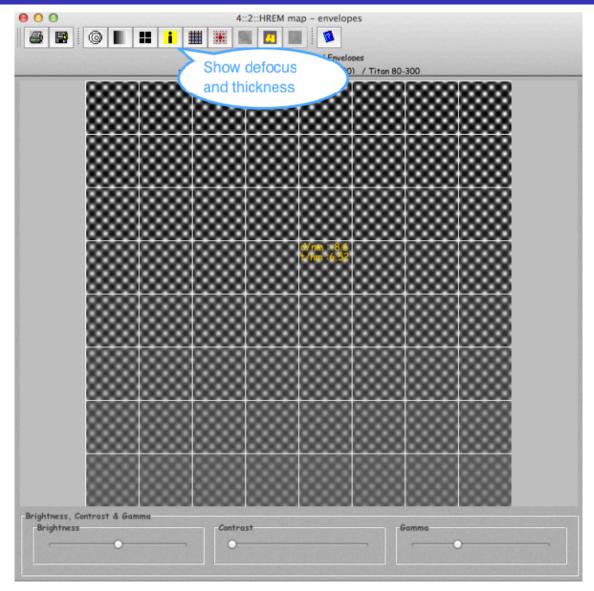


Projected potential of the slice.

Notice that:

► A table of the projected potential can be displayed, printed and exported to Mathematica.

## HREM map



Specimen thickness and defocus are displayed for each image.

Notice that:

Images are made of 2 x 2 unit cells.

#### Interactive image calculation and display

F	resnel propagator Phase object function Projected potential Absorptive Start / Stop calculation	potential Atom position HAADF image HREM map Super-cell image Nano-diffraction	
	Start Stop	Specimen thickness = 9.77 nm	
Illumination Imaging	Iteration Multislice Obj. lens Cs & C5 Shift 🕨	Map Plot Projection	
Multislice iterations Start after Number Increment Atomic Form Factor DTSB EJK Map options Atomic cols Sove Map	2 0 12 24 36 48 60 0 8 0 12 24 36 48 60 0 2 0 12 24 36 48 60 0 2 0 12 24 6 8 10 0 PRDW WK WKc XRoy Sove image Sove wave Show SAED	Curve si::Thickness : 0.54309 Plot 9.0::Intensity Out of the second seco	Gamma ( Bright -
Montage Beam plot	WVI WWI Thickness O Argand O Diffraction O Image		Cent.

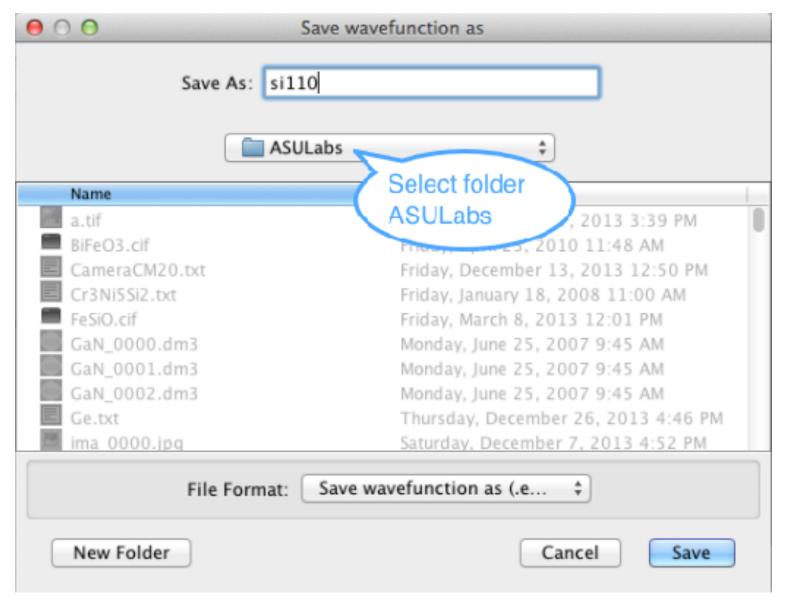
Select  $\odot$  Image and Plot and change specimen thickness.

Notice that:

- 1. Defocus is set in the Imaging tab as well as image size.
- 2. Most important aberrations can be varied in the Obj. lens tab.

## Iteration tab and $\odot$ Save wave

Redo the map calculation with the  $\odot$  Save wave radio button selected. You will be asked to name the wavefunctions.



Saving the wave functions for further imaging.

# Select Imaging $\implies$ HRTEM

⊖ ○ O Load way	vefunction			
ASULabs	÷			
Name 🔺	Date Modified			
4% si110TEM_0000.ems	Wednesday, January 1, 2014 3:33 PM			
🛱 si110TEM_0001.ems	Wednesday, January 1, 2014 3:33 PM			
印 si110TEM_0002.ems	Wednesday, January 1, 2014 3:33 PM			
印 si110TEM_0003.ems	Wednesday, January 1, 2014 3:33 PM			
<sup>학</sup> 5 si110TEM_0004.ems	Wednesday, January 1, 2014 3:33 PM			
🛱 si110TEM_0005.ems	Wednesday, January 1, 2014 3:33 PM			
<b>Fig</b> sil10TEM_0006.ems	Wednesday, January 1, 2014 3:33 PM			
5 sil10TEM_0007.ems	Wednesday, January 1, 2014 3:33 PM			
<b>Fig</b> si110TEM_0008.ems	Wednesday, January 1, 2014 3:33 PM			
Fig silloTEM_0009.ems	Wednesday, January 1, 2014 3:33 PM			
Sill1.txt	Sunday, December 29, 2013 5:11 PM			
Sill1.txtNANODIFF_0000.ems	Sunday, December 29, 2013 5:14 PM			
Si111.txtNANODIFF_0001.ems	Sunday, December 29, 2013 5:14 PM			
File Format: Load wavefunction (.ems) ‡				
Cancel Open				
Load a wave function.				

a 🗟 😫 🛋 📕 🎩 🕸			
Controls  Abernations Coherence Dark field Defocu	s DefocusSeries Drift å Noise Imaging Microscope 🕨	Wavefunction display	
	s Derocusseries Drift a Noise Intiging Microscope P	O Real	• Imaginary
		Amplitude     Positive	<ul> <li>Phase</li> <li>Negative</li> </ul>
✓ 2nd order 3rd order ►	C <sub>c</sub> ( Cc   W <sub>00</sub> ) [mm] 2.0		C rugania
Amplitude Angle	C <sub>01</sub> (I   W <sub>11</sub> ) [nm] 0.0 0.0		Image CTF Wavefunction
W20: Z W22: A1	$c_{10} (\mathbf{Z}   \mathbf{W}_{20}) [rm]$ 20.0		0.7755105 defecus: 20.0 Tetensity
1 1	$c_{12} (A_1   W_{22}) [mm] 0.0 0.0$	Show the image	s - s, r adroca - co, a - the birly
	C <sub>21</sub> (38 <sub>2</sub>   W <sub>31</sub> ) [rm] 0.0 0.0		
		Charles and the second	
•	$c_{23} (A_2   W_{33}) [mm] 0.0 0.0$		00000000
	$c_{30} (c_3   W_{40}) [mm]$ -0.03	0000	00000000
	C <sub>32</sub> (4S <sub>3</sub>   W <sub>42</sub> ) [µm] 0.0 0.0	0.000	100000000
	C <sub>34</sub> ( A <sub>3</sub>   W <sub>44</sub> ) [µm] 0.0 0.0	640404	
		0000	00000000
			0000000000
Formula	1 (.2		
Reset	$\frac{1}{2} \left( u^2 + v^2 \right) \lambda$	0.000	
		(0,0)	
			000000000
		040404	00000000
		040404	000000000
		2000	00000000
			— (1,0,0)
		Min : 0.584559	5, max : 1.0276718, contrast : 0.08955503

Imager: HRTEM image.

The imager dialogue allows to change interactively many HRTEM imaging parameters.

# Imager dialogue: wavefunction

Controls           Aberrations         Coherence         Dark field         Defocus         DefocusSeries         Drift & Noise         Imaging         Microscope         Imaging	Wavefunction display
	Real     O Imaginary     Amplitude     Phase
	Amplitude     Phase     Positive     Negative
✓ 2nd order 3rd order ► C <sub>e</sub> ( Cc   W <sub>00</sub> ) [mm] 2.0	
Amplitude         Angle         C <sub>01</sub> ( I   W <sub>11</sub> ) [rm]         0.0         0.0	Image CTF Wavefunction
W20: Z W22: A1 C <sub>10</sub> (Z   W <sub>20</sub> ) [rm] 20.0	
C <sub>12</sub> (A <sub>1</sub>   W <sub>22</sub> ) [nm] 0.0 0.0	
$C_{21} (3B_2   W_{31}) [nm] 0.0 0.0$	
$C_{23} (A_2   W_{33}) [m] 0.0 0.0$	
$c_{30} (c_3   W_{40}) [mm] = 0.03$	
$C_{32}(4S_3   W_{42}) [ \mu m ] 0.0 0.0$	
C <sub>34</sub> ( A <sub>3</sub>   W <sub>46</sub> ) [µm] 0.0 0.0	
Formula	
Reset $\frac{1}{2} (u^2 + v^2) \lambda$	

Imager: wavefunction.

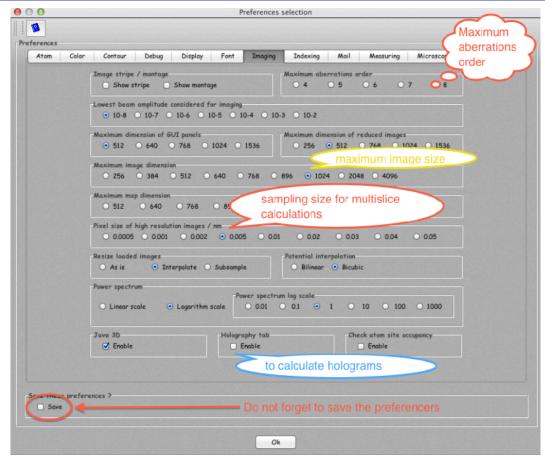
#### Interactive imaging: Stobbs factor

0	HREM imager::si::[0, 0, 1]::(0.000, 0.000, 0.000)::Titan 80-300	0   FEI Titan 80-300 Cs corrected   300.0	
🔛 🛩 📗 🞩	1		
ols Camera MTF Aberrat	tions Coherence Dark field Defocus DefocusSeries Drift & Noise Imaging 🕨	O Real O Amplitude	<ul> <li>Imaginary</li> <li>Phase</li> </ul>
	Cameras MTF/PSF	• Positive	<ul> <li>Negative</li> </ul>
	Default comera		Image CTF Wavefunction
	O Pixel size [µm] 24 Rows 1024 Columns 1024		ckness : 9.7756195, defocus : -9.0::Intensity
	MSC		
	Pixel size [µm] 24 Rows 1024 Columns 1024		
	<b>* * = *</b>		
		(0, <mark>1,0</mark> )	~~~
	Load camera MTF		
TEM			$\sim \sim \sim$
Magnifica	ation (ASULabs/cameraMTF	txt	~~~~
Options			~~~~
Show MTF	Show properties		(1.0,0)
Image properties Minimum : 0.1466	654 Maximum : 2.14146 Mean : 0.805143 Contrast : 0.499234		

Taking into account the camera MTF.

To see the contrast attenuation due to the camera MTF, change the microscope magnification.

# Wavefront aberrations: **Parameters** $\implies$ **Preferences**

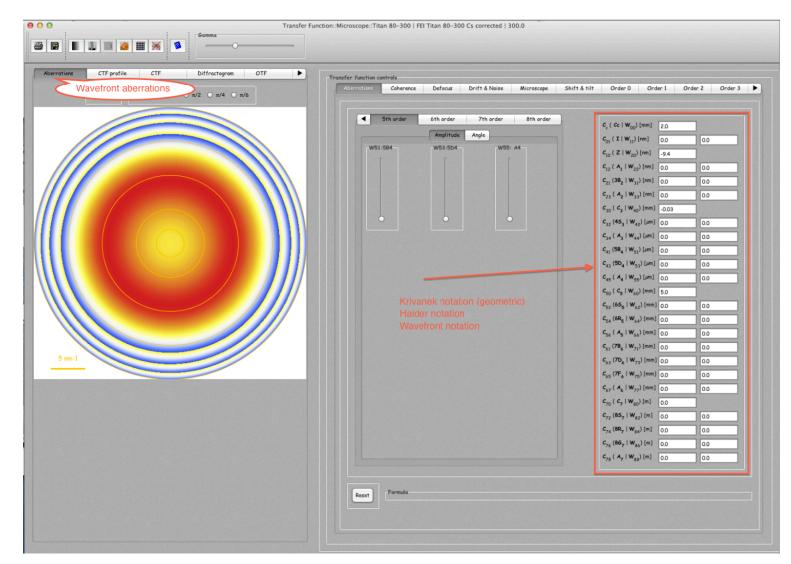


Selecting the wavefront aberrations order.

jems can display aberrations to 8<sup>th</sup> order. The order is selected in Imaging tab. This tab sets several imaging parameters. The most important are:

- 1. Pixel size (should not be ¿0.01 nm).
- 2. Java 3D (should be enable when OpenGL is installed).
- 3. Lowest beam amplitude considered for imaging ( $10^{-6}$  usually).

# Wavefront aberrations: **Drawing** $\implies$ **Transfer fucntion**



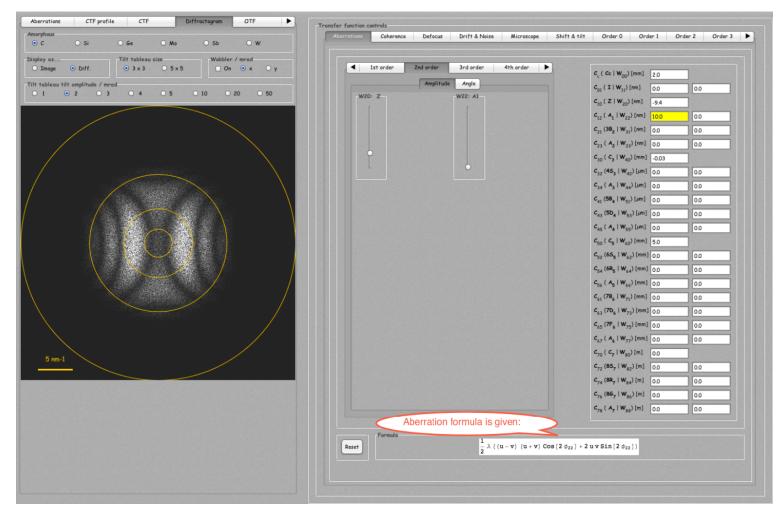
Dialogue to display wavefront aberration, CTF profile, CTF, Diffractogram, ...

#### Wavefront aberrations: 2-fold astigmatism

$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	
Aberrations       CTF profile       CTF       Diffractogram       OTF       Image         Amarphass $\odot$ C       Si       Ge       Ma       SS       W         Display es       Tilt tableau size       Wabler / mrad       On $\odot$ x       Y         Tilt tableau tilt amplitude / mrad       On $\odot$ x       Y         VIII tableau tilt amplitude / mrad       On $\odot$ x       Y         VIII tableau tilt amplitude / mrad       On $\odot$ x       Y         VIII tableau tilt amplitude / mrad       On $\odot$ x       Y         VIII tableau tilt amplitude / mrad       On $\odot$ x       Y         O I       2       3       4       5       10       20       50	
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1 🗅 📥
Amerphass         O C       Si       Ge       Mo       Sb       W         Display as       Tilt tableau size       Wabbler / mrad       On       Ox       Y         Tilt tableau tilt amplitude / mrad       On       Ox       Y         Tilt tableau tilt amplitude / mrad       On       Ox       Y         W20:       Z       W22:       All       V       Ox         W20:       Z       W22:       V       W22:       C <sub>1</sub> C <sub>1</sub> C <sub>1</sub> C <sub>10</sub> C 1       V       Ox       Ox       Ox       Ox       Ox       C <sub>10</sub> <	
$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Order 3
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	
Amplitude	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	
C <sub>12</sub> (A,  W <sub>22</sub> ) [m] 100 00	
SATTORIZARI COMPANYARIA CARACTERIA CARACTERIA	
10 nm 2 fold 00 00	
astigmatism	
C <sub>30</sub> (C <sub>3</sub> [W <sub>40</sub> )[mm] _0.03	
C <sub>22</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> (98 <sub>4</sub>   W <sub>51</sub> )[ <i>m</i> ] 0.0 0.0	
C <sub>43</sub> (50 <sub>4</sub>   W <sub>53</sub> ) [µm] 00 00	
G <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] 50	
C <sub>52</sub> (65 <sub>5</sub>   W <sub>62</sub> ) [mm] 0.0 0.0	
C <sub>s4</sub> (64 <sub>5</sub>   W <sub>s4</sub> ) [mm] 00 00	
$c_{ss}(A_{s} W_{ss})$ [m] $0.0$ 0.0	
C <sub>s1</sub> (77B <sub>6</sub>   W <sub>71</sub> )[mm] 0.0 0.0	
$C_{s3} (7D_{s}   W_{73}) [mm]_{00}$ 0.0	
$C_{65}(TF_6   W_{75}) [mm] 0.0 0.0$	
$c_{bT}(A_b   W_{TT}) [mm] 0.0 0.0$	
$C_{70}(C_{7}   W_{00}) [m] = 0.0$	
C <sub>72</sub> (85 <sub>7</sub>   W <sub>82</sub> ) [m] 0.0 0.0	
C <sub>74</sub> (8R <sub>2</sub>   W <sub>34</sub> ) [m] 0.0 0.0	
$\begin{array}{c} c_{7_{5}}(86_{7}   w_{ac})(m) & 0.0 & 0.0 \\ c_{7_{5}}(4_{7}   w_{ac})(m) & 0.0 & 0.0 \\ \end{array}$	
C <sub>76</sub> (A <sub>7</sub>   W <sub>80</sub> ) [m] 00 00	
Formda	
Reset $\frac{1}{2} \lambda ((u - v) (u + v) \cos [2 \phi_{22}] + 2 u v \sin [2 \phi_{22}])$	

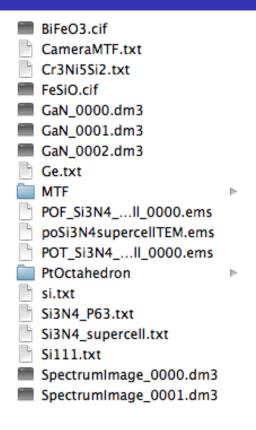
10 nm 2-fold astigmatism (Krivanek:  $C_{12}$ , Haider  $A_1$ , Wavefront  $W_{22}$ ).

#### Diffractogram: 2-fold astigmatism



10 nm 2-fold astigmatism (Krivanek:  $C_{12}$ , Haider  $A_1$ , Wavefront  $W_{22}$ ).

# ASULabs folder



The ASULabs folder contains:

- 1. .cif files (BiFeO3 and FeSiO crystal structures).
- 2. MTF folder with .dat files for determining the camera MTF (1024, 1024, signed short, Little endian).
- 3. Gatan images (.dm3)
- 4. Si3N4 unit cell and super-cell.
- 5. Folder PtOctahedron with a large super-cell cut into  $\approx$  0.2 nm slices (PtOct\_0000.txt, ...).

# Suggestions 1

I suggest you:

- 1. Open the Si3N4.txt crystal file (**File**  $\implies$  **Open**).
- 2. Display the structure in 3-D (**Drawing**  $\implies$  **Perspective**).
- 3. Display the SAED pattern (**Drawing**  $\implies$  **Diffraction**).
- 4. Do HRTEM image simulation (Imaging  $\implies$  Multislice) or (Imaging  $\implies$  Blochwave).
- 5. Open the Si3N4\_supercell.txt crystal file (File  $\implies$  Open).
- 6. Display the structure in 3-D (**Drawing**  $\implies$  **Perspective**).
- 7. Display the SAED pattern (**Drawing**  $\implies$  **Diffraction**).
- 8. Do HRTEM image simulation (Imaging  $\implies$  Multislice) using tab Super-cell image. In tab Multislice have the radio buttons  $\odot$  Load phase-object and  $\odot$  Save phase-object set.

Make sure that aberrations are reset!

Remember that any drawing or table has its own popup menu and that a tip text is attached to any control.

I suggest also that you:

- Open the PtOct\_0000.txt crystal file (of folder PtOctahedron) (File ⇒ Open). It contains the atoms position of the first slice of a large model (Pt octahedron model by Prof. Ernst).
- 2. Do HRTEM image simulation (Imaging  $\implies$  Multislice) using tab Super-cell image.
- 3. Add to the super-cells table all the other slices using ++. You can display the model made of the stack of slices.
- Make sure that ⊙ Save of tab Iteration-Wavefunction is selected. To see an image after each slice have the ⊙ Show image <sup>2</sup> of tab Iteration selected.
- 5. Select the first slice of the table (PtOct\_0000.txt). Start the calculation (Start). You will be asked to give a name to the wavefunctions files.
- Load the last wave function in the HRTEMImager (Imaging ⇒ HRTEMImager. Change the imaging parameters in order to how aberrations affect HRTEM images.

<sup>&</sup>lt;sup>2</sup>You can close all the images using **Window**  $\implies$  **Close All**.

# Documentation jemsLinux64.zip jemsMacOSX.mpkg.pkg.zip jemsWindows7.zip jemsWindowsXP.zip

- Copy the .zip file compatible with your PC operating system.
- Do not open it, but use Extract All in order to unzip the file.

#### Extracting jems

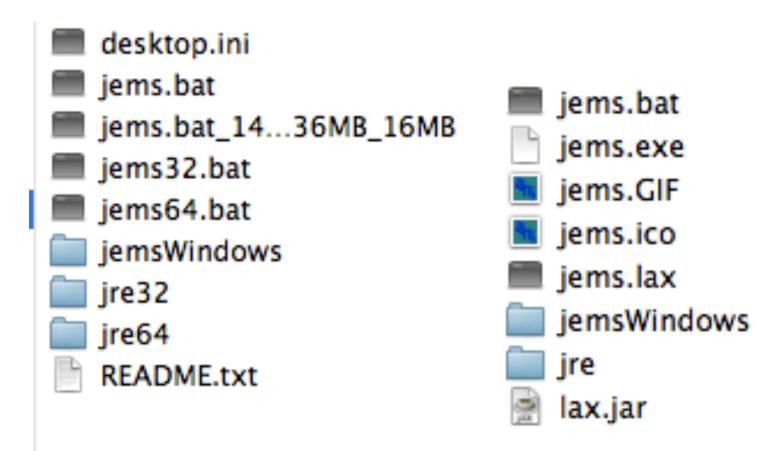


Figure: Windows 7 or 8 version: jems started either using jems32.bat or jems64.bat depending on Windows being 32 or 64 bits.

Figure: Windows XP (only 32 bits).

For Windows 7 after having determine the version 32 (or 64) copy jems32.bat (or jems64.bat) to jems.bat. jems modifies jems.bat.