

Diffraction and Image Simulation Laboratory Notes

2019 CCEM Summer School on Electron Microscopy
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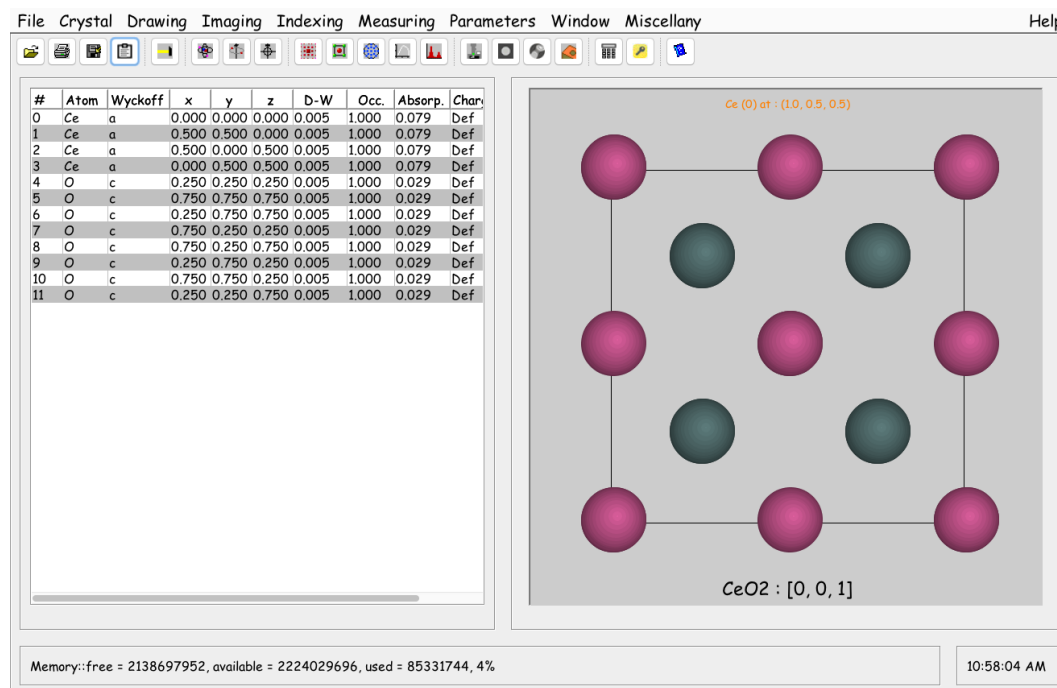
May 15, 2019

Starting jems

Start jems ¹ with this icon:



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



The screenshot shows the JEMS software interface. The top menu bar includes File, Crystal, Drawing, Imaging, Indexing, Measuring, Parameters, Window, Miscellany, and Help. Below the menu is a toolbar with various icons. The main window is divided into two panels. The left panel contains a table of atom positions:

#	Atom	Wyckoff	x	y	z	D-W	Occ.	Absorp.	Char.
0	Ce	a	0.000	0.000	0.000	0.005	1.000	0.079	Def
1	Ce	a	0.500	0.500	0.000	0.005	1.000	0.079	Def
2	Ce	a	0.500	0.000	0.500	0.005	1.000	0.079	Def
3	Ce	a	0.000	0.500	0.500	0.005	1.000	0.079	Def
4	O	c	0.250	0.250	0.250	0.005	1.000	0.029	Def
5	O	c	0.750	0.750	0.750	0.005	1.000	0.029	Def
6	O	c	0.250	0.750	0.750	0.005	1.000	0.029	Def
7	O	c	0.750	0.250	0.250	0.005	1.000	0.029	Def
8	O	c	0.750	0.250	0.750	0.005	1.000	0.029	Def
9	O	c	0.250	0.750	0.250	0.005	1.000	0.029	Def
10	O	c	0.750	0.750	0.250	0.005	1.000	0.029	Def
11	O	c	0.250	0.250	0.750	0.005	1.000	0.029	Def

The right panel shows a [001] projection of the unit cell. It features a 3x3 grid of pink spheres representing Cerium (Ce) atoms and a 2x2 grid of dark green spheres representing Oxygen (O) atoms. The text 'Ce (0) at : (1.0, 0.5, 0.5)' is displayed above the grid, and 'CeO2 : [0, 0, 1]' is displayed below the grid. At the bottom of the window, there is a status bar showing memory usage: 'Memory::free = 2138697952, available = 2224029696, used = 85331744, 4%' and the time '10:58:04 AM'.

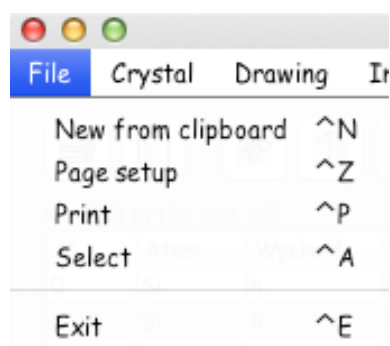
Main jems window, atoms position (left panel) and [001] projection of the unit cell (right) of default crystal structure.

¹<http://www.jems-saas.ch>

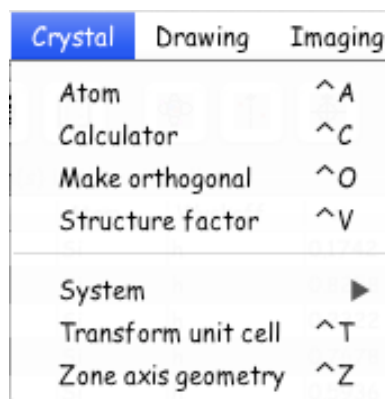
jems MenuBar: part 1

File Crystal Drawing Imaging Indexing Measuring Parameters Window Miscellany

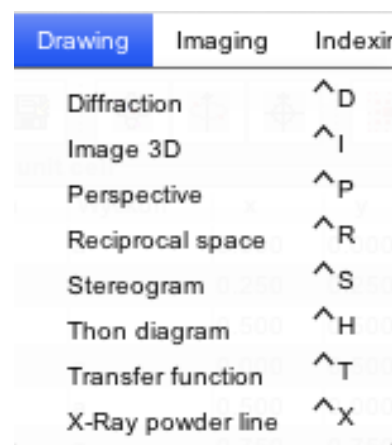
jems MenuBar.



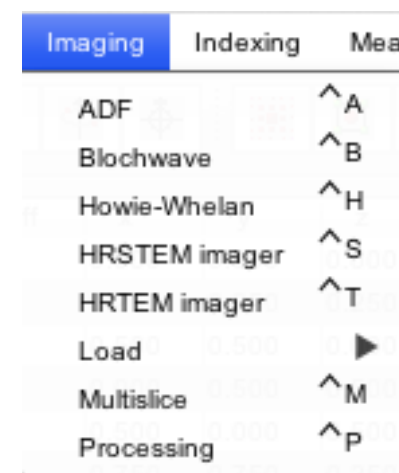
File menu: to select a crystal structure.



Crystal menu: to define crystal structures.

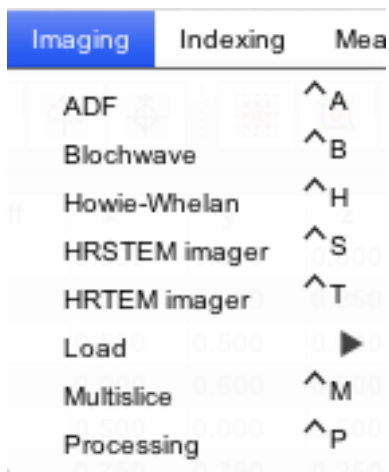


Drawing menu: to draw crystal structures, diffraction patterns.



Imaging menu: to perform Blochwave or multislice calculations.

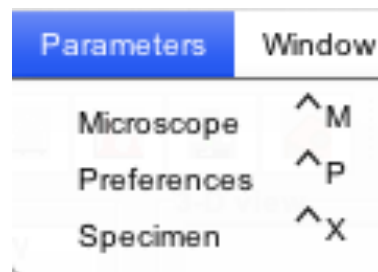
jems MenuBar: part 2



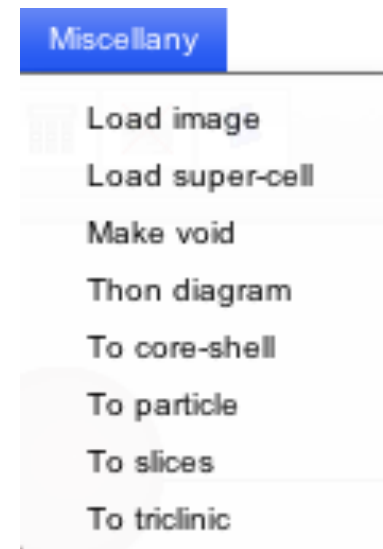
Indexing menu: to index diffraction patterns.



Measuring menu: to measure camera MTF, specimen thickness.



Parameters menu: to configure jems, define microscope or specimen properties.

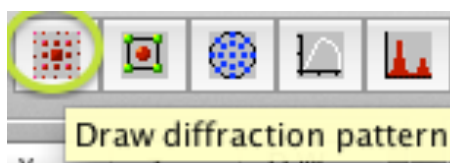


Miscellany menu: to load or create super-cells.

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:



Main window left panel

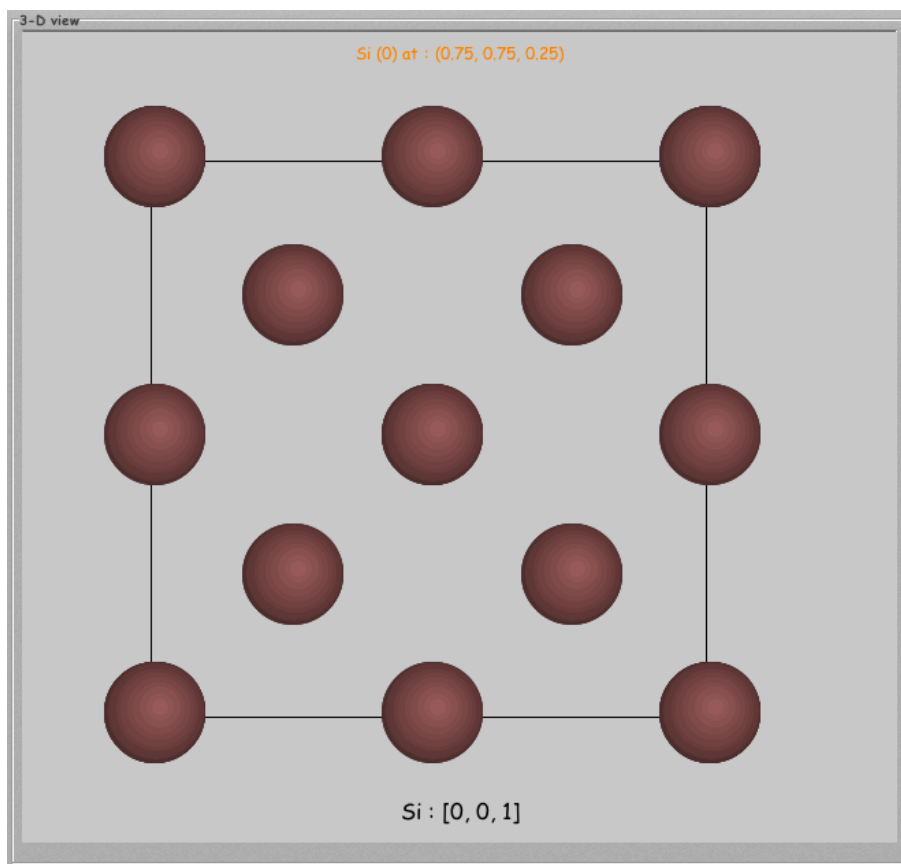
#	Atom	Wyckoff	x	y	z	D-W	Occ.	Absorp.	Charge	AFF
0	Si	a	0.000	0.000	0.000	0.0049	1.000	0.029	Def	0
1	Si	a	0.250	0.250	0.250	0.0049	1.000	0.029	Def	0
2	Si	a	0.500	0.500	0.000	0.0049	1.000	0.029	Def	0
3	Si	a	0.000	0.500	0.500	0.0049	1.000	0.029	Def	0
4	Si	a	0.500	0.000	0.500	0.0049	1.000	0.029	Def	0
5	Si	a	0.750	0.750	0.250	0.0049	1.000	0.029	Def	0
6	Si	a	0.250	0.750	0.750	0.0049	1.000	0.029	Def	0
7	Si	a	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.

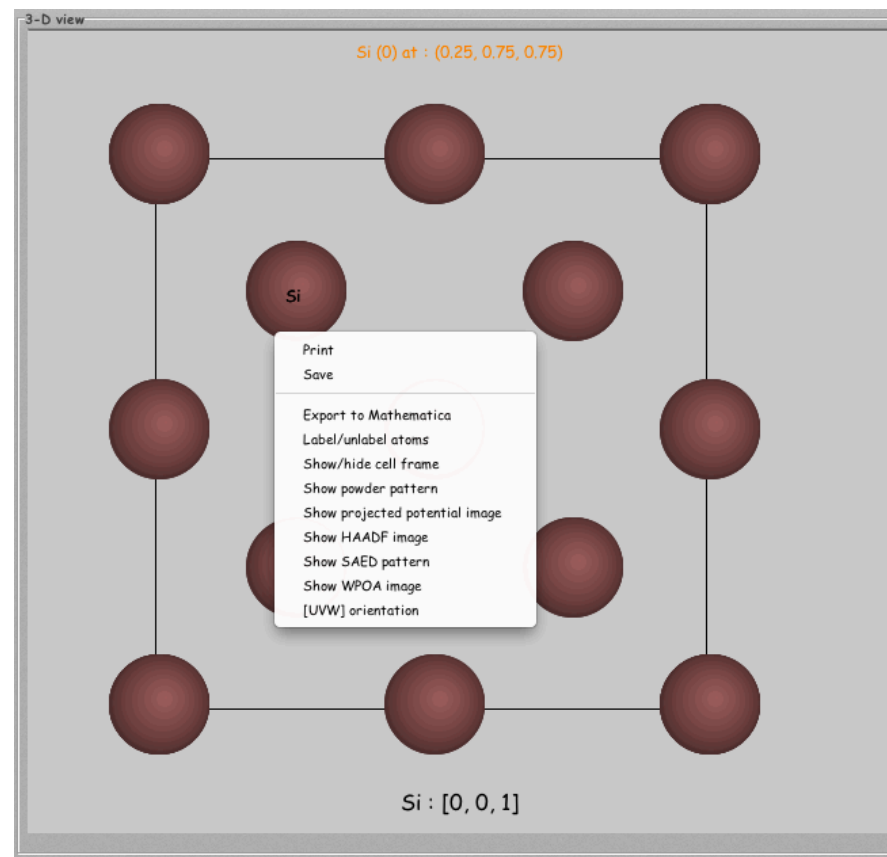
With the alternate non-centric $Fd\bar{3}m$ space group the Si structure contains 8 atoms. Only the atom at Wyckoff position a, $(x, y, z) = (0, 0, 0)$, must be defined. All the other atom positions are generated by the symmetry operations of the space-group.

- ▶ 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 $[\text{nm}^2]$
- ▶ 1.000: site occupancy $[0, 1[$.
- ▶ 0.029: absorption coefficient.
- ▶ Def: charge.
- ▶ 0: Atomic Form Factor source (Doyle-Turner or Smith-Burge).

Main window right panel



The right panel shows a projection of a silicon unit cell. Note that all atoms of the FCC Bravais lattice are shown.

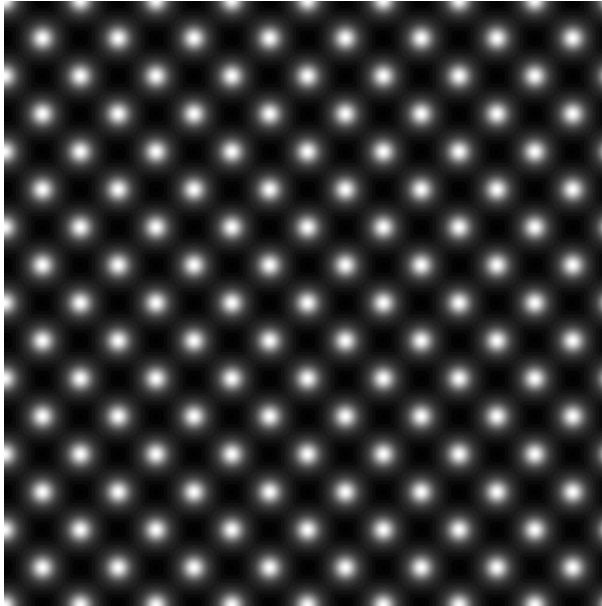


A mouse click on an atom position labels the atom and a right mouse click displays a popup menu (Ctrl-mouse click on Mac OSX).

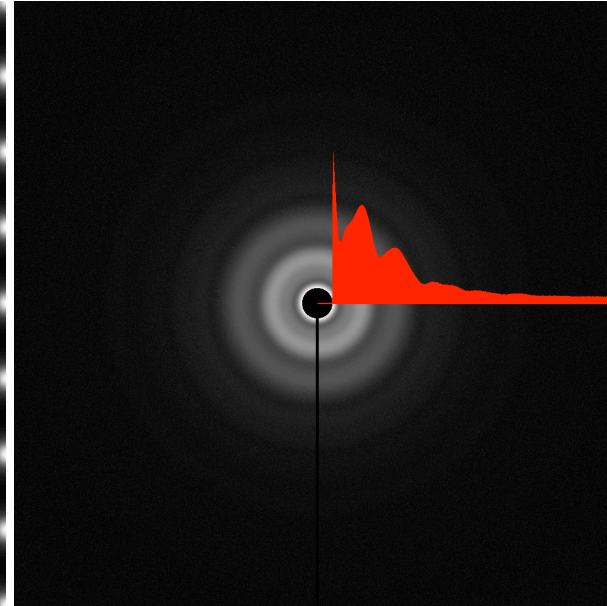
Note that a popup menu is attached to many drawings and tables. The popup menu of the right panel allows to:

- ▶ 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



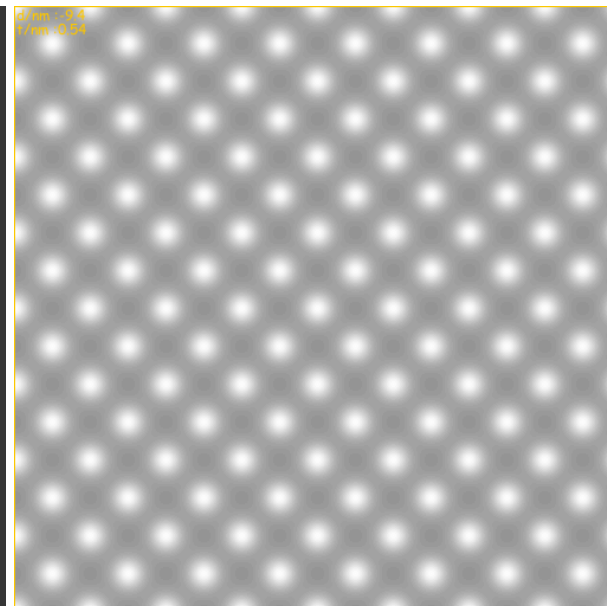
Si HAADF (FEI Titan pico).



Si powder pattern (randomly oriented Si unit cell).



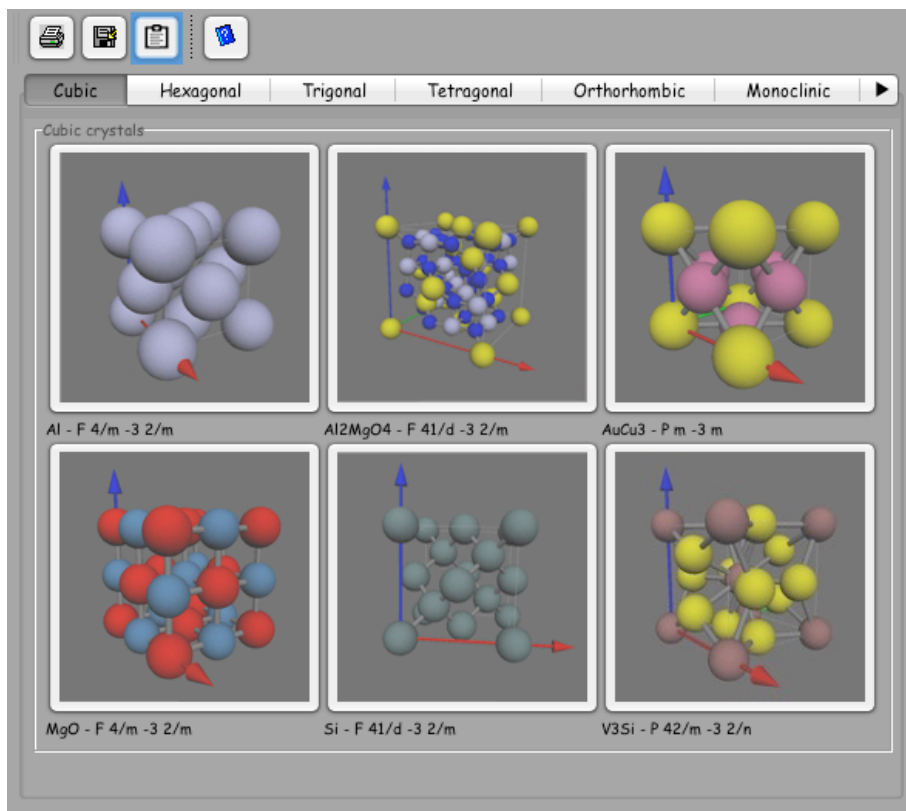
Si [001] kinematical selected area diffraction pattern.



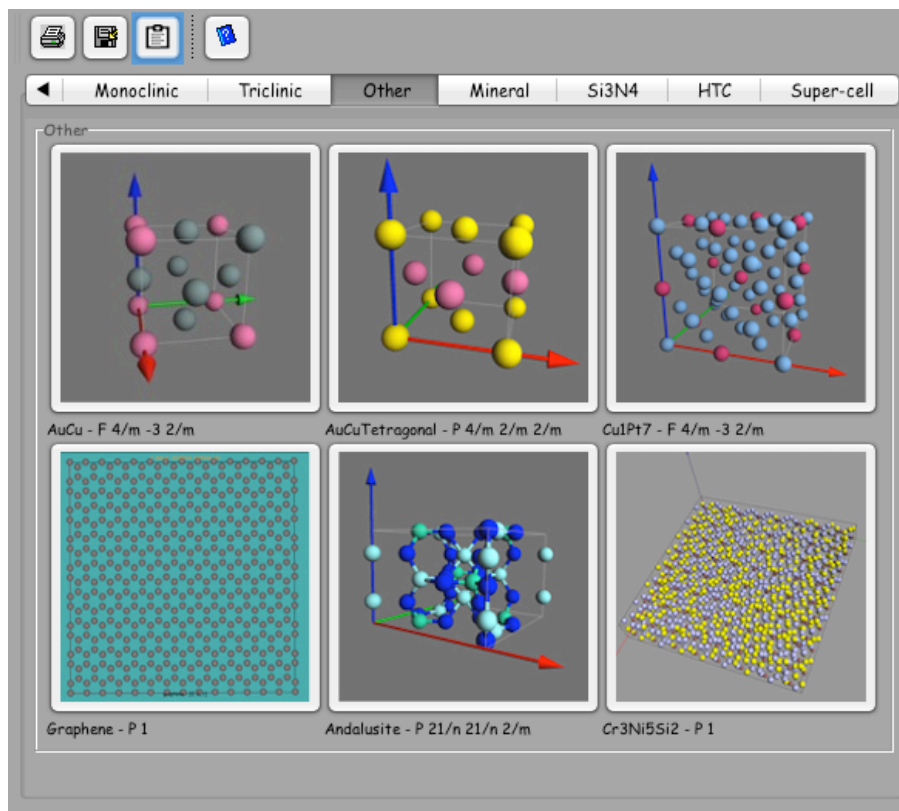
Si HRTEM image (WPOA) approximation.

jems student edition crystal structures

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

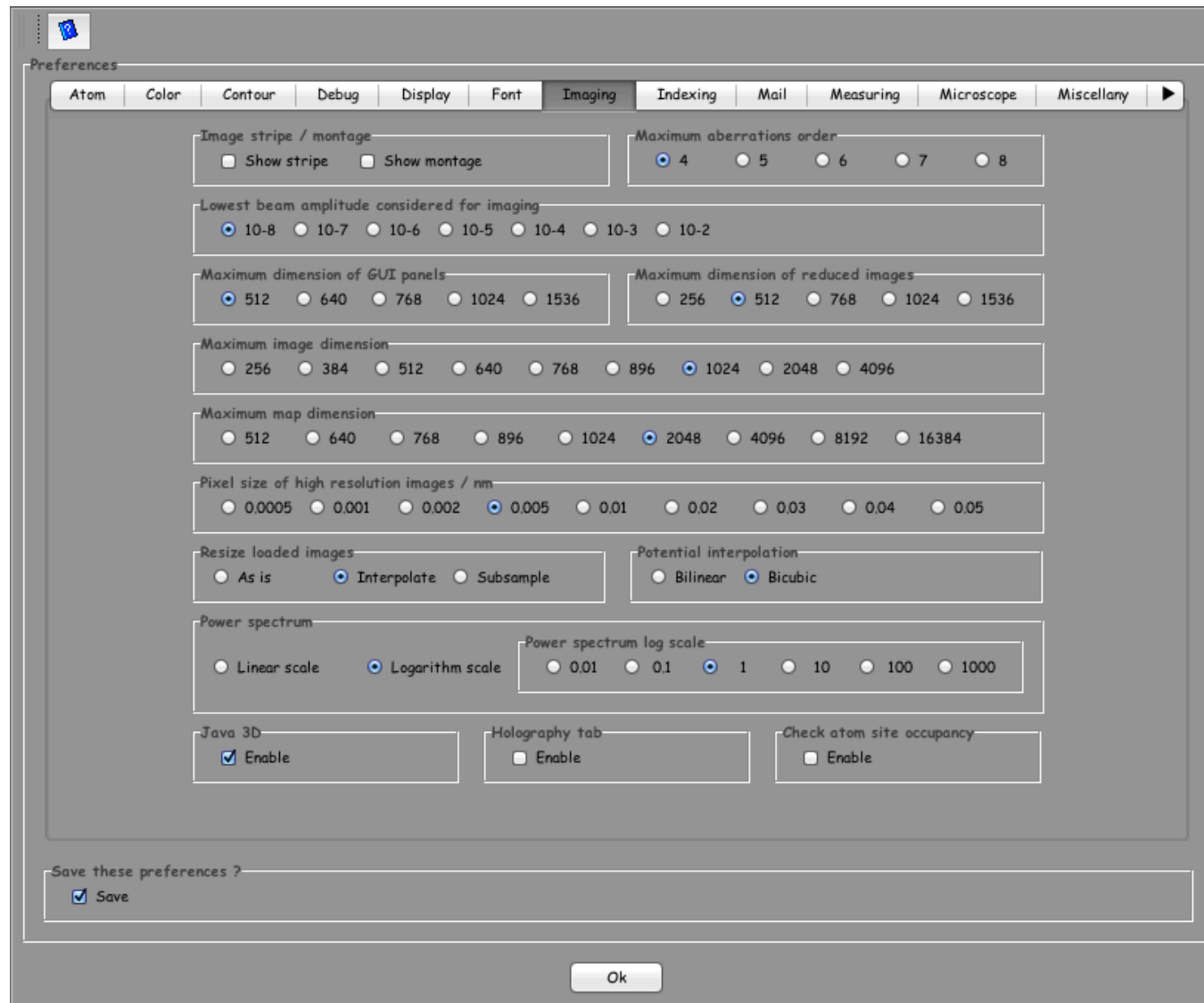


6 different *Cubic* crystals can be selected.



6 different *Other* crystals.

Displaying structures using OpenGL



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.

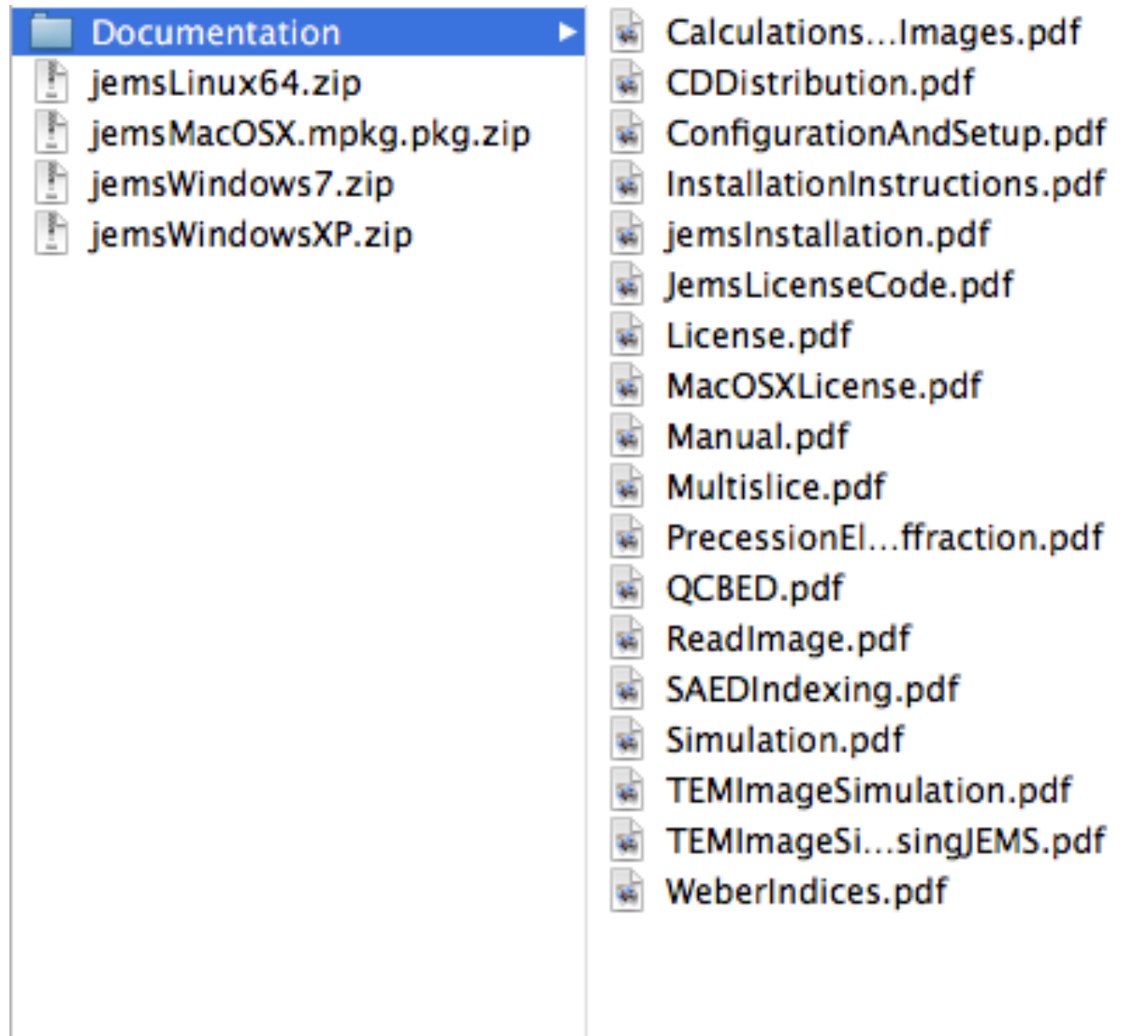
Today's *HRTEM image simulation lab*

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.

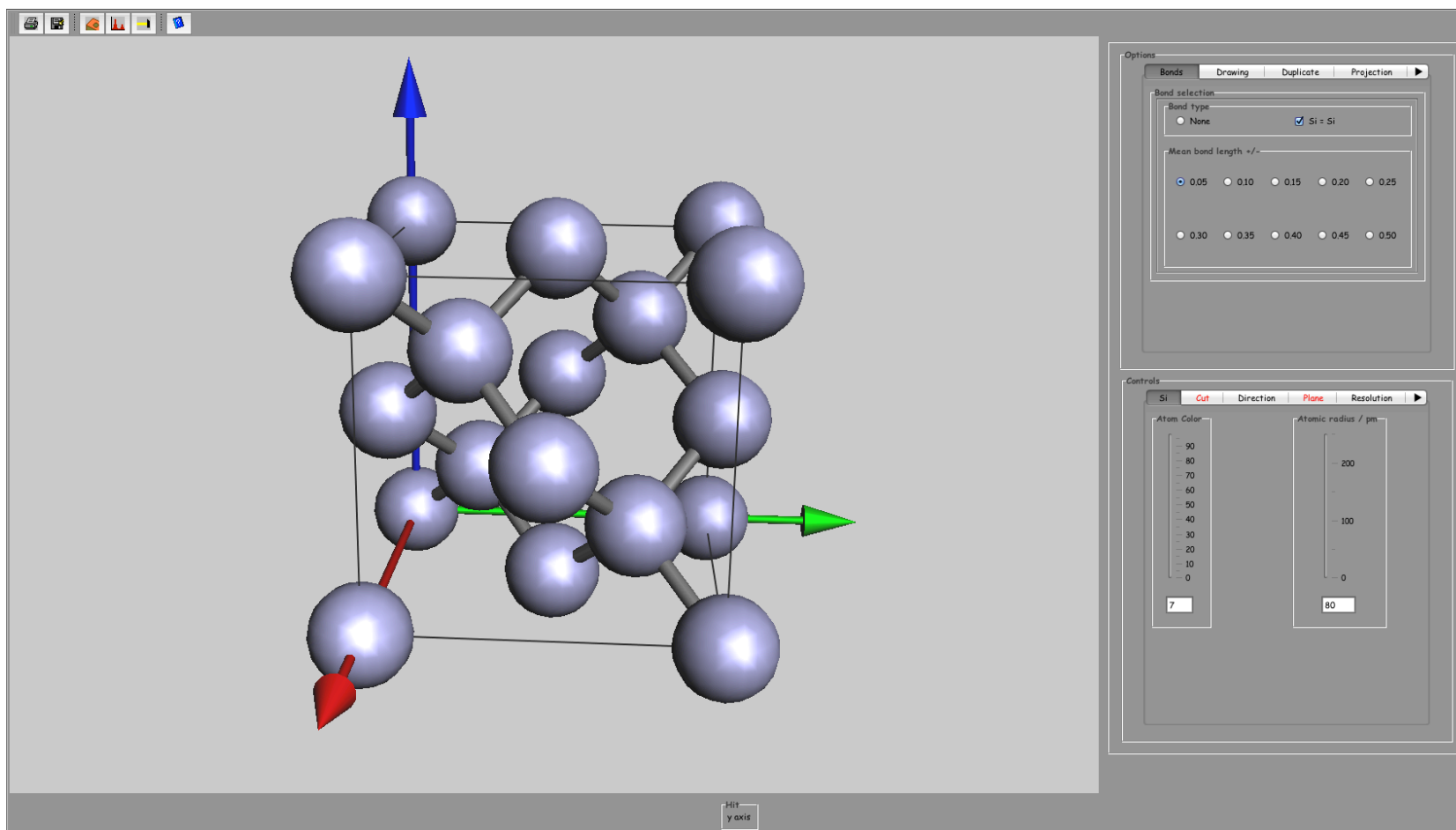
We will finally learn how to define a super-cell and use it to perform HRTEM image simulation. More information is available in jems [../pdfFiles](#) folder.

Documentation folder



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

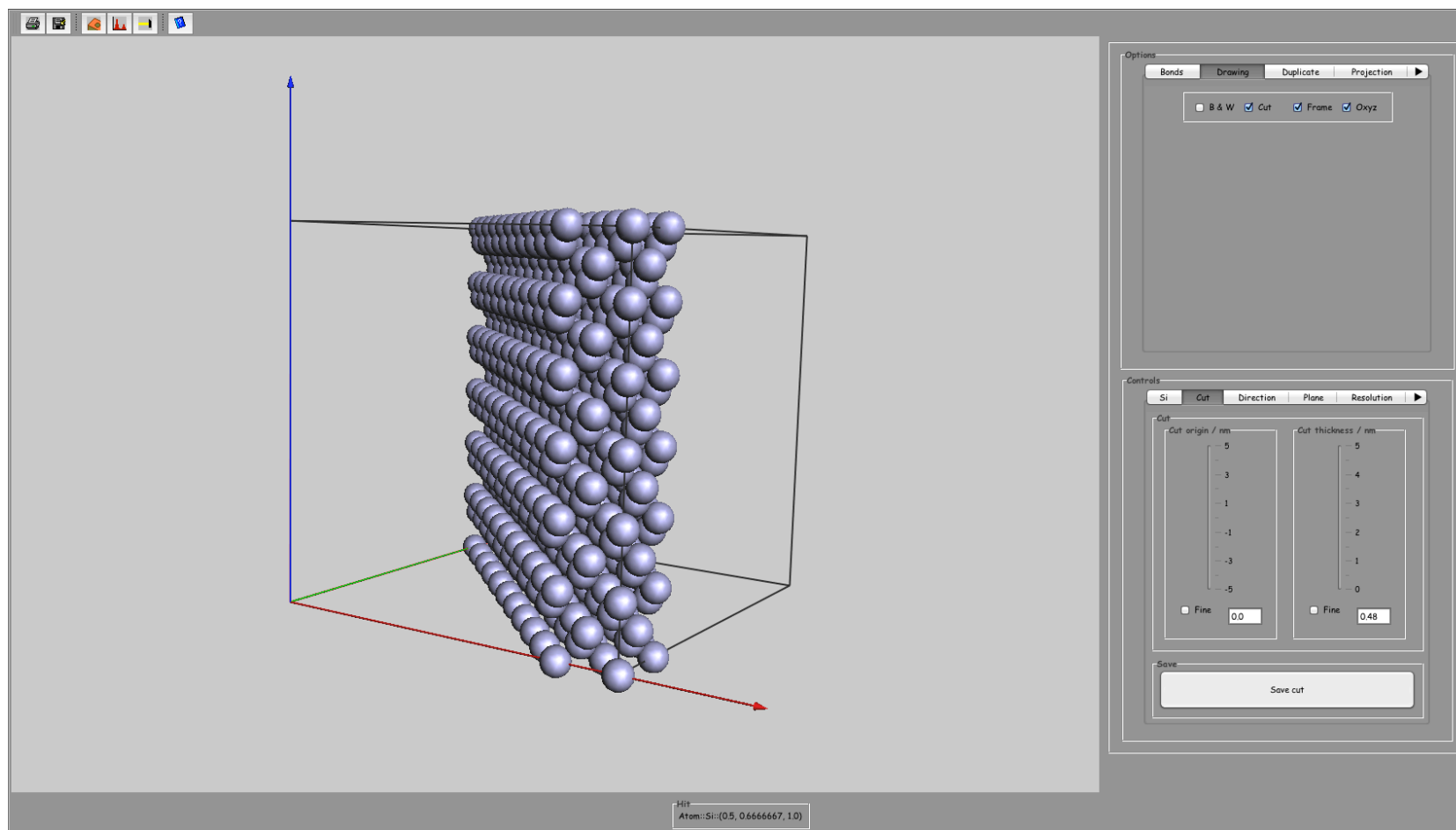
Use **Drawing** \implies **Perspective** (or the associated tool button) to display the Si structure in 3-D.



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.

The screenshot displays a software interface for calculating structure factors. On the left is a table with columns: #, (h,k,l), d* / nm-1, Vr / V, Vi / V, Ampli / V, Phase / Deg, and Ext. / nm. The table lists 36 rows of data for various (hkl) reflections. On the right are control panels. The top panel has three sliders for h max, k max, and l max, each set to 5. Below them is a text box showing 'Default maximum spacing : 15.946 [nm-1]'. The middle panel has a text box for '(h,k,l) number : 701'. The bottom panel is titled 'Atomic Form Factor' and includes radio buttons for DT5B, EJK, PRDW, WK, WKc, and XRay, with a checked checkbox for 'Relativistic correction'.

#	(h,k,l)	d* / nm-1	Vr / V	Vi / V	Ampli / V	Phase / Deg	Ext. / nm
0	(0, 0, 0)	0.000	22.08305	0.64041	22.09233	1.66111	
1	(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
6	(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
9	(2, 0, 0)	3.68263	0.000	0.000	0.000	0.000	0.000
10	(-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

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

Tool buttons icons structure factors dialogue



Print



Save



Make



Reduce



Powder



Rings



Help

Multiplicity

#	(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
24	(3, 1, 1)	6.10695	2.78815	-2.64629	3.84403	-43.50469	198.75513
6	(4, 0, 0)	7.36526	4.08513	0.12377	4.08701	1.73543	186.93735
24	(3, 3, 1)	8.02611	1.72516	1.84124	2.52317	46.86418	302.79852
24	(4, 2, 2)	9.02057	2.95358	0.10605	2.95549	2.05641	258.50374
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
48	(5, 3, 1)	10.89337	1.1245	-1.03409	1.5277	-42.60172	500.09381
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
8	(4, 4, 4)	12.75701	1.63906	0.07731	1.64088	2.70042	465.5881
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
48	(7, 3, 1)	14.14341	0.64281	0.71141	0.95881	47.89956	796.78354
6	(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
12	(6, 6, 0)	15.62408	1.11251	0.06005	1.11413	3.08944	685.68855
24	(8, 2, 2)	15.62408	1.11251	0.06005	1.11413	3.08944	685.68855
8	(5, 5, 5)	15.94626	0.50415	0.56243	0.75531	48.12776	1011.43011
48	(7, 5, 1)	15.94626	0.56243	-0.50415	0.75531	-41.87224	1011.43011

Multiplicity

h max. 5

k max. 5

l max. 5

Default maximum spacing : 15.946 [nm-1]

(h,k,l) number : 25

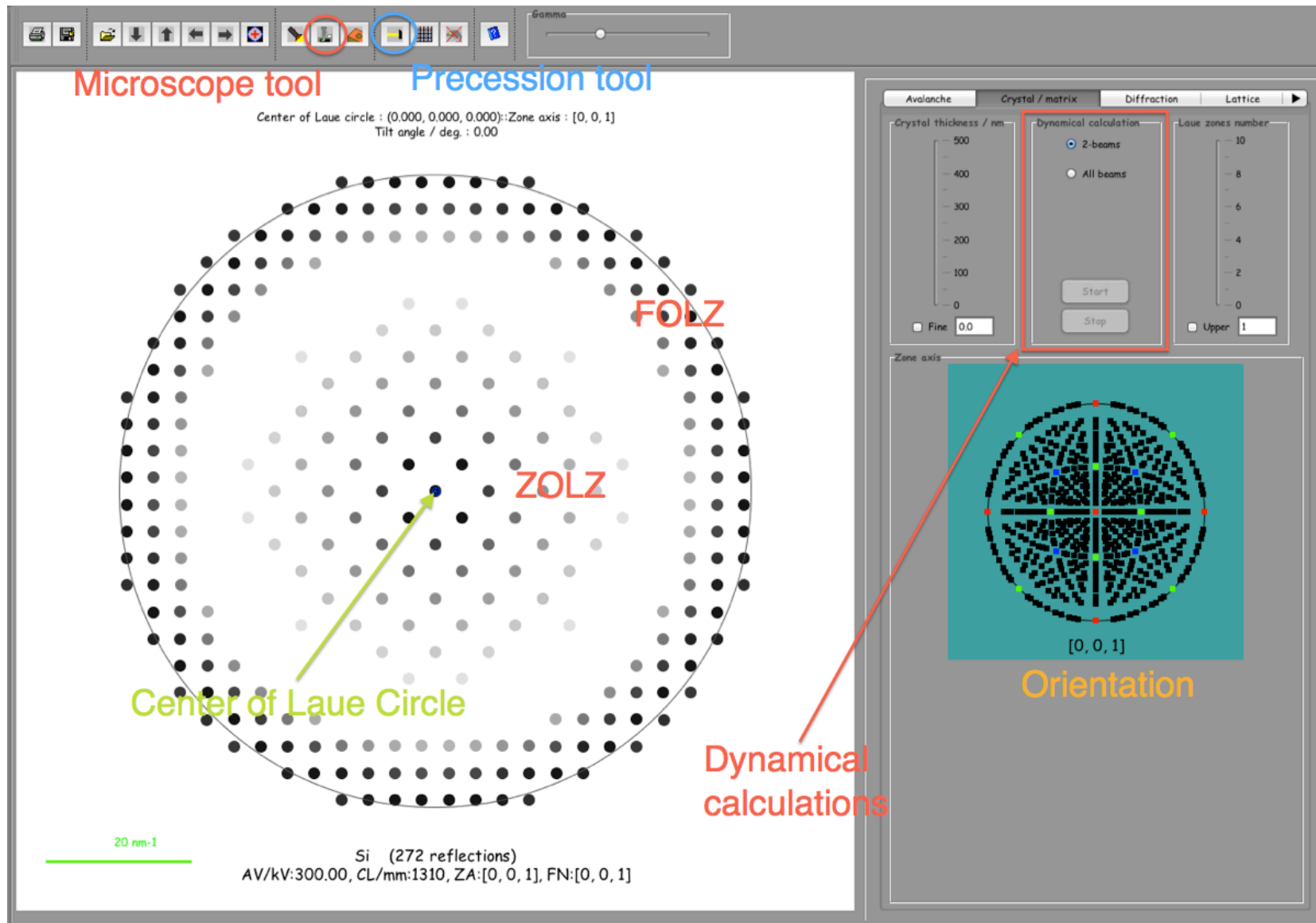
Atomic Form Factor

DTSB EJK PRDW WK WKc XRay

Relativistic correction Atomic form factors

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

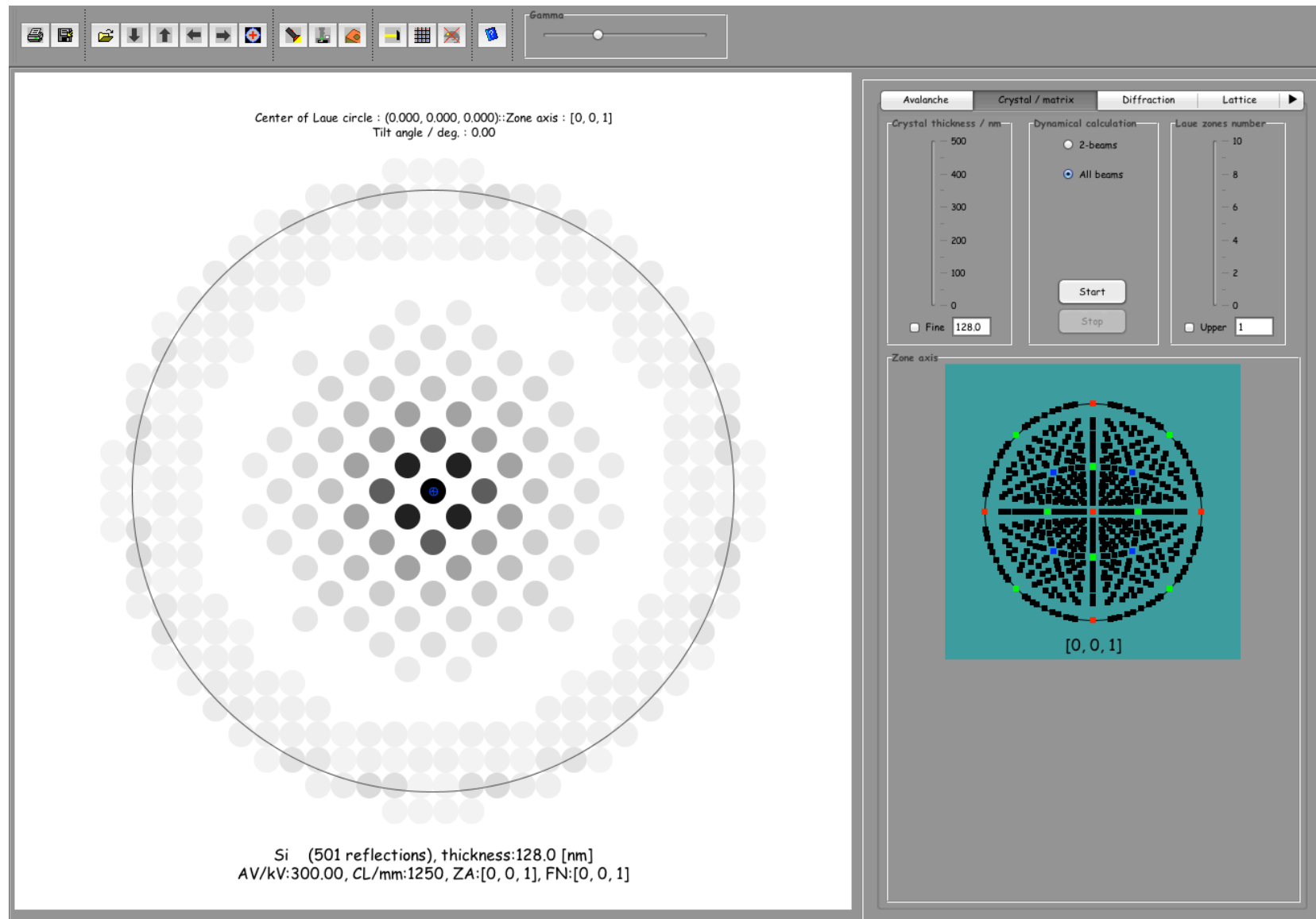
SAED kinematical diffraction



ZOLZ and FOLZ intensities are scaled independently.

Use check box 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.

SAED dynamical diffraction



Dynamical SAED

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

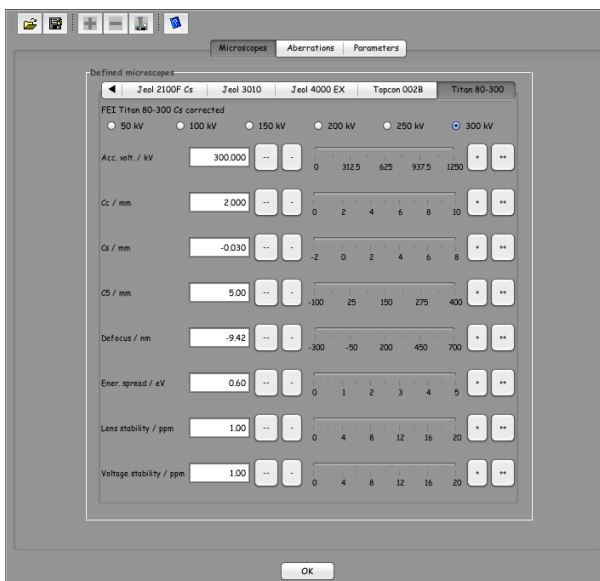
Two methods:

- ▶ 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 50λ .

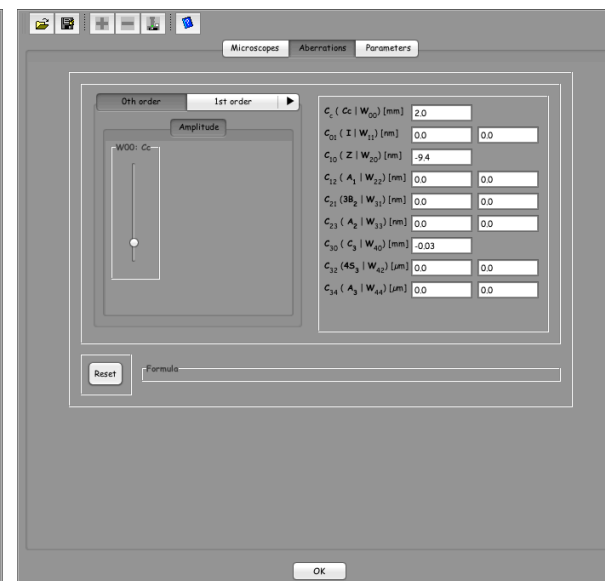
Imaging \implies Blochwave

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

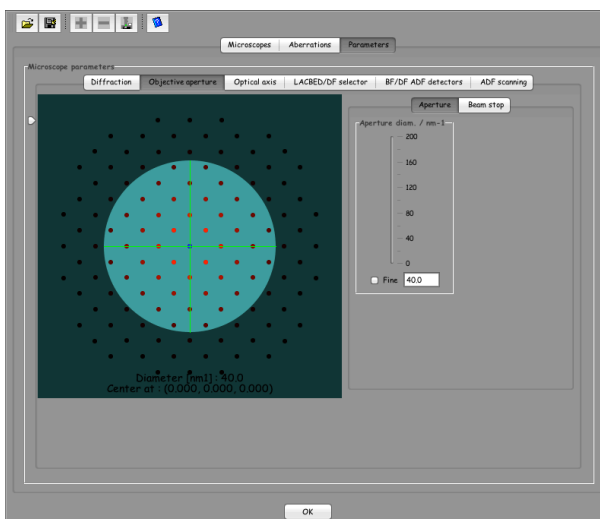
Select the microscope: Parameters \implies Microscope



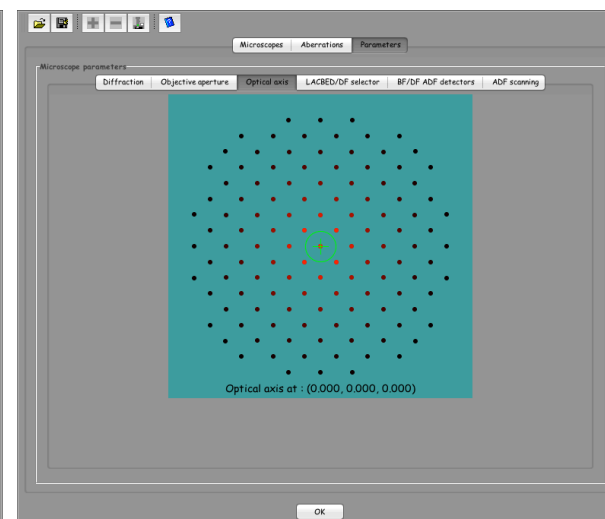
Select a microscope. When not available, edit a new one \oplus



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

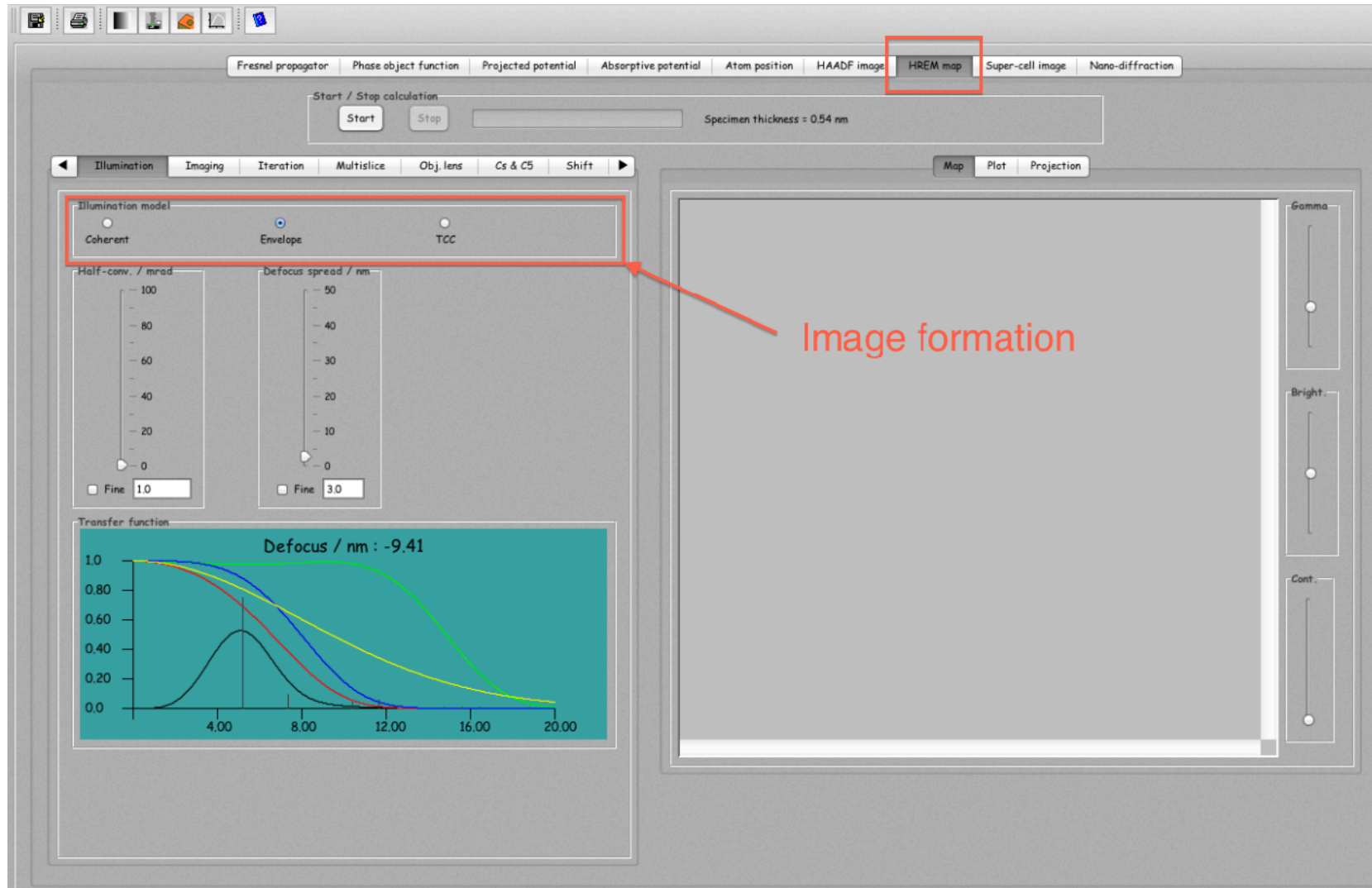


Objective aperture diameter \geq information transfer.



Optical axis can be moved to simulated dark field images.

Open the multislice dialogue: Imaging \implies Multislice

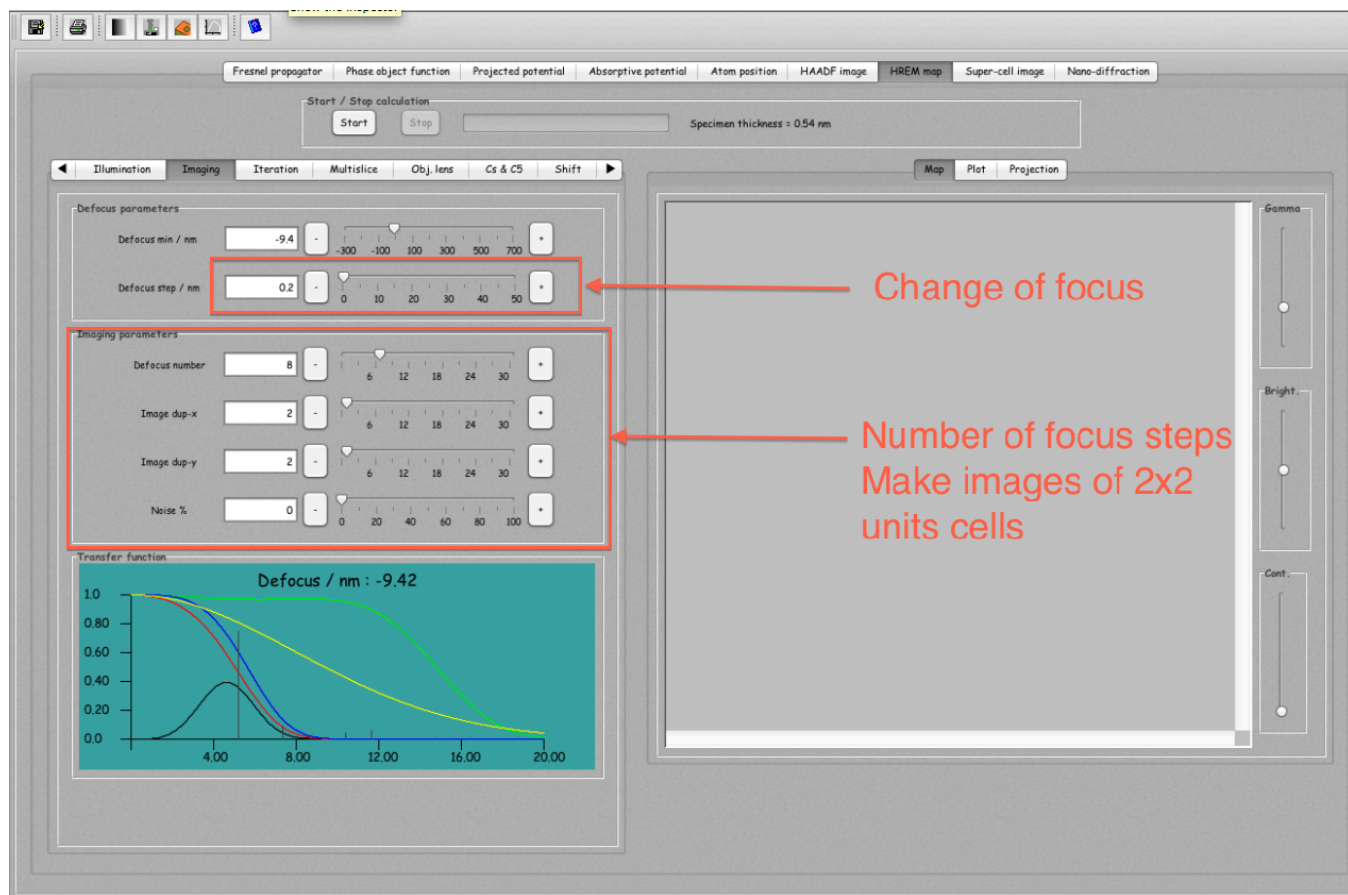


HRTEM image calculation by multislice approach.

The HRTEM map tab is automatically selected.

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

Select the Imaging tab

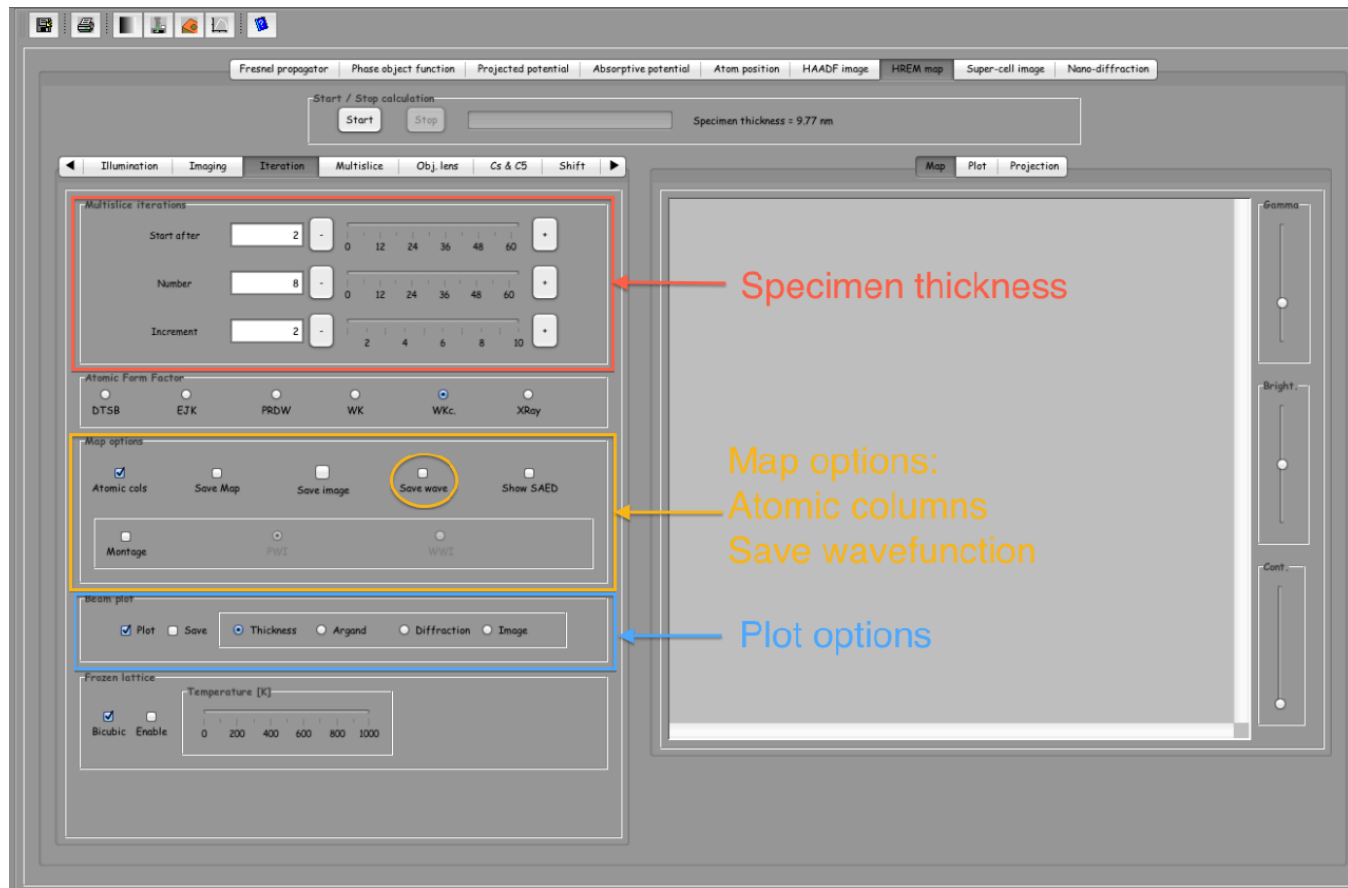


HRTEM image calculation by multislice approach.

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.

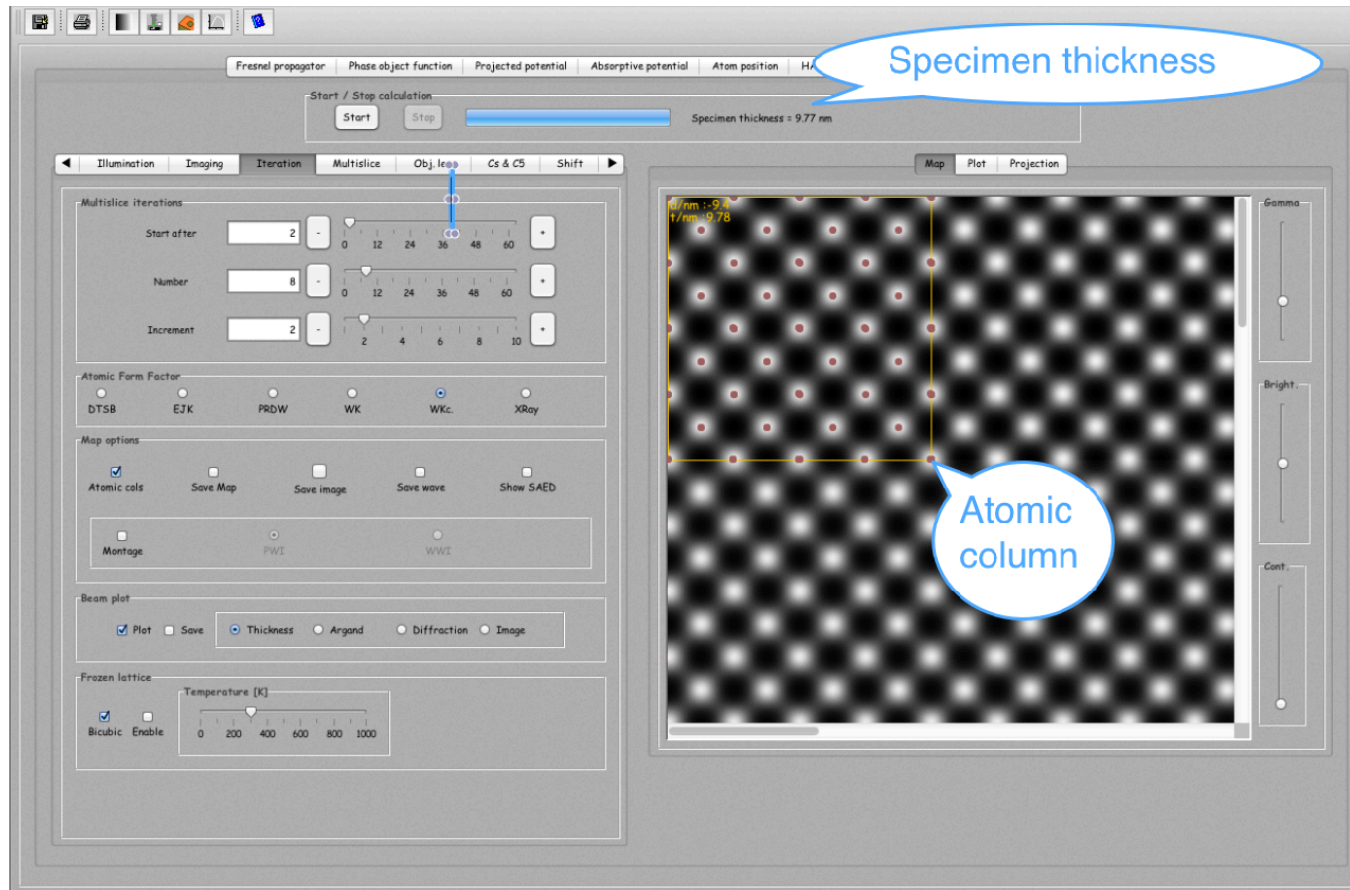
Select the Iteration tab



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.

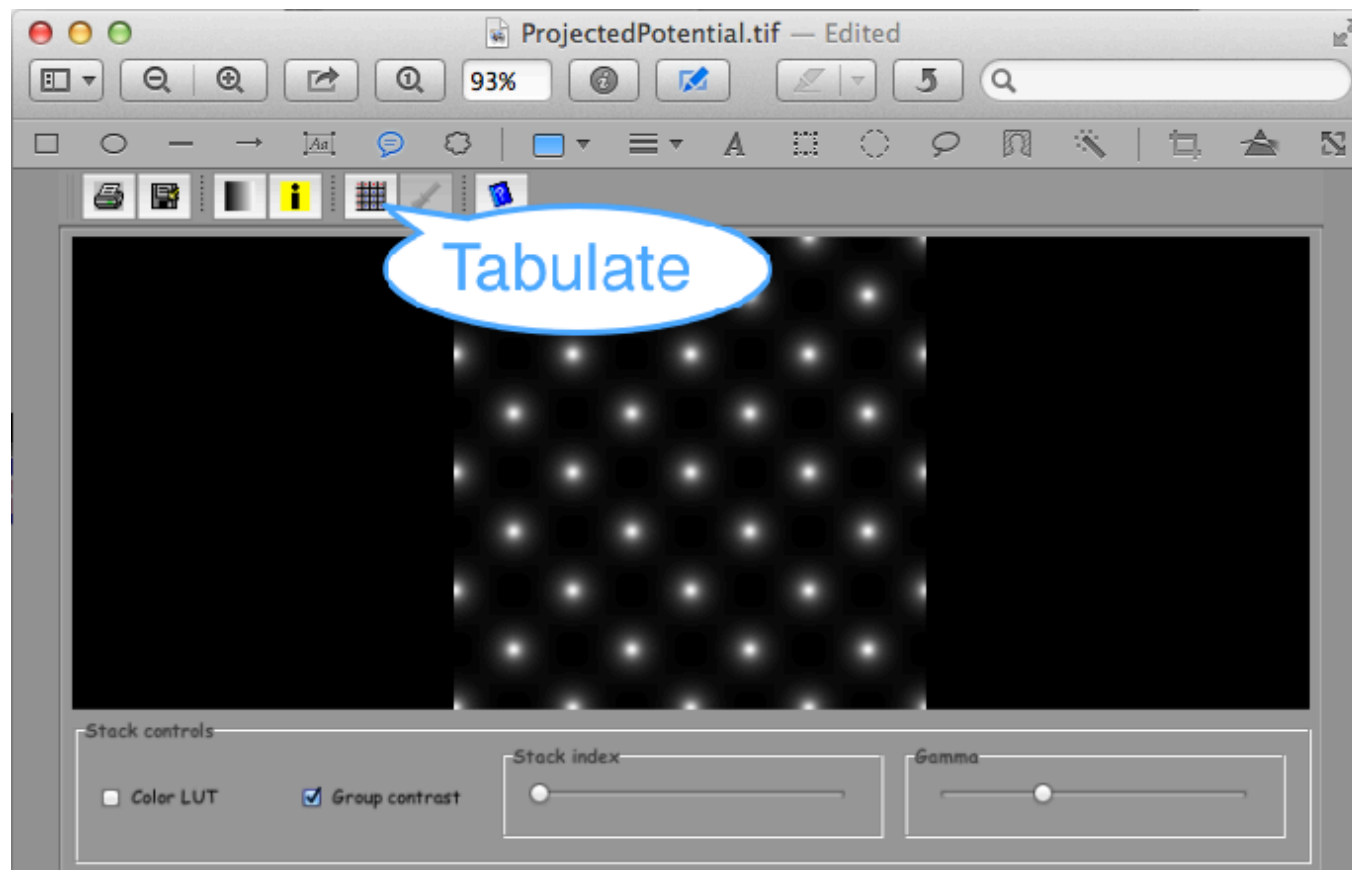


`start` calculates the map.

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

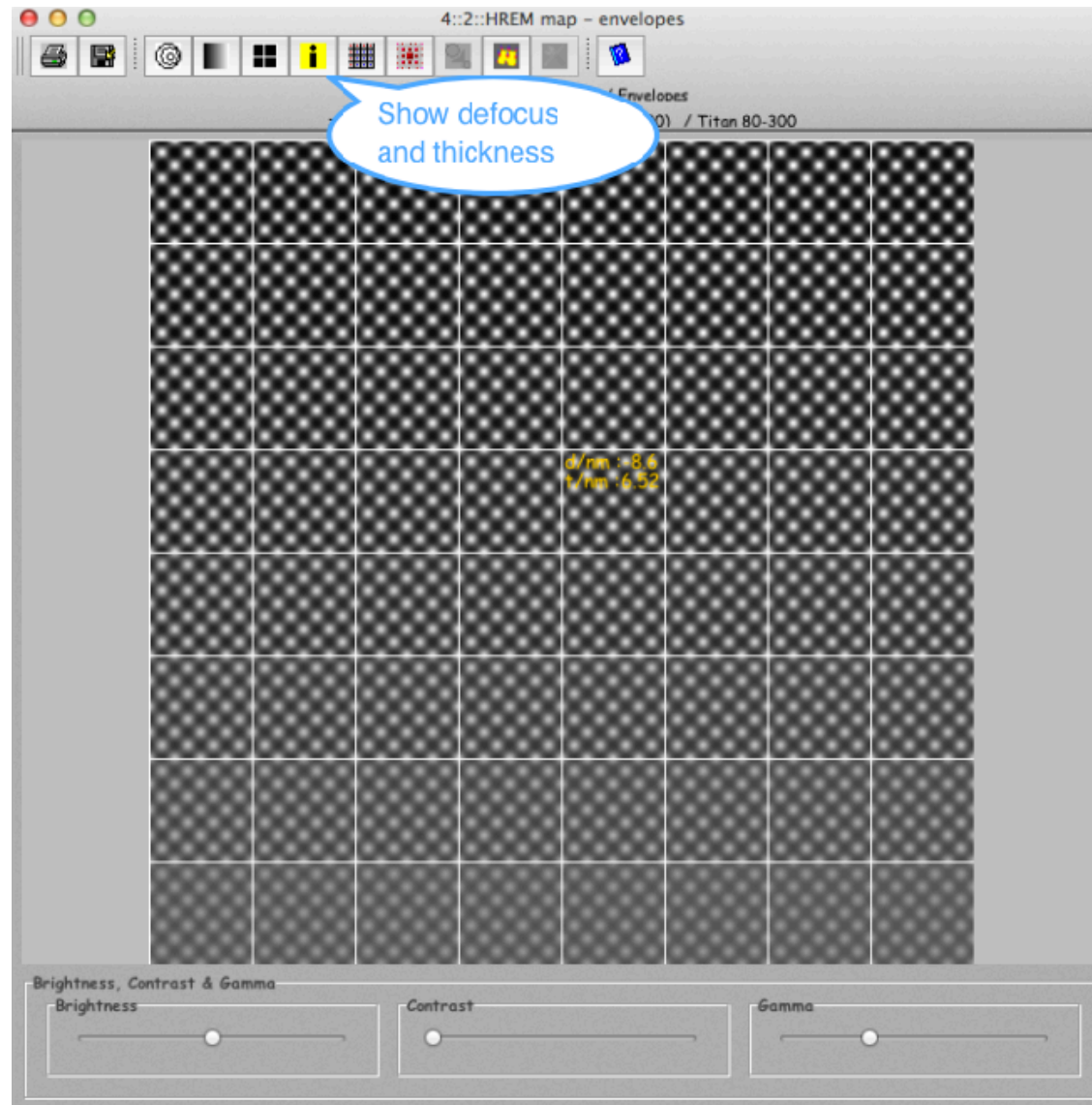


Projected potential of the slice.

Notice that:

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

HREM map

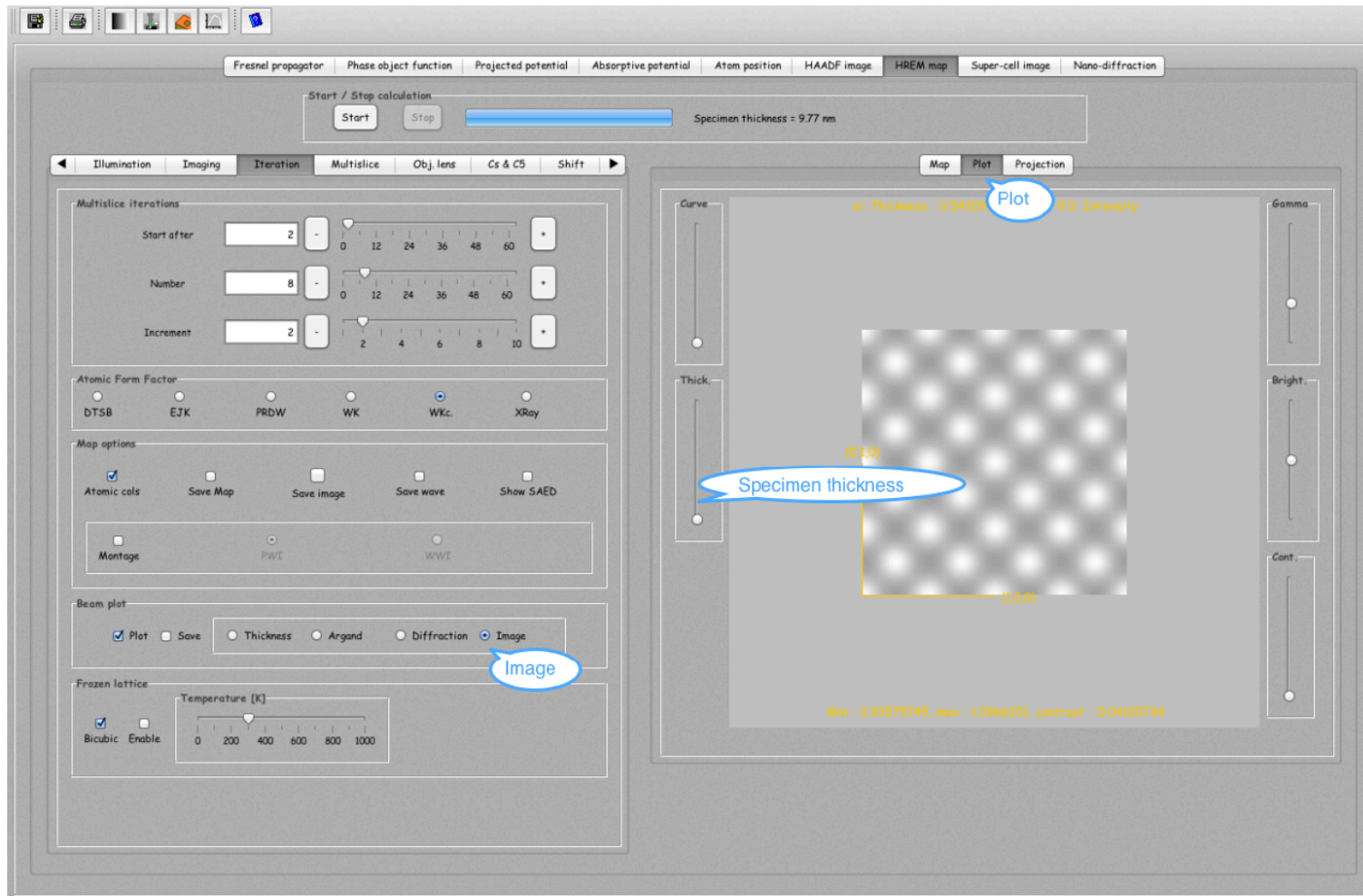


Specimen thickness and defocus are displayed for each image.

Notice that:



- ▶ Images are made of 2 x 2 unit cells.

Interactive image calculation and display




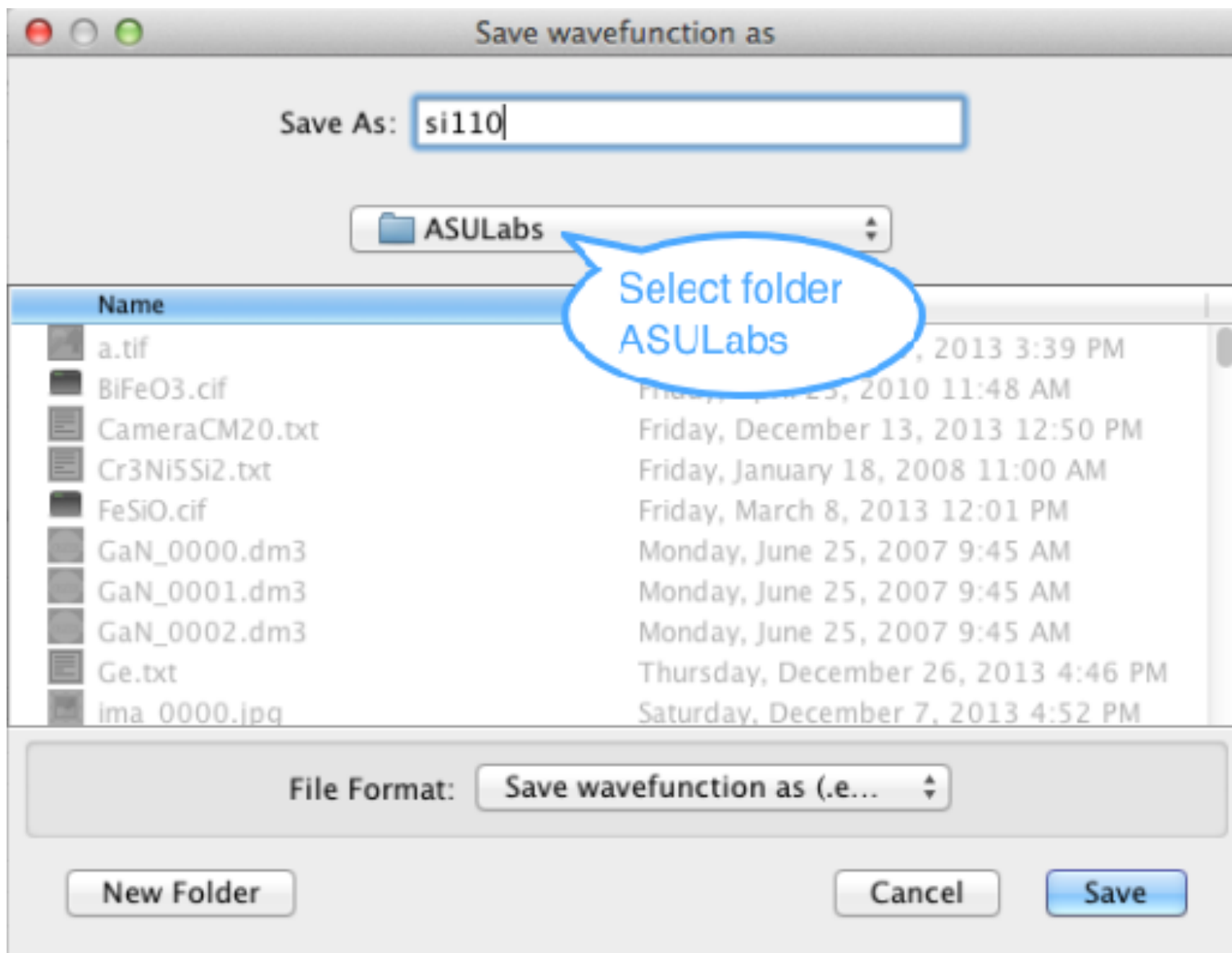
Select  Image and  Plot and change specimen thickness.

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.

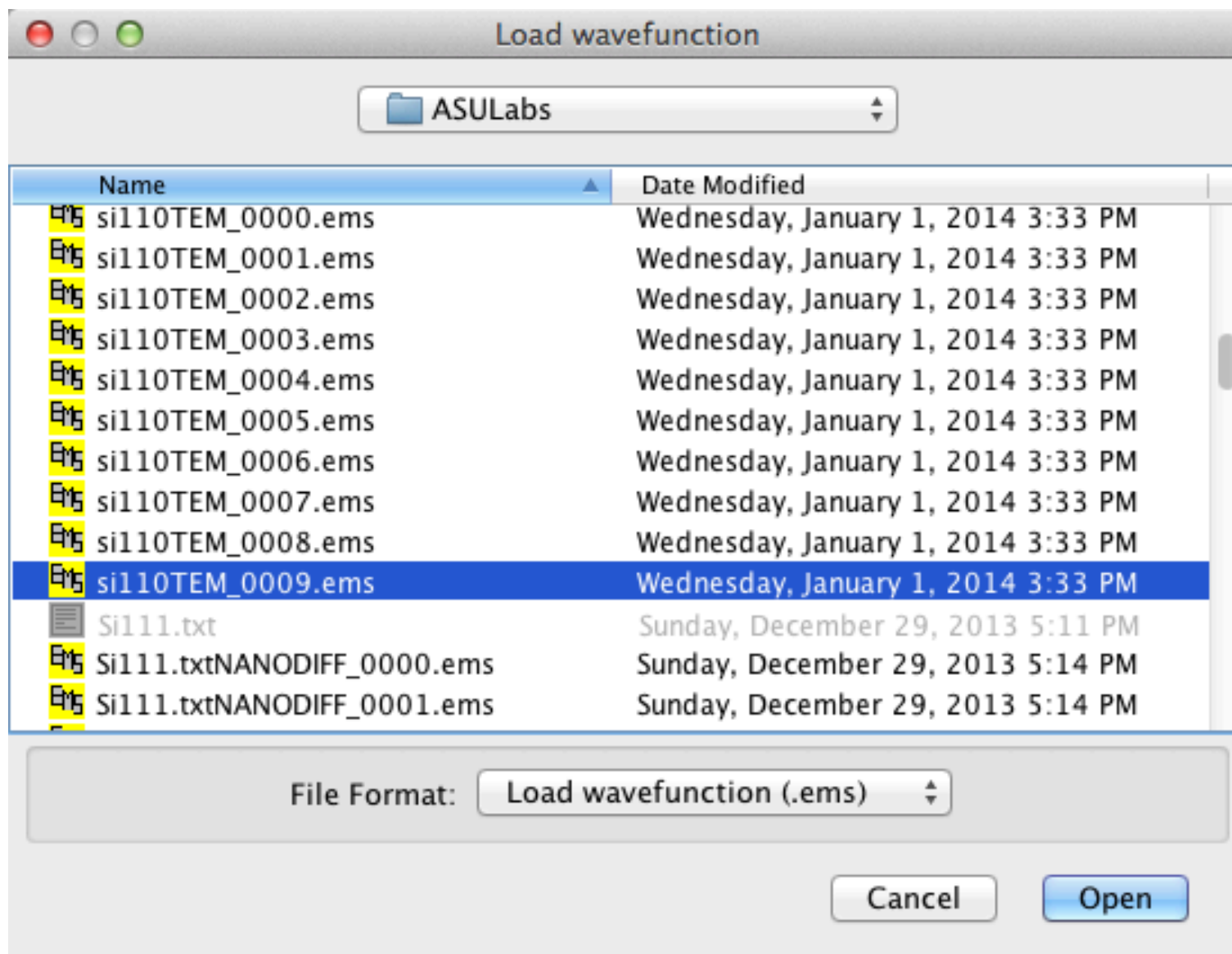
Iteration tab and Save wave

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



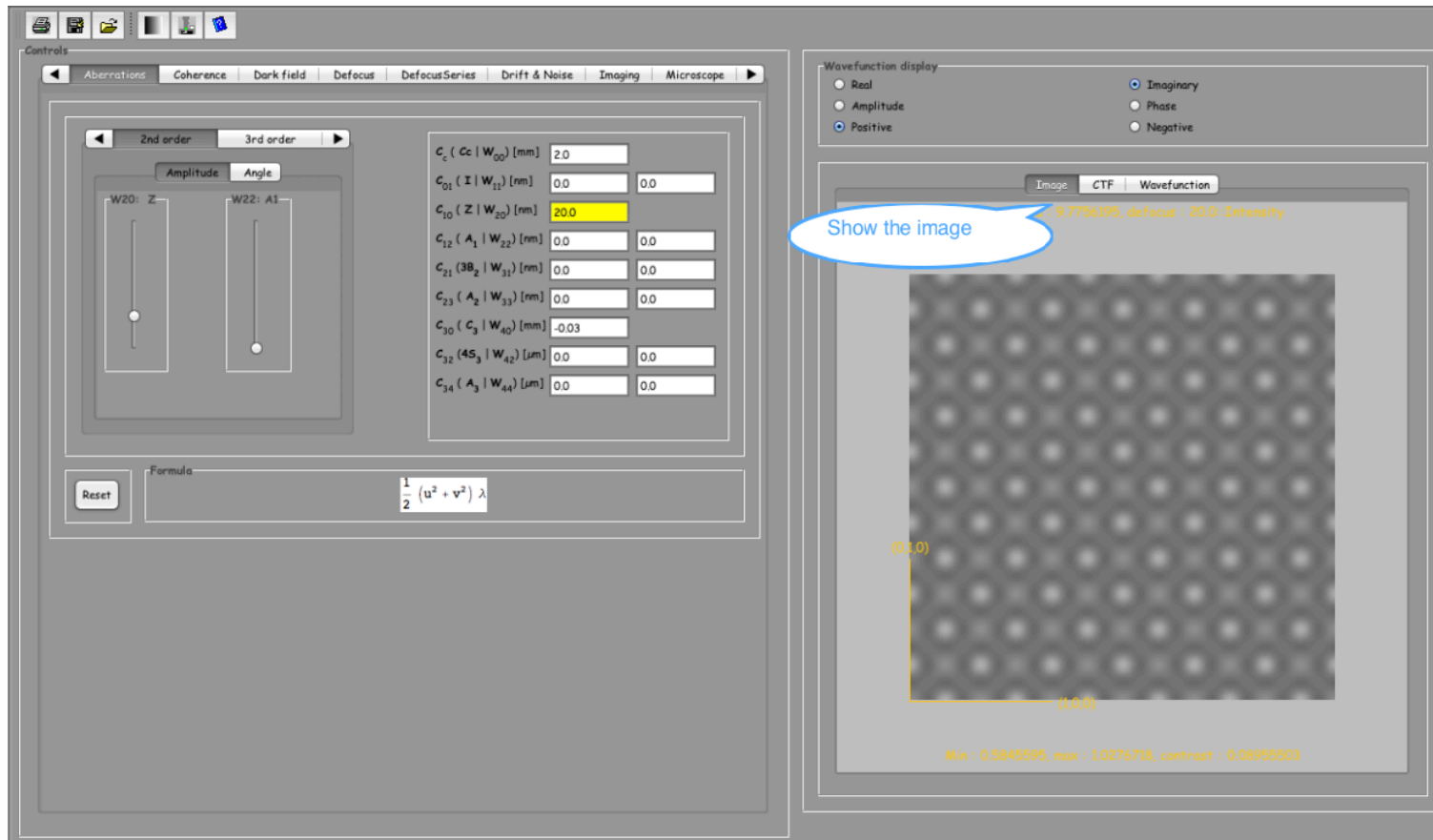
Saving the wave functions for further imaging.

Select Imaging \implies HRTEM



Load a wave function.

Imager dialogue: image



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

2nd order 3rd order

Amplitude Angle

W20: Z W22: A1

$C_c (C_c | W_{00}) [nm]$ 2.0

$C_{01} (I | W_{11}) [nm]$ 0.0 0.0

$C_{10} (Z | W_{20}) [nm]$ 20.0

$C_{12} (A_1 | W_{22}) [nm]$ 0.0 0.0

$C_{21} (3B_2 | W_{31}) [nm]$ 0.0 0.0

$C_{23} (A_2 | W_{33}) [nm]$ 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

$C_{34} (A_3 | W_{44}) [\mu m]$ 0.0 0.0

Reset Formula $\frac{1}{2} (u^2 + v^2) \lambda$

Wavefunction display

Real Imaginary

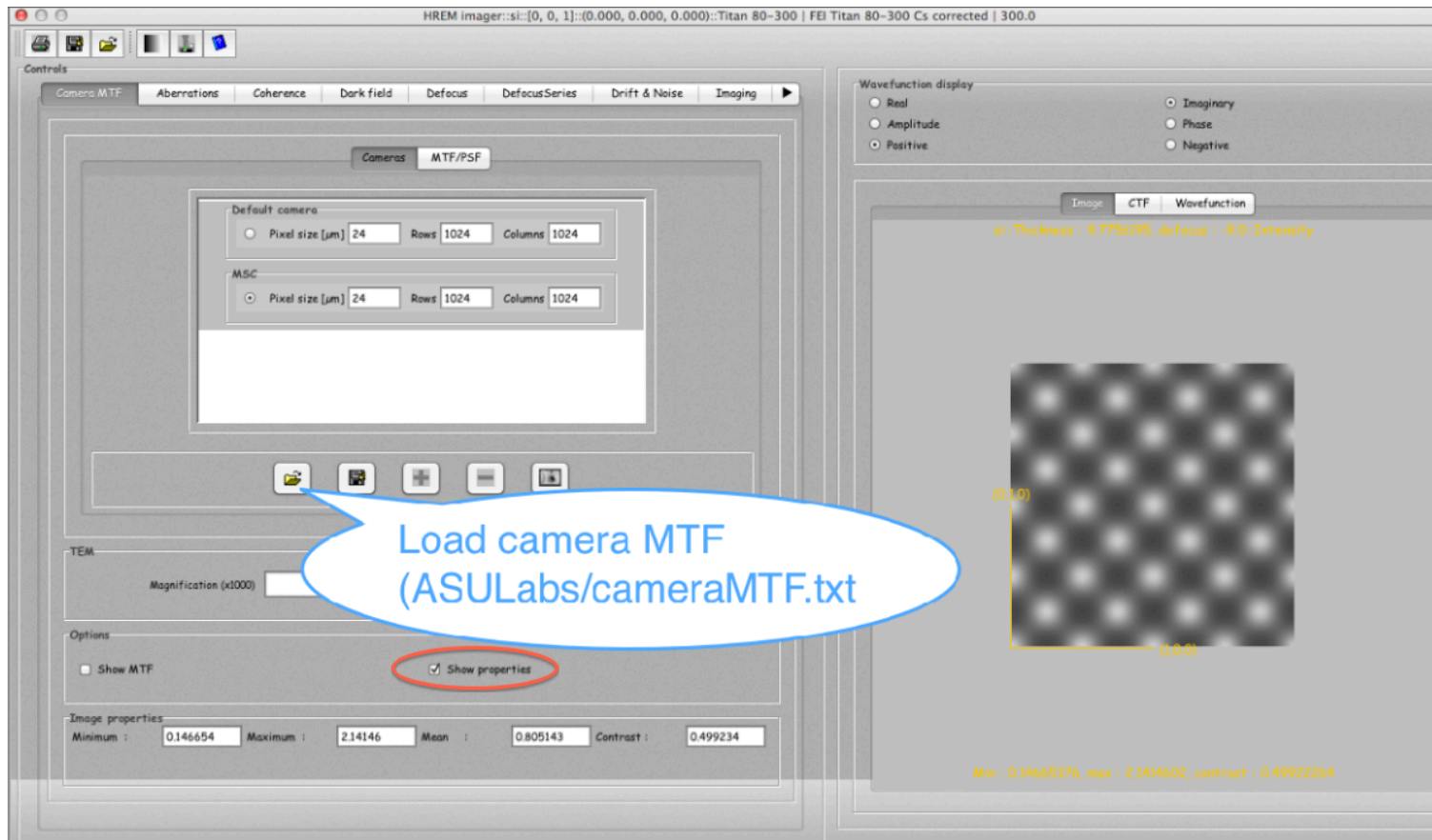
Amplitude Phase

Positive Negative

Image CTF Wavefunction

Imager: wavefunction.

Interactive imaging: Stobbs factor

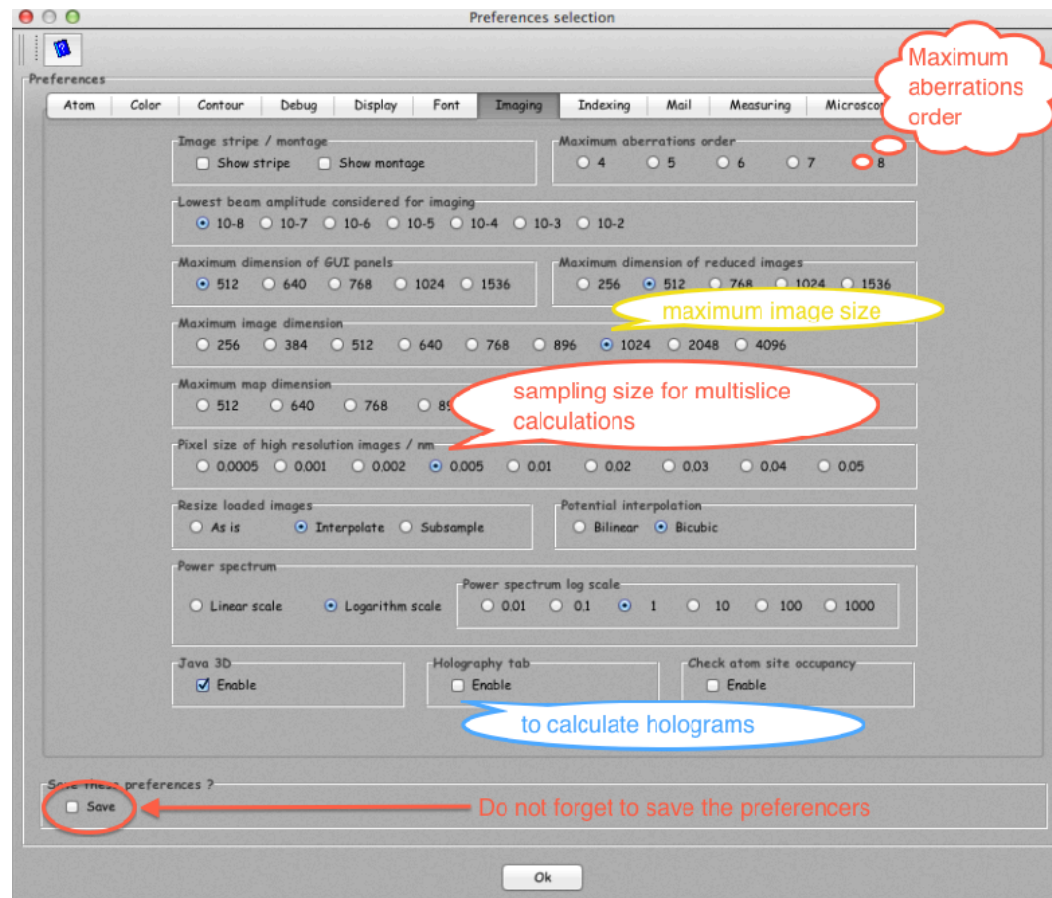


Load camera MTF
(ASULabs/cameraMTF.txt)

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 8th 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 function

The screenshot shows a software interface titled "Transfer Function::Microscope: Titan 80-300 | FEI Titan 80-300 Cs corrected | 300.0". The interface is divided into several sections:

- Left Panel:** Displays a circular wavefront aberration plot with a color gradient from blue (low) to red (high). A red oval highlights the text "Wavefront aberrations" above the plot. A scale bar at the bottom left indicates "5 nm⁻¹".
- Top Panel:** Contains tabs for "Aberrations", "CTF profile", "CTF", "Diffractogram", and "OTF". A "Gamma" slider is also present.
- Right Panel (Transfer function controls):** Contains tabs for "Aberrations", "Coherence", "Defocus", "Drift & Noise", "Microscope", "Shift & tilt", and "Order 0" through "Order 3". It features three vertical sliders for "5th order", "6th order", and "7th order" with sub-labels "W51: 5B4", "W53: 5D4", and "W55: A4".
- Bottom Right Panel:** A table of aberration coefficients with their respective notations and values. A red arrow points from the "5th order" sliders to this table.

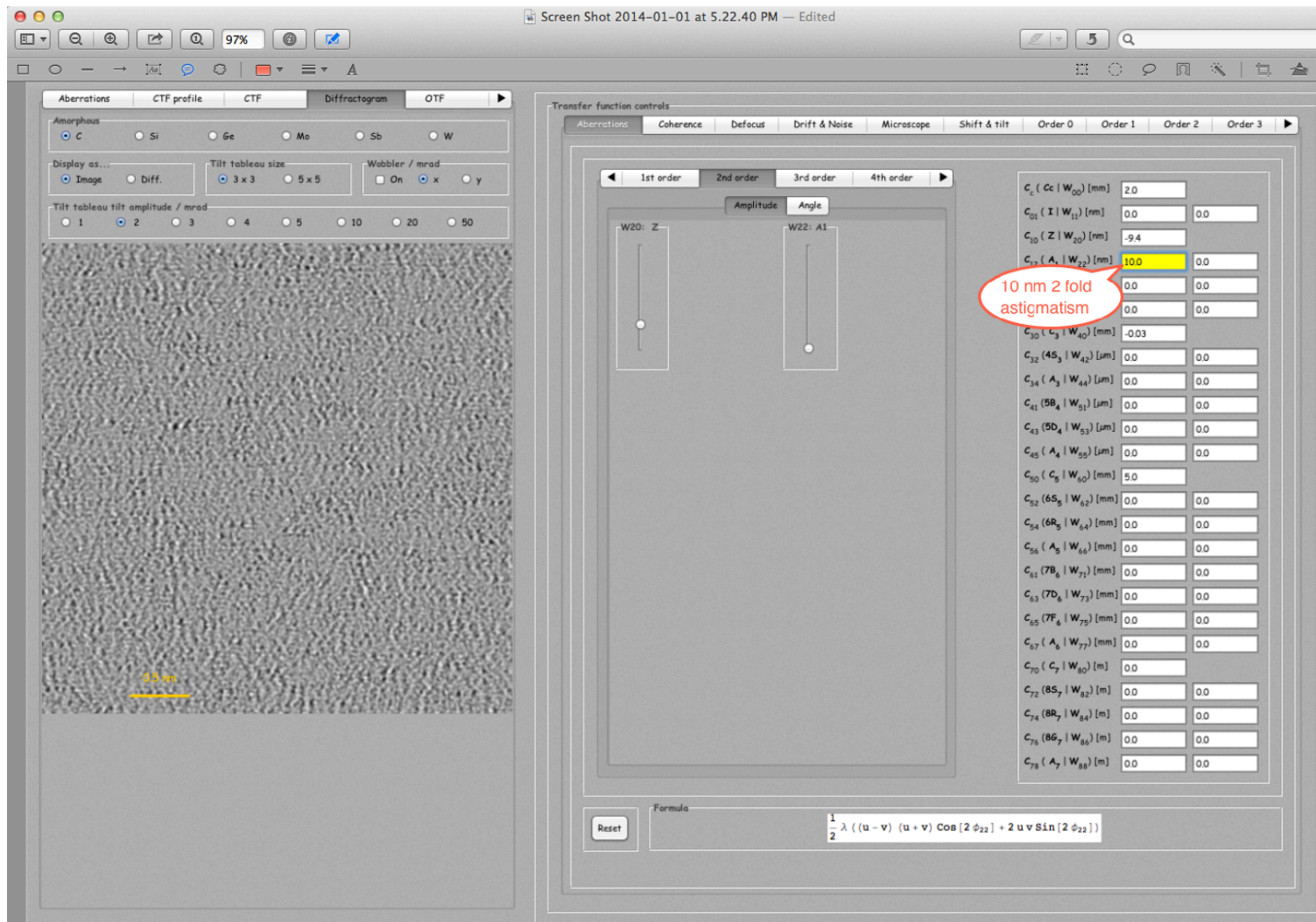
Legend for notations:

- Krivanek notation (geometric)
- Haider notation
- Wavefront notation

Notation	Value	
$C_c (C_c W_{00})$ [mm]	2.0	
$C_{01} (I W_{11})$ [nm]	0.0	0.0
$C_{10} (Z W_{20})$ [nm]	-9.4	
$C_{12} (A_1 W_{22})$ [nm]	0.0	0.0
$C_{21} (3B_2 W_{31})$ [nm]	0.0	0.0
$C_{23} (A_2 W_{33})$ [nm]	0.0	0.0
$C_{30} (C_3 W_{40})$ [mm]	-0.03	
$C_{32} (4S_3 W_{42})$ [μm]	0.0	0.0
$C_{34} (A_3 W_{44})$ [μm]	0.0	0.0
$C_{41} (5B_4 W_{51})$ [μm]	0.0	0.0
$C_{43} (5D_4 W_{53})$ [μm]	0.0	0.0
$C_{45} (A_4 W_{55})$ [μm]	0.0	0.0
$C_{50} (C_5 W_{60})$ [mm]	5.0	
$C_{52} (6S_5 W_{62})$ [nm]	0.0	0.0
$C_{54} (6R_5 W_{64})$ [nm]	0.0	0.0
$C_{56} (A_5 W_{66})$ [nm]	0.0	0.0
$C_{61} (7B_6 W_{71})$ [nm]	0.0	0.0
$C_{63} (7D_6 W_{73})$ [nm]	0.0	0.0
$C_{65} (7F_6 W_{75})$ [nm]	0.0	0.0
$C_{67} (A_6 W_{77})$ [nm]	0.0	0.0
$C_{70} (C_7 W_{80})$ [m]	0.0	
$C_{72} (8S_7 W_{82})$ [m]	0.0	0.0
$C_{74} (8R_7 W_{84})$ [m]	0.0	0.0
$C_{76} (8G_7 W_{86})$ [m]	0.0	0.0
$C_{78} (A_7 W_{88})$ [m]	0.0	0.0

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

Wavefront aberrations: 2-fold astigmatism



Screen Shot 2014-01-01 at 5.22.40 PM — Edited

Aberrations CTF profile CTF Diffraction OTF

Amorphous C Si Ge Mo Sb W

Display as... Image Diff. Tilt tableau size 3 x 3 5 x 5 Wobbler / mrad On x y

Tilt tableau tilt amplitude / mrad 1 2 3 4 5 10 20 50

Transfer function controls

Aberrations Coherence Defocus Drift & Noise Microscope Shift & tilt Order 0 Order 1 Order 2 Order 3

1st order 2nd order 3rd order 4th order

Amplitude Angle

-W20: Z -W22: A1

$C_c (C_c | W_{00}) [mm]$ 2.0

$C_{01} (I | W_{11}) [nm]$ 0.0 0.0

$C_{10} (Z | W_{20}) [nm]$ -9.4

$C_{12} (A_1 | W_{22}) [nm]$ 10.0 0.0

$C_{20} (C_2 | W_{40}) [mm]$ -0.03

$C_{32} (4S_3 | W_{42}) [\mu m]$ 0.0 0.0

$C_{34} (A_3 | W_{44}) [\mu m]$ 0.0 0.0

$C_{41} (5B_4 | W_{51}) [\mu m]$ 0.0 0.0

$C_{43} (5D_4 | W_{53}) [\mu m]$ 0.0 0.0

$C_{45} (A_4 | W_{55}) [\mu m]$ 0.0 0.0

$C_{50} (C_5 | W_{60}) [mm]$ 5.0

$C_{52} (6S_5 | W_{62}) [mm]$ 0.0 0.0

$C_{54} (6R_5 | W_{64}) [mm]$ 0.0 0.0

$C_{56} (A_5 | W_{66}) [mm]$ 0.0 0.0

$C_{61} (7B_6 | W_{71}) [mm]$ 0.0 0.0

$C_{63} (7D_6 | W_{73}) [mm]$ 0.0 0.0

$C_{65} (7F_6 | W_{75}) [mm]$ 0.0 0.0

$C_{67} (A_6 | W_{77}) [mm]$ 0.0 0.0

$C_{70} (C_7 | W_{80}) [m]$ 0.0

$C_{72} (8S_7 | W_{82}) [m]$ 0.0 0.0

$C_{74} (8R_7 | W_{84}) [m]$ 0.0 0.0

$C_{76} (8G_7 | W_{86}) [m]$ 0.0 0.0

$C_{78} (A_7 | W_{88}) [m]$ 0.0 0.0

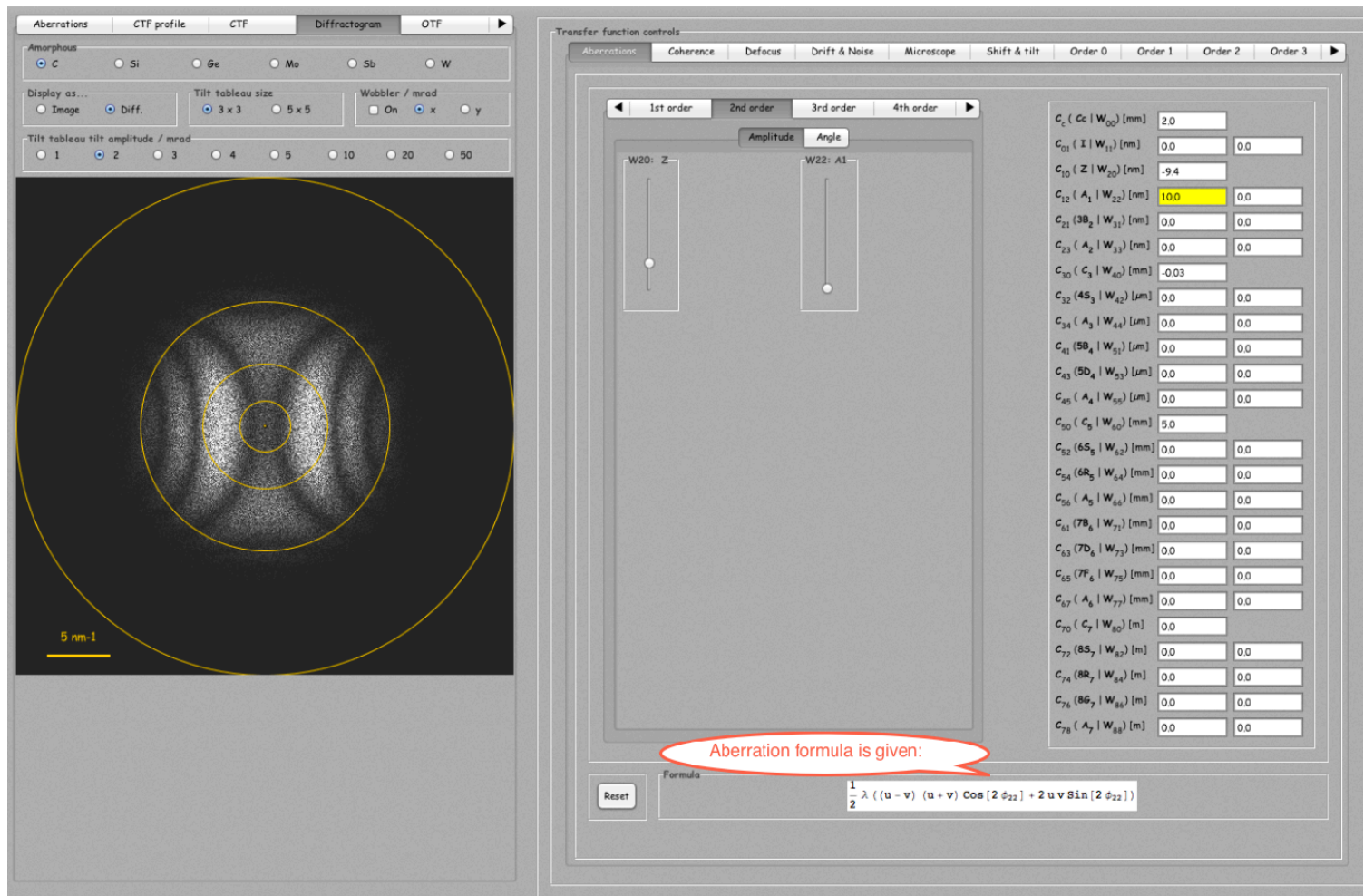
Formula

$$\frac{1}{2} \lambda ((u - v) (u + v) \cos[2 \phi_{22}] + 2 u v \sin[2 \phi_{22}])$$

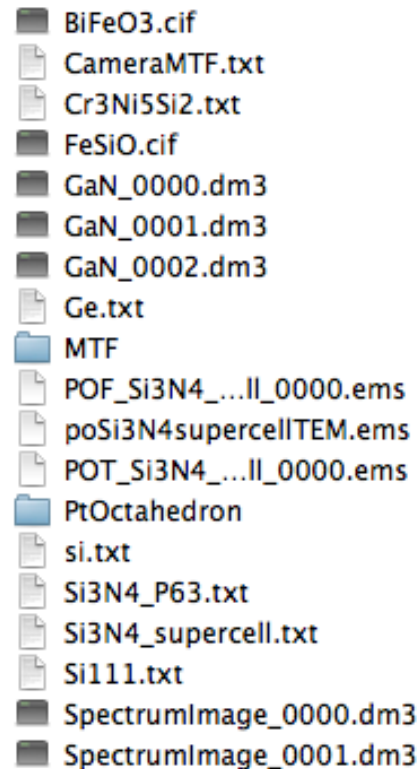
Reset

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}).



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 ≈ 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 Load phase-object and Save phase-object set.

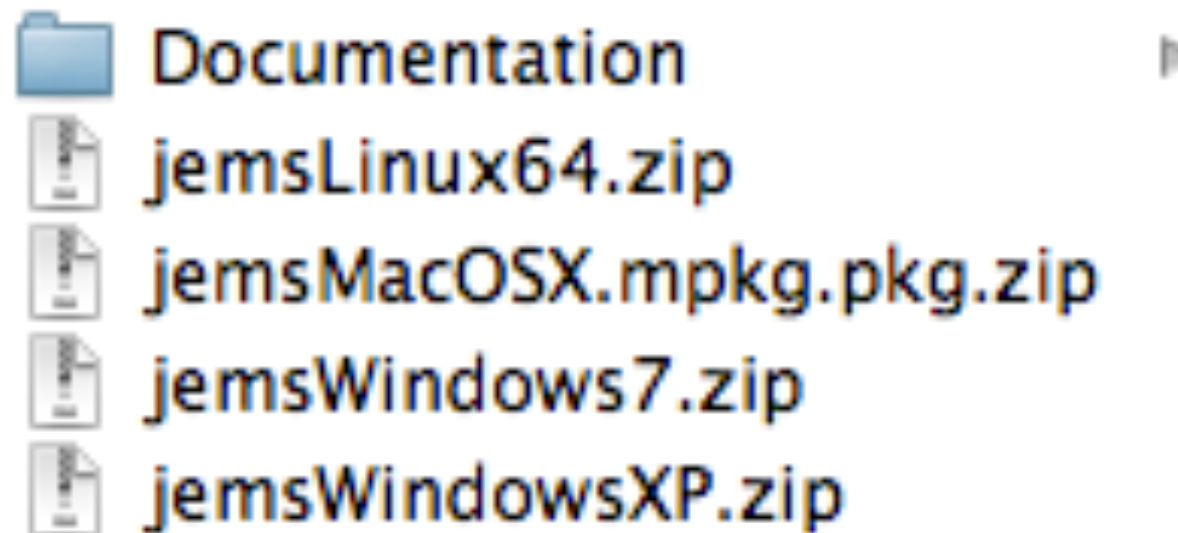
Make sure that aberrations are reset!

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:

1. Open the PtOct_0000.txt crystal file (of folder PtOctahedron) (**File** \implies **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.
4. Make sure that Save of tab `Iteration-Wavefunction` is selected. To see an image after each slice have the Show image ² 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.
6. Load the last wave function in the HRTEMImager (**Imaging** \implies **HRTEMImager**). Change the imaging parameters in order to how aberrations affect HRTEM images.

²You can close all the images using **Window** \implies **Close All**.



- ▶ 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

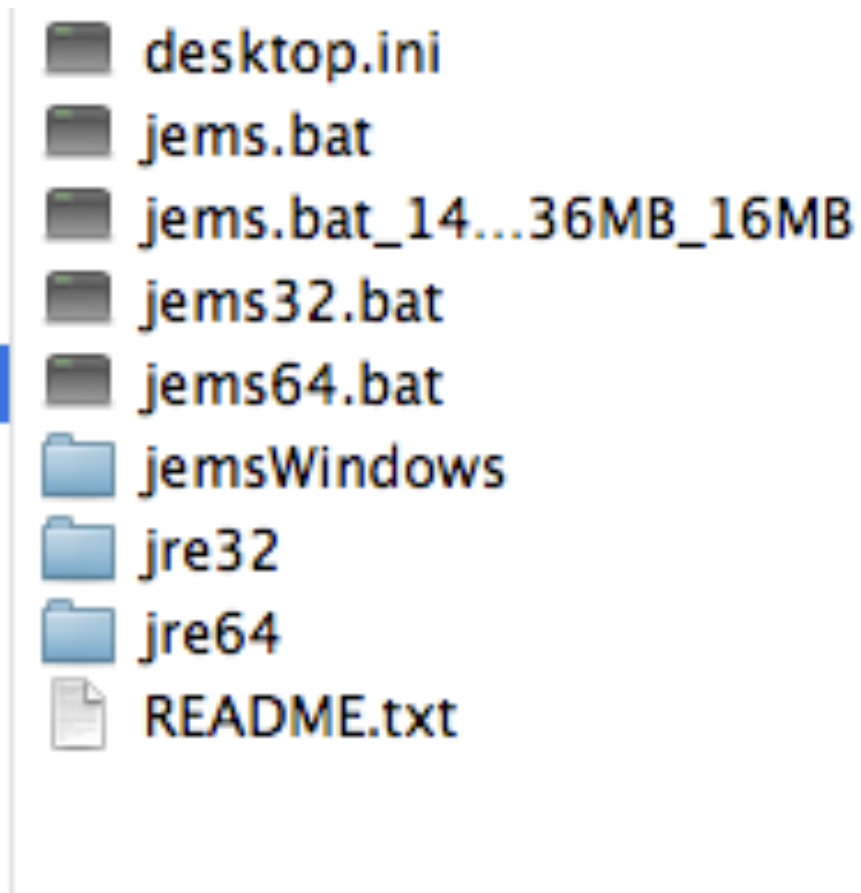


Figure: Windows 7 or 8 version: jems started either using jems32.bat or jems64.bat depending on Windows being 32 or 64 bits.

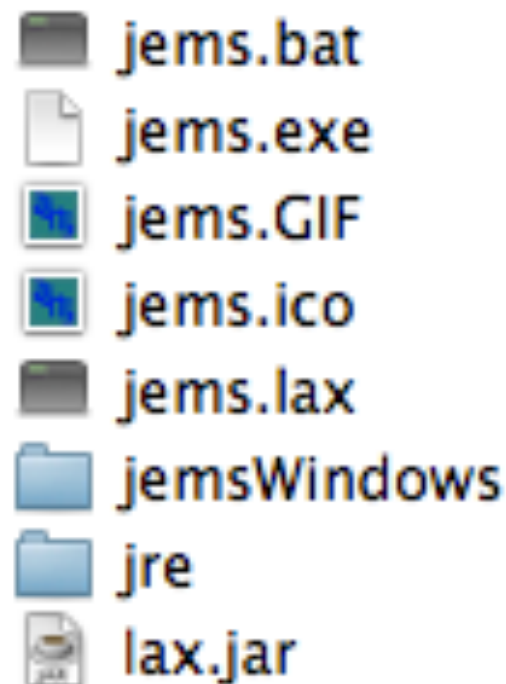


Figure: Windows XP (only 32 bits).

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