

# Image Simulation Laboratory Notes

Winter School on High Resolution Electron Microscopy  
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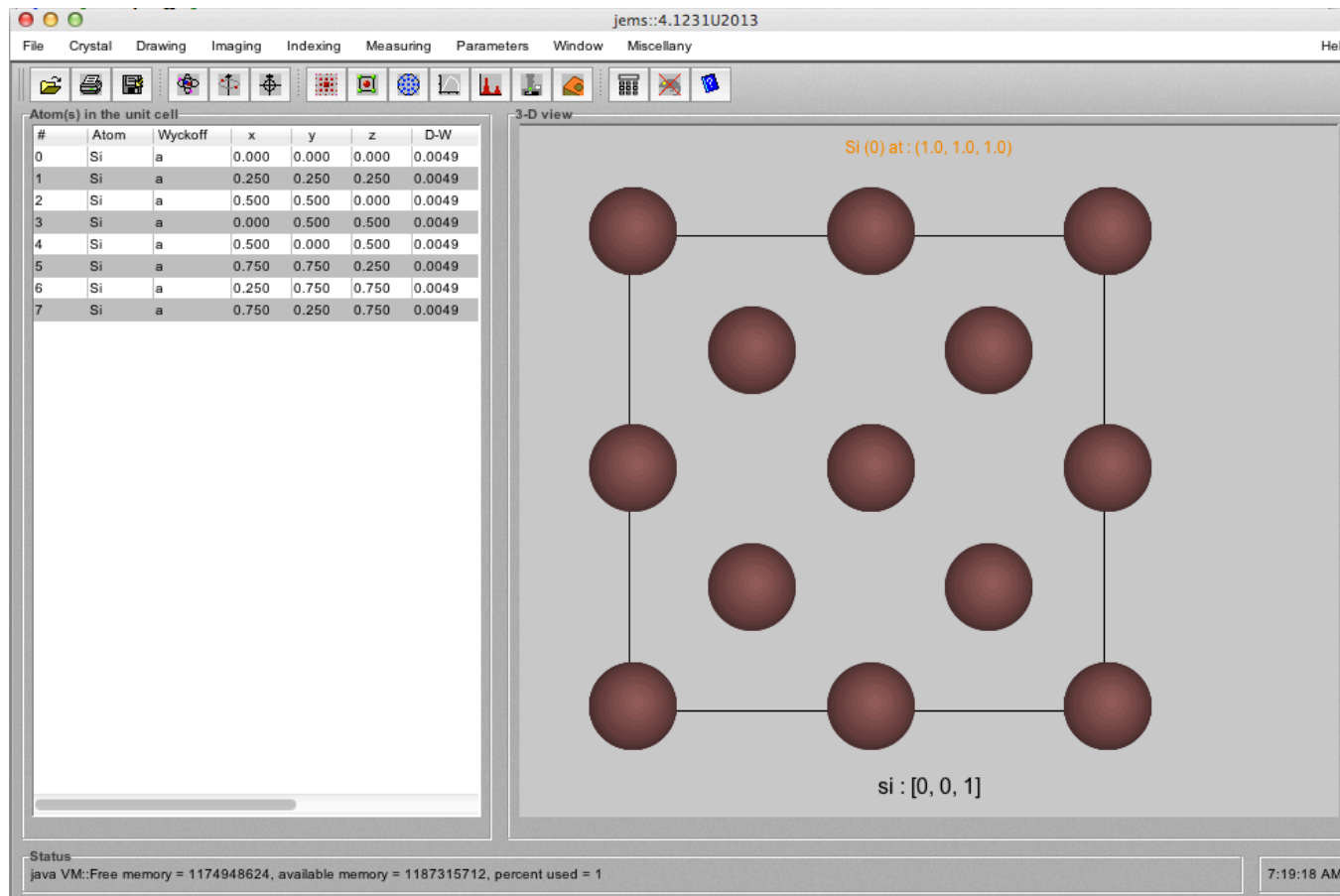
December 29, 2014

# Starting jems

Start jems with this icon:



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



The screenshot shows the JEMS software interface. The title bar reads 'jems::4.1231U2013'. The menu bar includes 'File', 'Crystal', 'Drawing', 'Imaging', 'Indexing', 'Measuring', 'Parameters', 'Window', 'Miscellany', and 'Help'. The toolbar contains various icons for file operations and crystal structure manipulation. The main window is divided into two panels. The left panel, titled 'Atom(s) in the unit cell', contains a table with the following data:

#	Atom	Wyckoff	x	y	z	D-W
0	Si	a	0.000	0.000	0.000	0.0049
1	Si	a	0.250	0.250	0.250	0.0049
2	Si	a	0.500	0.500	0.000	0.0049
3	Si	a	0.000	0.500	0.500	0.0049
4	Si	a	0.500	0.000	0.500	0.0049
5	Si	a	0.750	0.750	0.250	0.0049
6	Si	a	0.250	0.750	0.750	0.0049
7	Si	a	0.750	0.250	0.750	0.0049

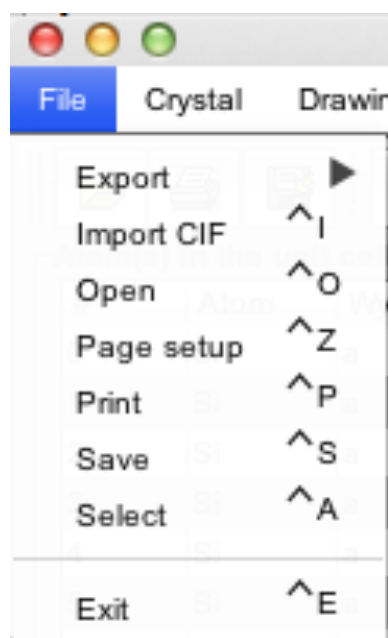
The right panel, titled '3-D view', shows a 3D projection of the Si crystal structure. It displays a 3x3 grid of dark red spheres representing Si atoms. The top-left atom is labeled 'Si (0) at: (1.0, 1.0, 1.0)'. The bottom-right atom is labeled 'si : [0, 0, 1]'. The status bar at the bottom shows 'Status: java VM: Free memory = 1174948624, available memory = 1187315712, percent used = 1' and the time '7:19:18 AM'.

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

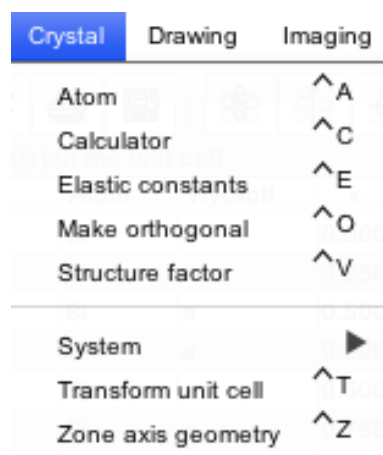
# jems MenuBar: part 1

File Crystal Drawing Imaging Indexing Measuring Parameters Window Miscellany

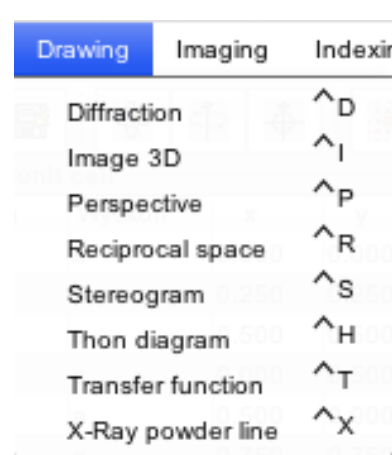
jems MenuBar.



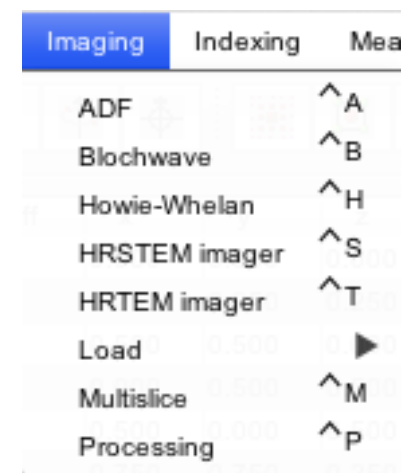
File menu: to import, open, or save crystal structures.



Crystal menu: to define crystal structures.

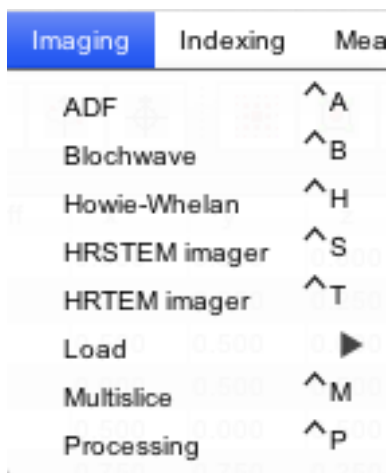


Drawing menu: to draw crystal structures, diffraction patterns.



Imaging menu: to perform Blochwave or multislice calculations.

# jems MenuBar: part 2



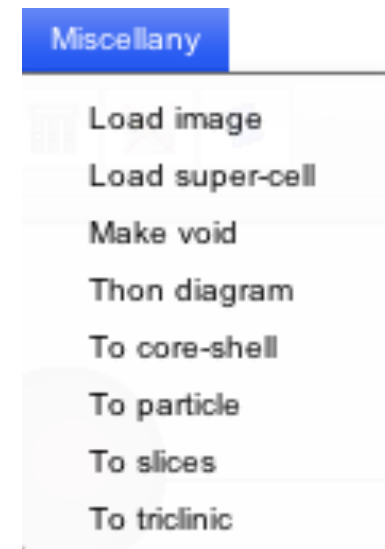
Indexing menu: to index diffraction patterns.



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

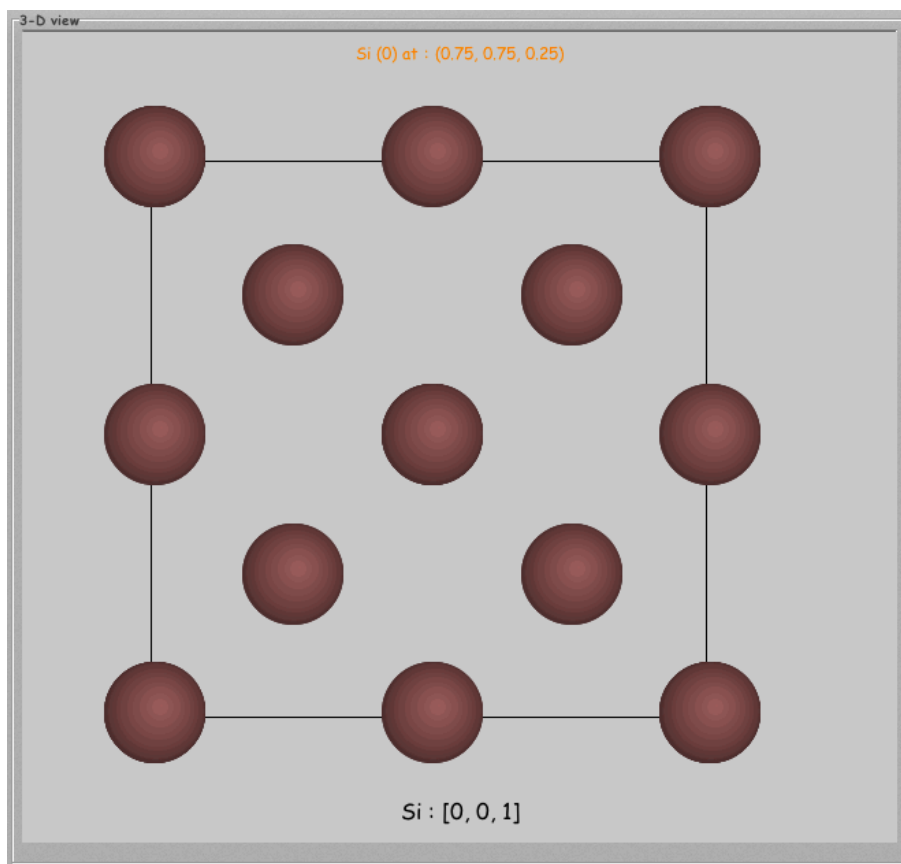
#	Atom	Wyckoff	x	y	z	D-W	Occ.	Absorp.	Charge	AFF
0	Si	a	0.000	0.000	0.000	0.0049	1.000	0.029	Def	0
1	Si	a	0.250	0.250	0.250	0.0049	1.000	0.029	Def	0
2	Si	a	0.500	0.500	0.000	0.0049	1.000	0.029	Def	0
3	Si	a	0.000	0.500	0.500	0.0049	1.000	0.029	Def	0
4	Si	a	0.500	0.000	0.500	0.0049	1.000	0.029	Def	0
5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

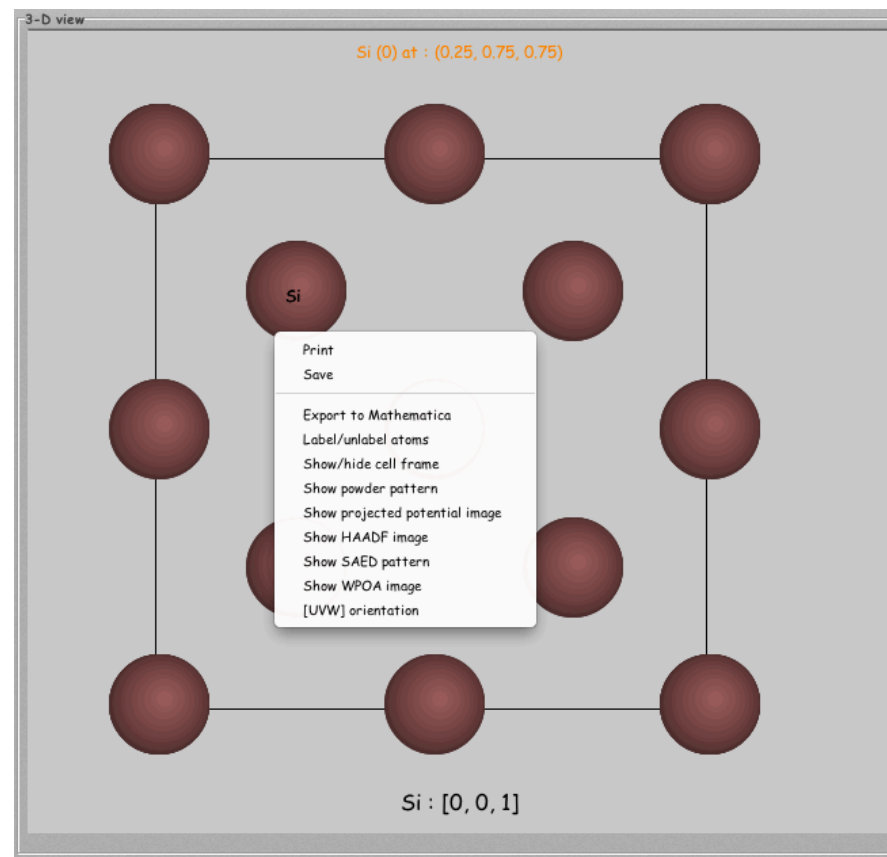
With the alternate non-centric  $Fd\bar{3}m$  space group the Si structure contains 8 atoms. Only the atom at Wyckoff position a,  $(x, y, z) = (0, 0, 0)$ , must be defined. All the other atom positions are generated by the symmetry operations of the space-group.

- ▶ 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.

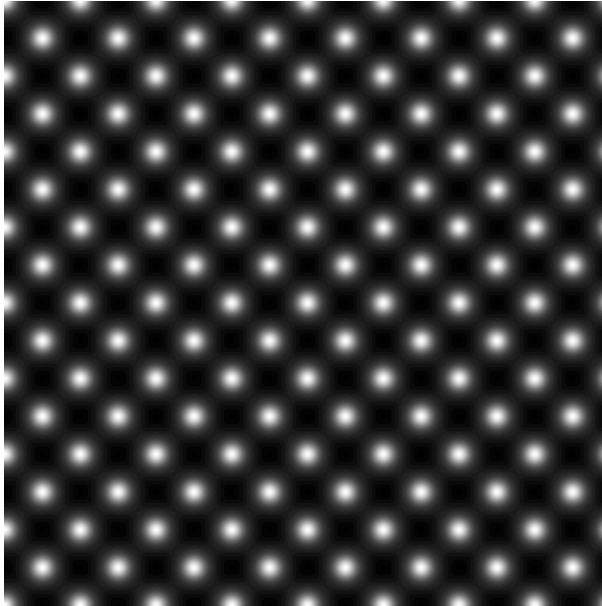


A mouse click on an atom position labels the atom and a right mouse click displays a popup menu (Ctrl-mouse click on Mac OSX).

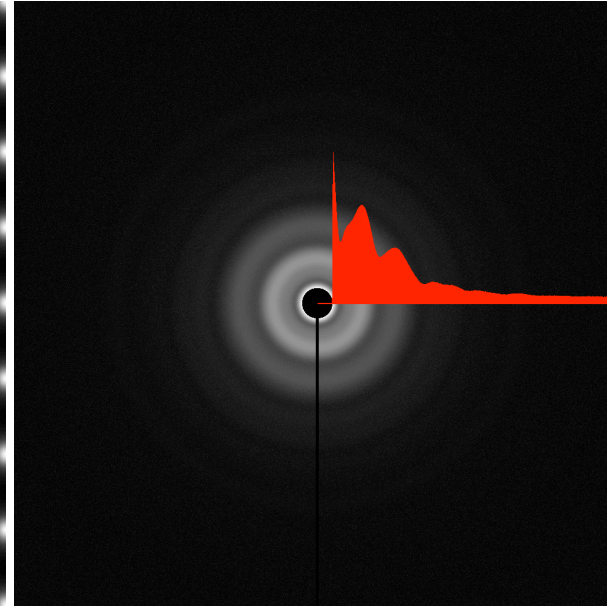
Note that a popup menu is attached to many drawings and tables. The popup menu of the right panel allows to:

- ▶ 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.

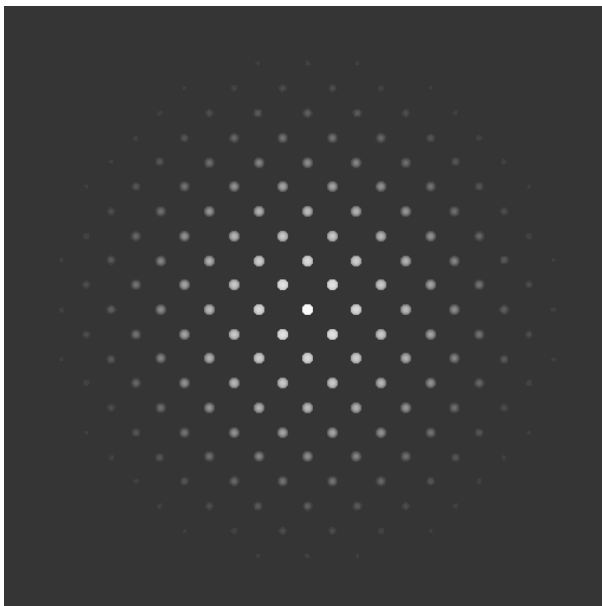
# Popup menus items



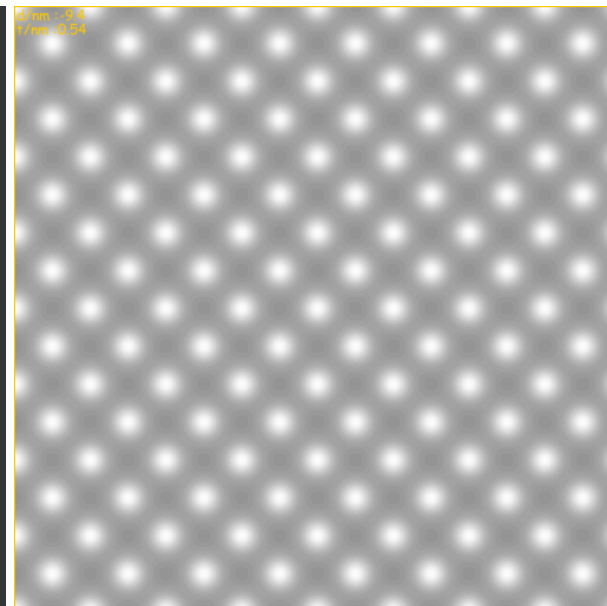
Si HAADF (FEI Titan pico).



Si powder pattern (randomly oriented Si unit cell).



Si [001] kinematical selected area diffraction pattern.



Si HRTEM image (WPOA) approximation.

# Defining a new model (crystal structure)

Several possibilities to define a new crystal structure:

- ▶ When the structure is present in `../jemsData/Cubic` or `../jemsData/Hexagonal`, ... load it with menu File, menu item Open (**File**  $\implies$  **Open**). jems crystal structures are text files that can be edited using TextEdit or any text processing program. jems structures are saved in .txt format by default <sup>1</sup>.
- ▶ When the structure is provided as a .cif file, load it using **File**  $\implies$  **Import**. You can check .cif files using program **Encifer**. jems creates .cif files (**File**  $\implies$  **Save**). More than 100'000 structures are available in crystallographic data bases such as:
  - ▶ American Mineralogist Crystal Structure DataBase ([http://www.minsocam.org/msa/crystal\\_database.html](http://www.minsocam.org/msa/crystal_database.html)).
  - ▶ Inorganic Crystal Structure Database - ICSD (<http://www.fiz-karlsruhe.de/icsd.html>).
  - ▶ Crystallography Open Database - COD (<http://www.crystallography.net>).
- ▶ When the structure has not yet been defined one should have available:
  - ▶ the lattice parameters (a,b, c,  $\alpha$ ,  $\beta$ ,  $\gamma$ ).
  - ▶ the space-group or the Regular Point System code (symmetry operations as  $\{x, y, z\}$ ,  $\{x + \frac{1}{2}, y, z\}$ , ...).
  - ▶ the atom types and positions.

<sup>1</sup>60 different crystal structures are also available under **File**  $\implies$  **Select**.

# Defining the germanium crystal structure

The simplest way to define the germanium structure consists in modifying the Si structure:

- ▶ Change the atom type ( $Si \rightarrow Ge$ ).
- ▶ Change the lattice parameter ( $0.54309 \rightarrow 0.5689$ ).

#	Atom	Wyckoff	x	y	z	D-W
0	Si	a	0.000	0.000	0.000	0.0049
1	Si	a	0.250	0.250	0.250	0.0049
2	Si	a	0.500	0.500	0.000	0.0049
3	Si	a	0.000	0.500	0.500	0.0049
4	Si	a	0.500	0.000	0.500	0.0049
5	Si	a	0.750	0.750	0.250	0.0049
6	Si	a	0.250	0.750	0.750	0.0049
7	Si	a	0.750	0.250	0.750	0.0049

3 toolbuttons to modify the Si structure into Ge structure.

They correspond to **Crystal**  $\Rightarrow$  **Atom**  $\Rightarrow$  , **Crystal**  $\Rightarrow$  **System**  $\Rightarrow$  **RPS code** and **Crystal**  $\Rightarrow$  **System**  $\Rightarrow$  **Space-group** respectively.

# Atom position

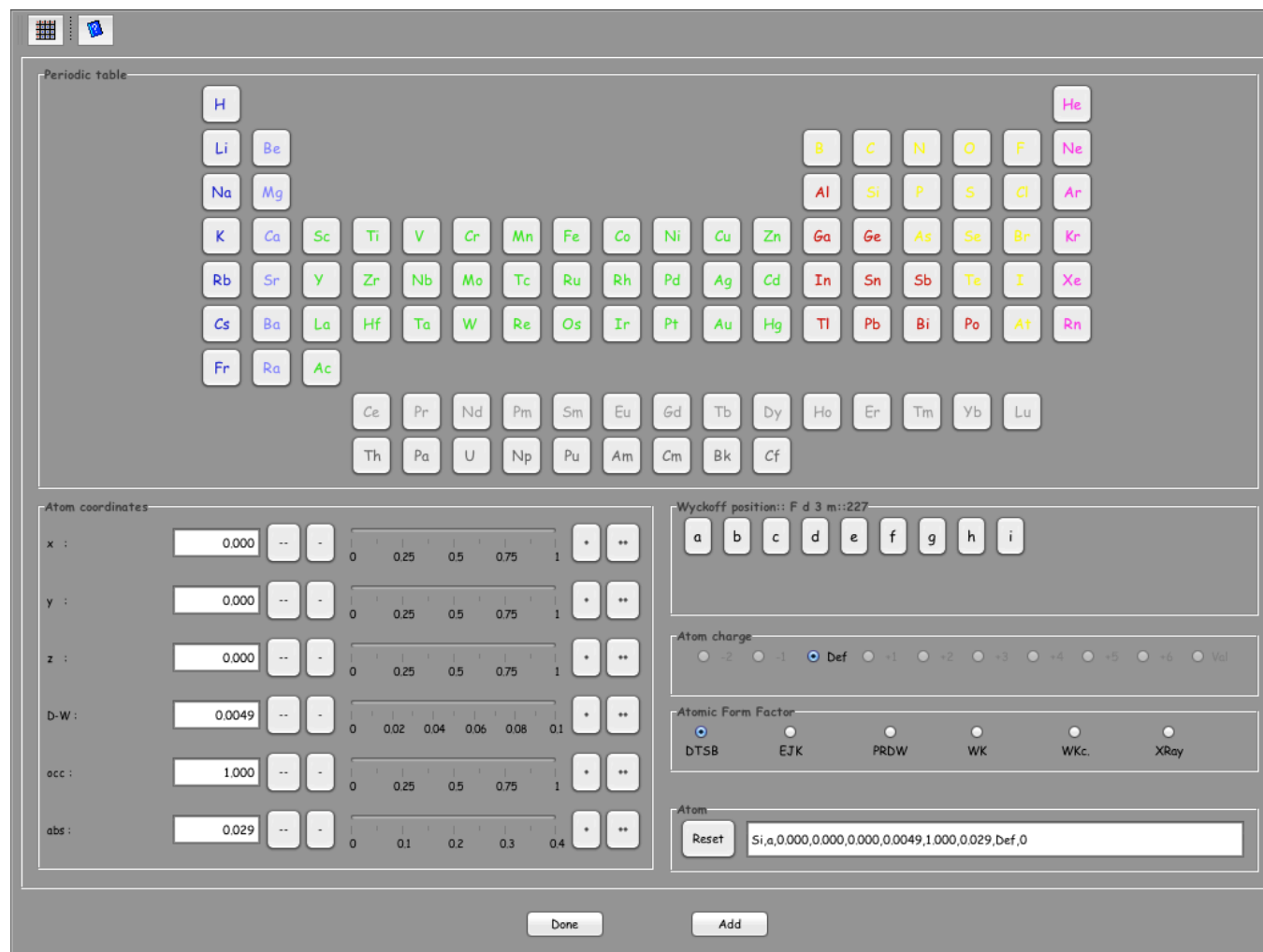
The atom position tool opens a dialogue that displays the atoms necessary to fully describe the structure. For Si F d-3m we only have to change symbol Si to symbol Ge.



3 menu items or icons to define a new crystal structure.

Select the atom and and push the **M** button to open the atom editor.

# Atom editor

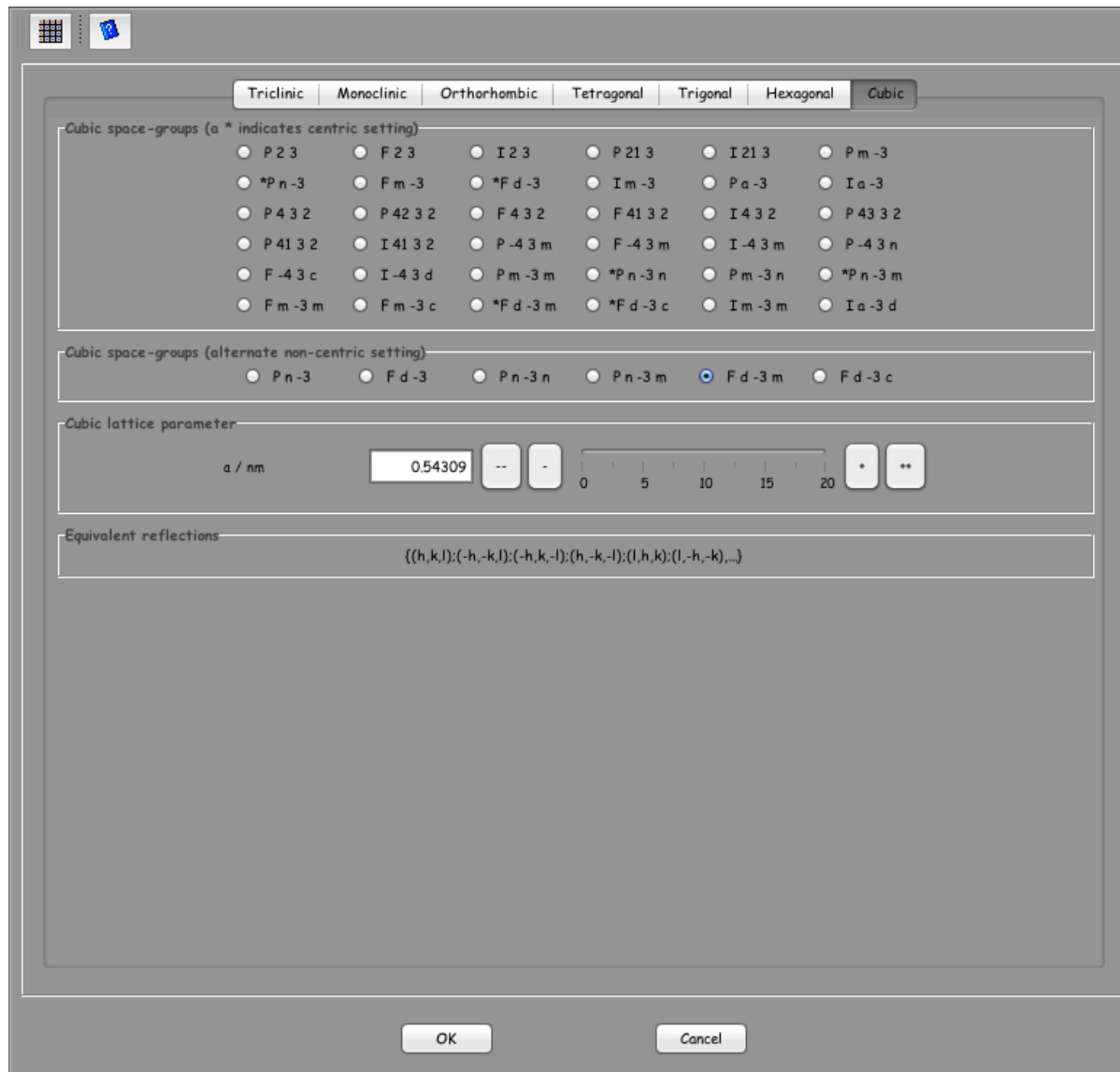


Atom editor allows to define the atom type, its  $(x, y, z)$  position ( $0 \leq (x, y, z) < 1$ ).

When the space-group is defined before launching the atom editor the appropriate Wyckoff position button (here a to i) set the  $(x, y, z)$  atom coordinates. Here only push the **Ge** to define Ge. Then push **Add** to replace Si by Ge in the atoms list. Finally close the dialogue (using **Done**) and close the atom definition dialogue (using **replace**).



# Ge lattice parameter and space-group selection



The space-group dialogue allows to set the space-group and lattice parameters of the Ge crystal.

Ge has space-group  $Fd-3m$  and only the  $a$  lattice parameter has to be set. You can use  $+$ ,  $++$ , ... together with keyboard keys **Alt**, **Ctrl**, **Cmd** or **Shift** to speed up the change. When set push **Ok** to close the dialogue.

# Saving the newly defined structure

The newly defined structure still appears as **Si** in the right panel. Save it under name Ge.txt. When loading or saving crystal structures, images, ... jems by default opens the folder containing the default crystal (i.e. the crystal that is loaded when jems starts).

The screenshot displays the JEMS software interface. On the left, a table titled "Atom(s) in the unit cell" lists the coordinates for 8 Germanium atoms. On the right, a 3-D view shows these atoms as green spheres in a diamond lattice structure. The status bar at the bottom indicates the current filename is "Ge : [0, 0, 1]".

Atom	Wyckoff	x	y	z	D-W
Ge	a	0.000	0.000	0.000	0.0049 1.
Ge	a	0.000	0.500	0.500	0.0049 1.
Ge	a	0.500	0.500	0.000	0.0049 1.
Ge	a	0.500	0.000	0.500	0.0049 1.
Ge	a	0.750	0.250	0.750	0.0049 1.
Ge	a	0.250	0.250	0.250	0.0049 1.
Ge	a	0.250	0.750	0.750	0.0049 1.
Ge	a	0.750	0.750	0.250	0.0049 1.

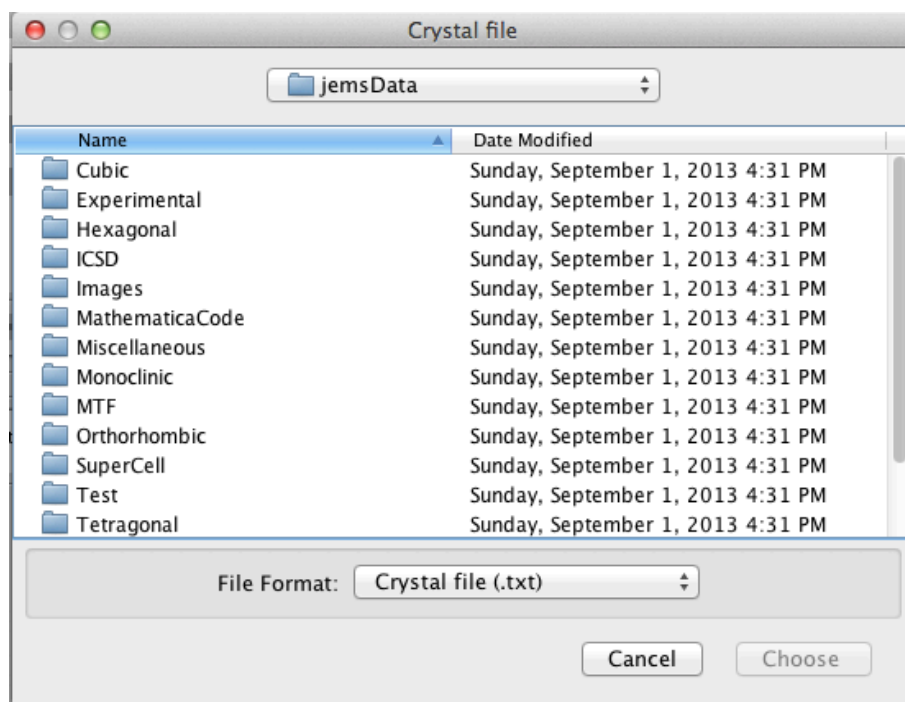
3-D view  
Ge (0) at : (0,0,0,1,0)  
Ge : [0, 0, 1]

Status  
java VM::Free memory = 2268352664, available memory = 2282749952, percent used = 1  
4:49:01 PM

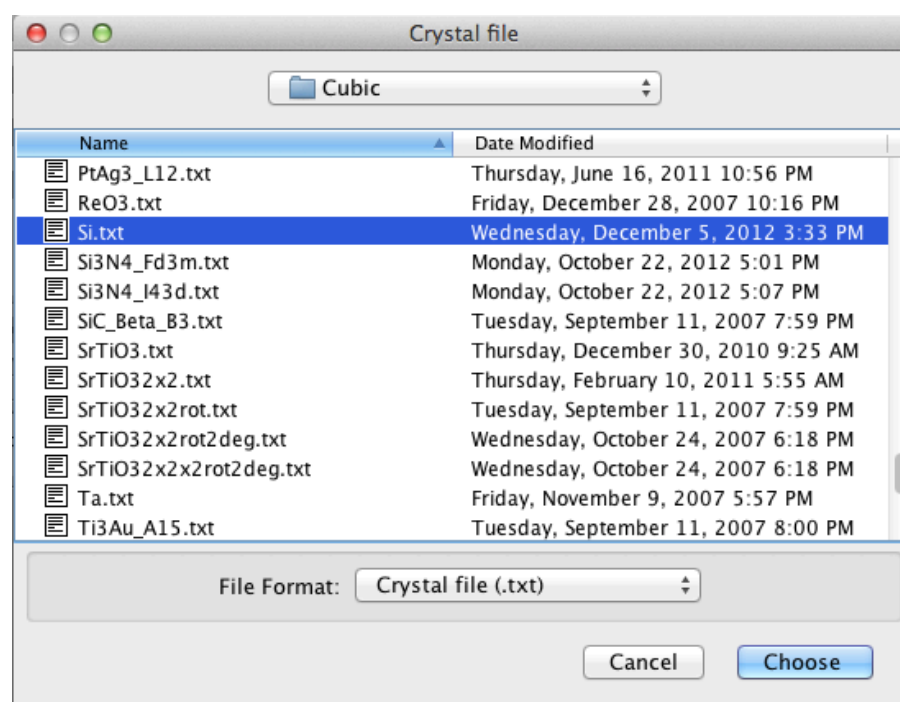
Saving the structure sets the crystal filename that labels the right panel.

# jems crystal structures

jems contains 150 different crystal structures (.txt). They are placed in different folders depending on their system (cubic, hexagonal, ...).



Crystal files are organised by crystal system.



Si crystal file.

# Importing .cif file

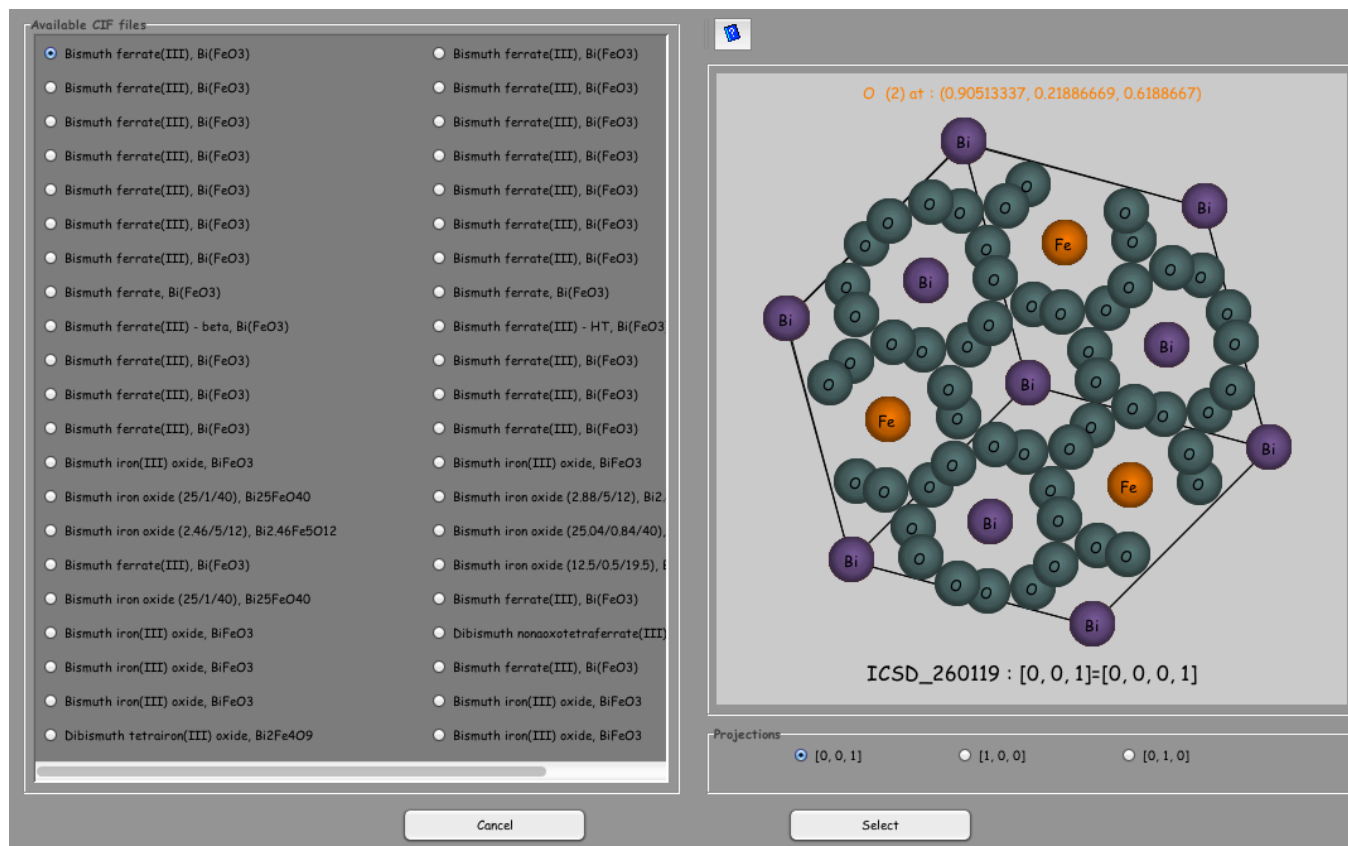
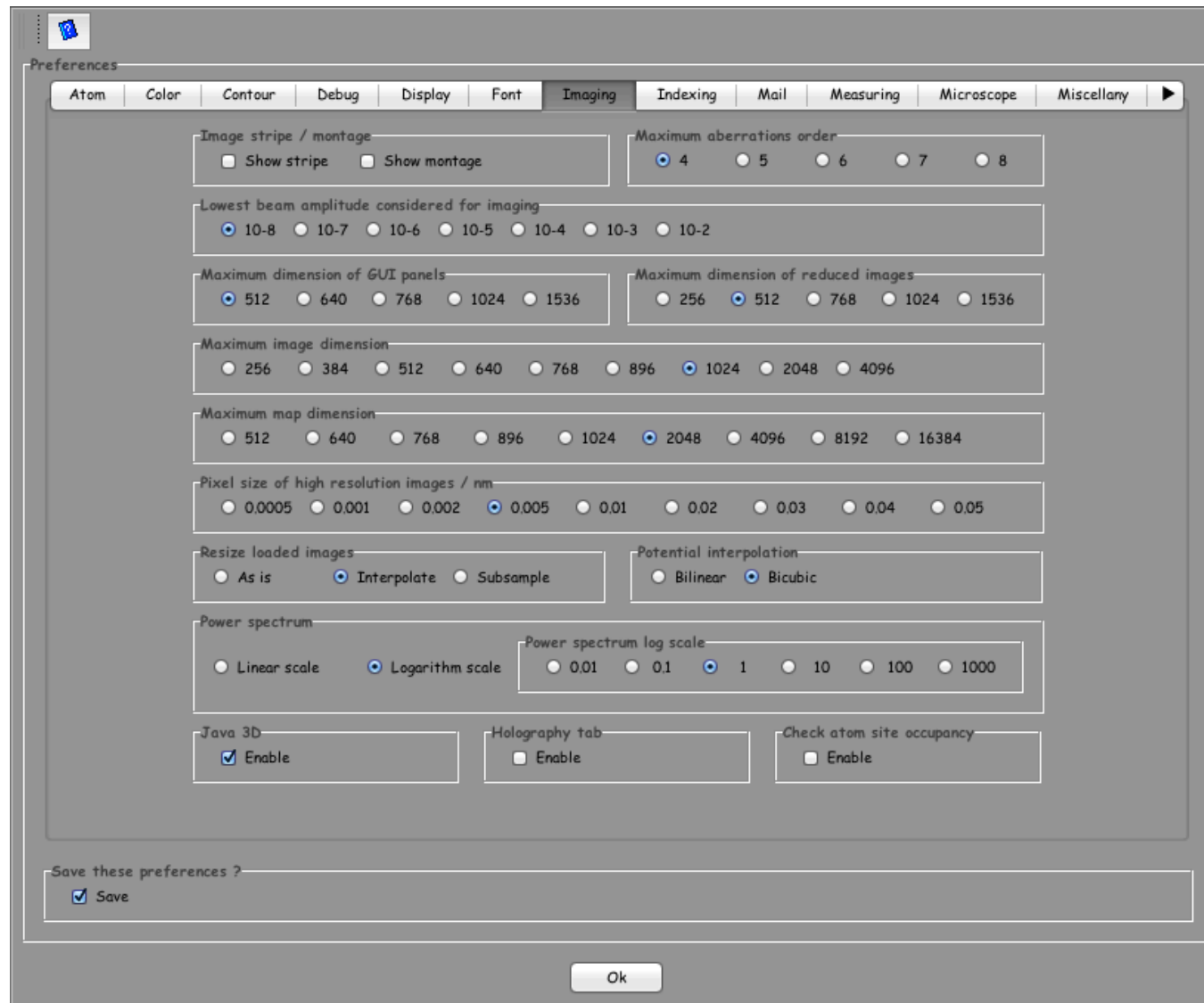


Figure: BiFeO3.cif file defines 50 different crystal structures.

Any one in the table can be projected along the [001], [100] or [010] directions before selecting it (**Select**). After loading the .cif structure it is advisable to verify its space-group setting.

# 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.

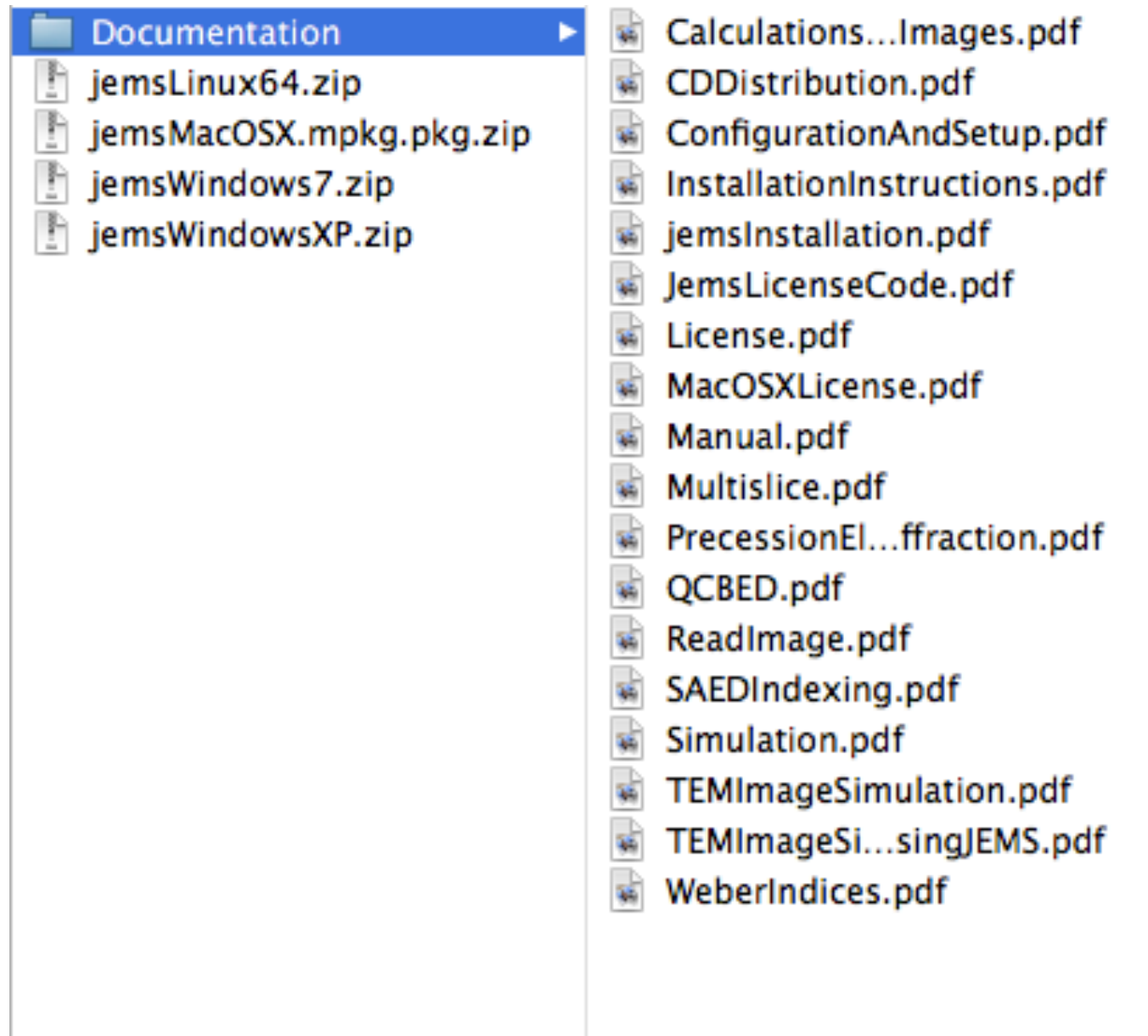
# Today's HRTEM image simulation lab

We have already seen how to load or define a crystal structure. I suggest to open the Si crystal structure available in folder ASU-Labs. 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.

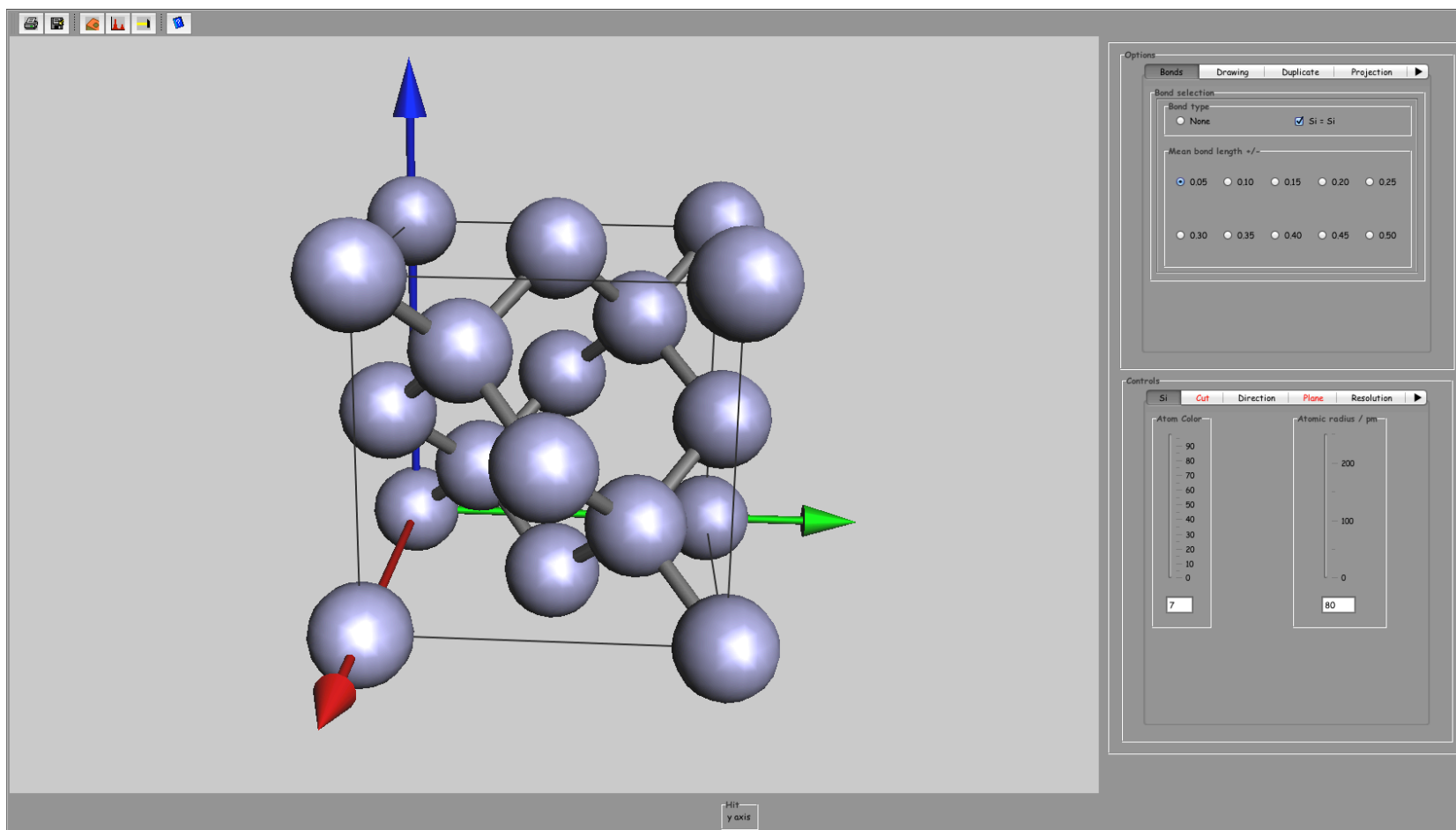
We will finally learn how to define a super-cell and use it to perform HRTEM image simulation. More information is available in jems [../pdfFiles](#) folder.

# 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.

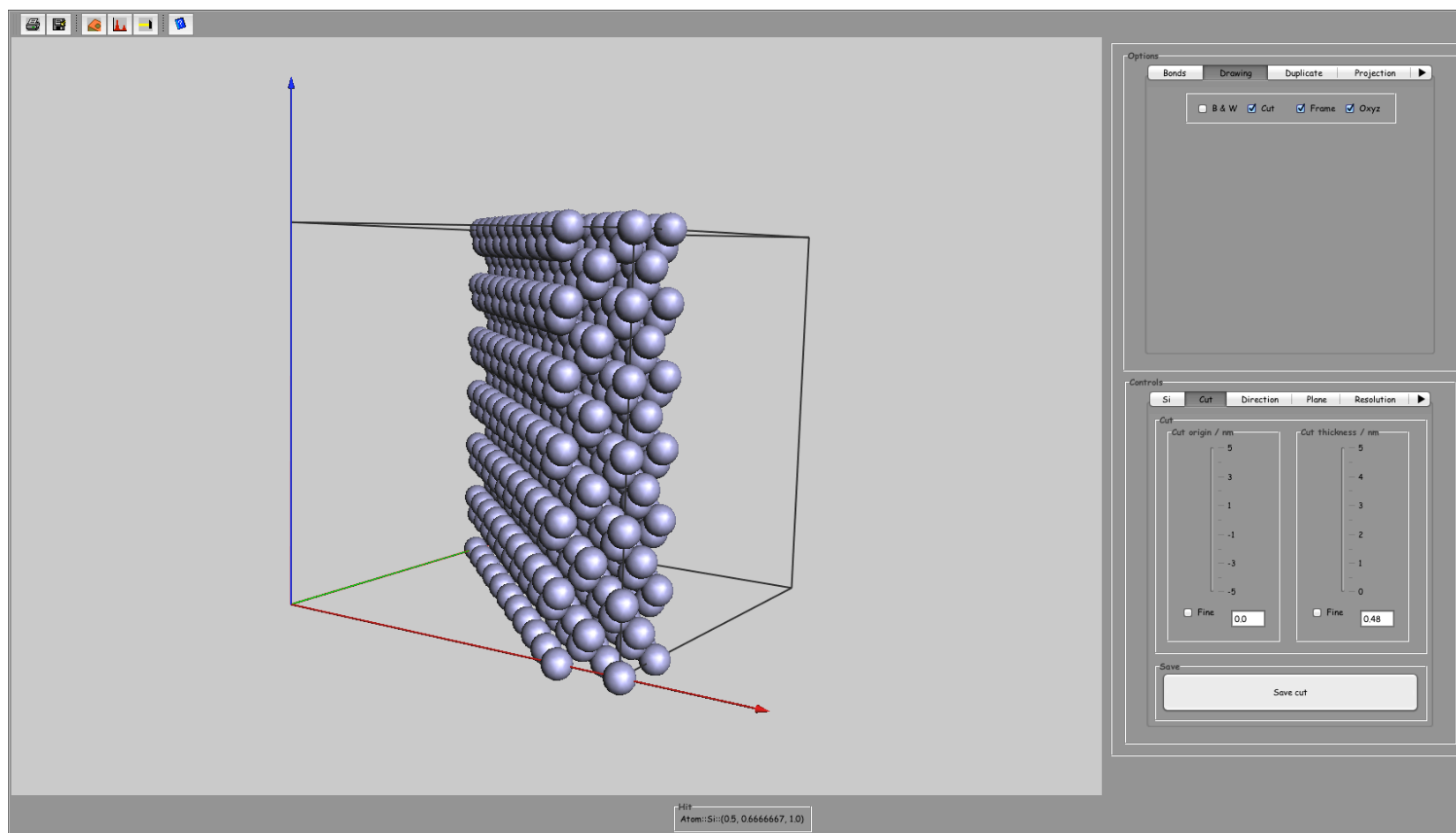


One can change the atom color, size or add bonds, cut the unit cell by parallel (hkl) planes, etc. One can also duplicate the unit cell in order to generate larger unit cells.



# 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 the following 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, including reflections like (0,0,0), (1,1,1), (1,-1,1), and (3,1,1). On the right, there are control panels. The top panel allows setting h max, k max, and l max, each with a numeric input (set to 5) and a slider (0 to 15). Below this is a box for 'Default maximum spacing : 15.946 [nm-1]'. The middle panel shows '(h,k,l) number : 701'. The bottom panel, titled 'Atomic Form Factor', has radio buttons for DT5B, EJK, PRDW, WK, WKc, and XRay, with a checked box 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

h max. 5

k max. 5

l max. 5

Default maximum spacing : 15.946 [nm-1]

(h,k,l) number : 25

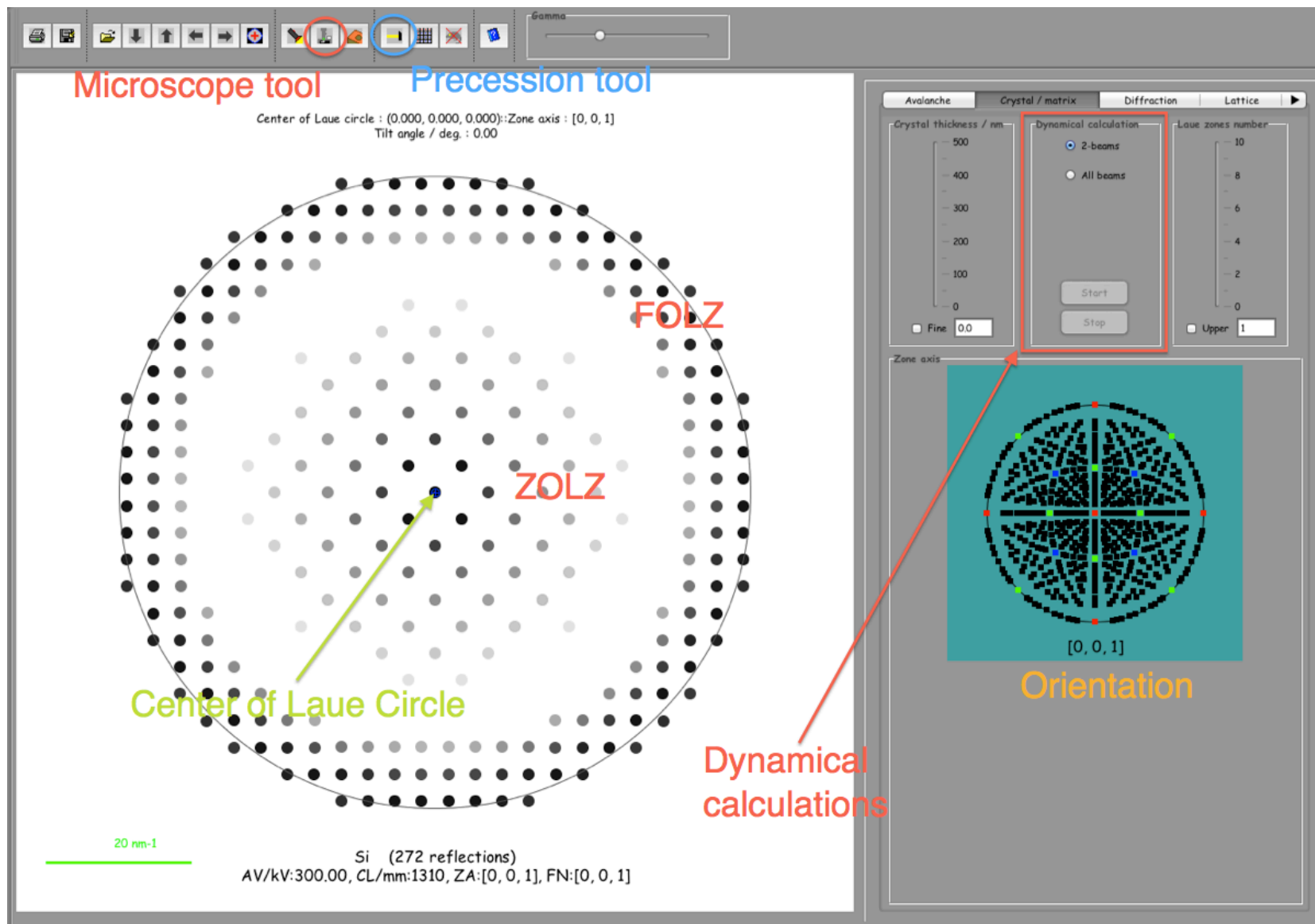
Atomic Form Factor

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).

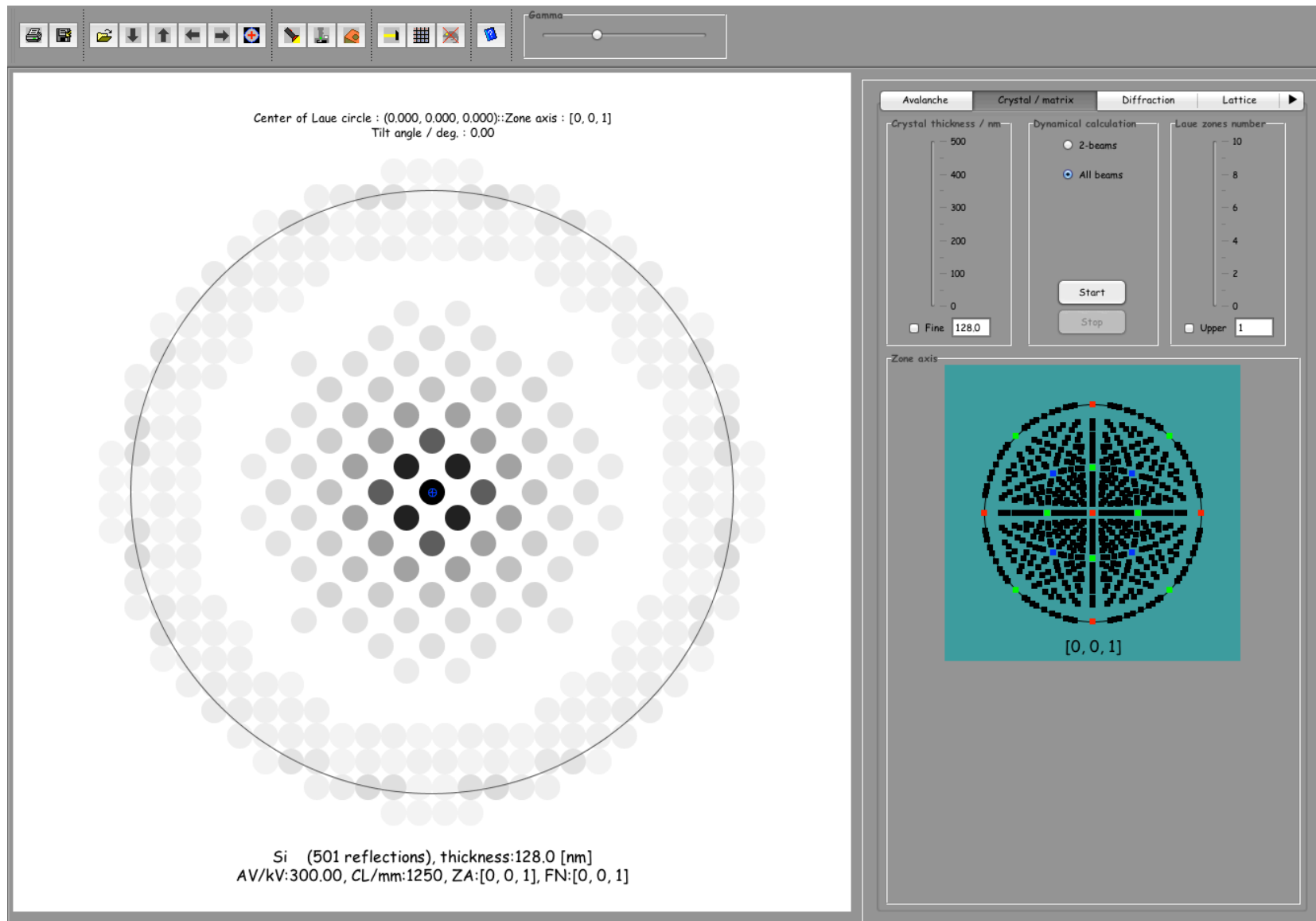
# SAED kinematical diffraction



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  $50 \lambda$ .

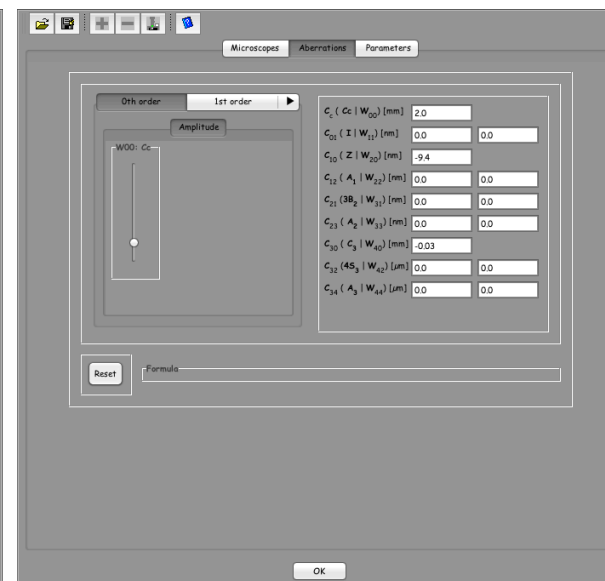
**Imaging  $\implies$  Blochwave**

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

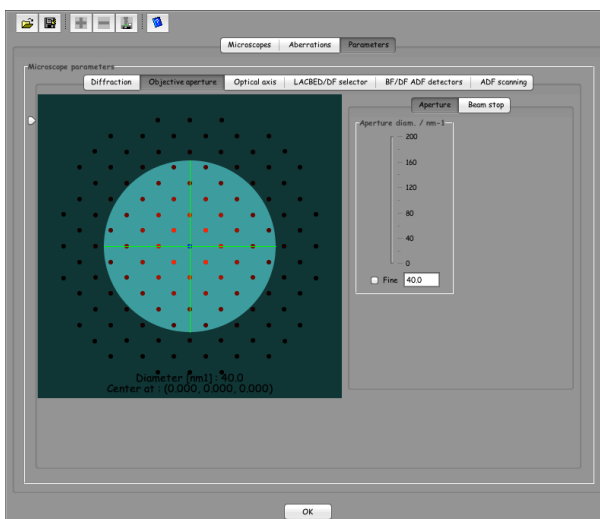
# Select the microscope: Parameters $\implies$ Microscope



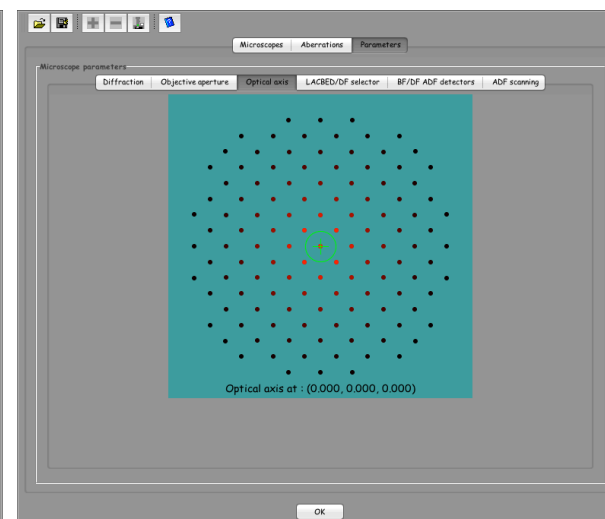
Select a microscope. When not available, edit a new one  $\oplus$



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



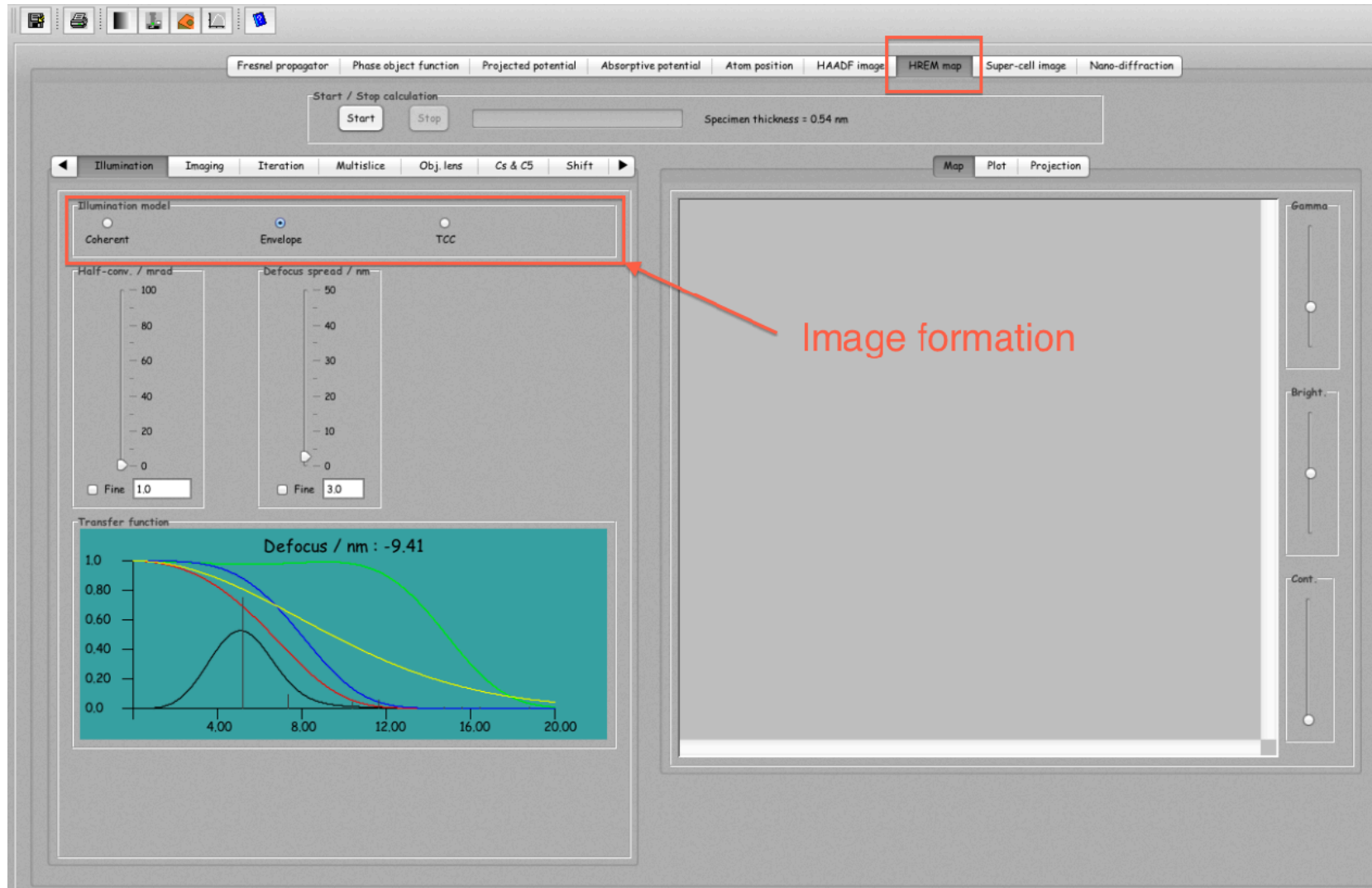
Objective aperture diameter  $\geq$  information transfer.



Optical axis can be moved to simulated dark field images.



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

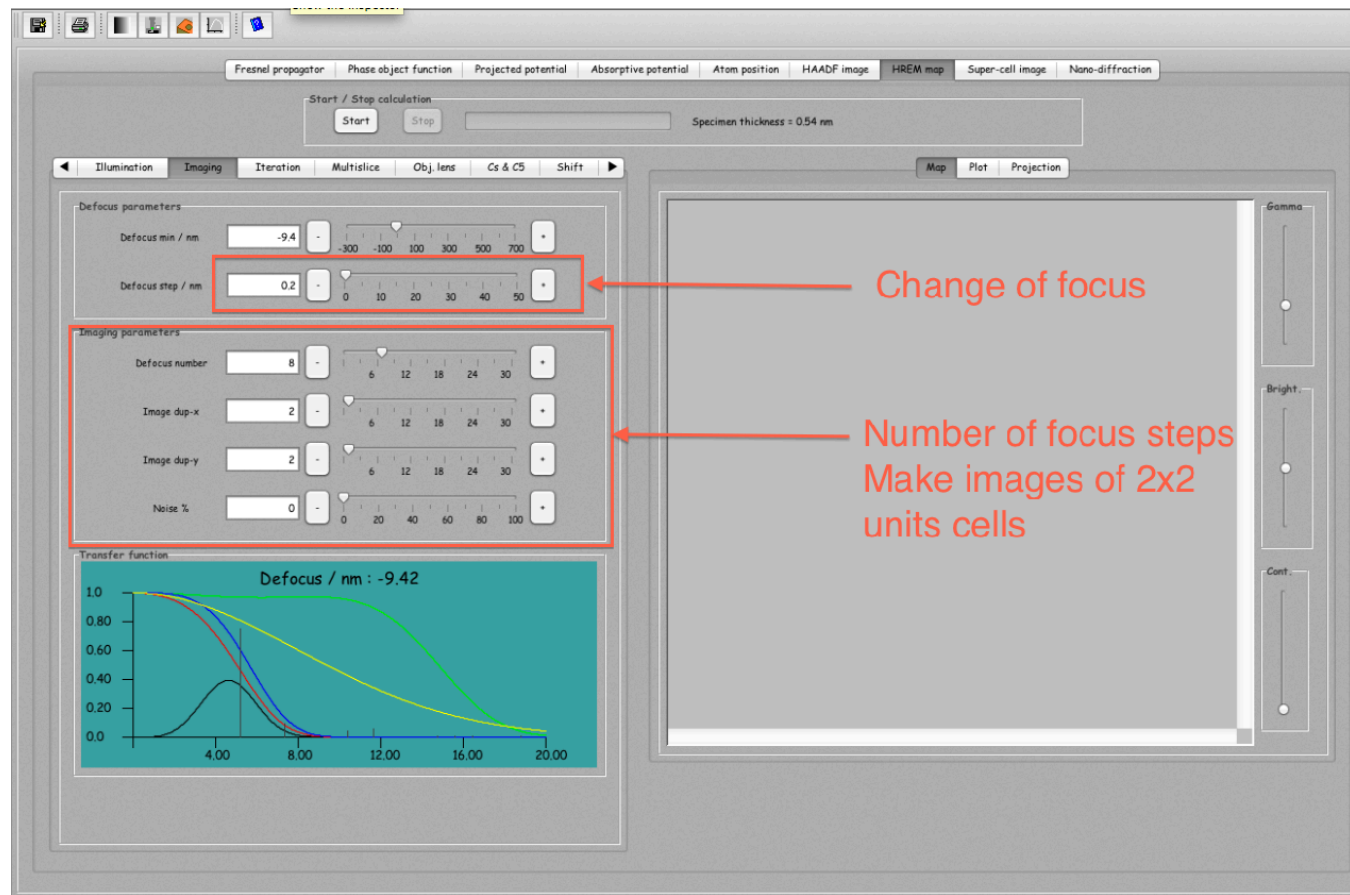


HRTEM image calculation by multislice approach.

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

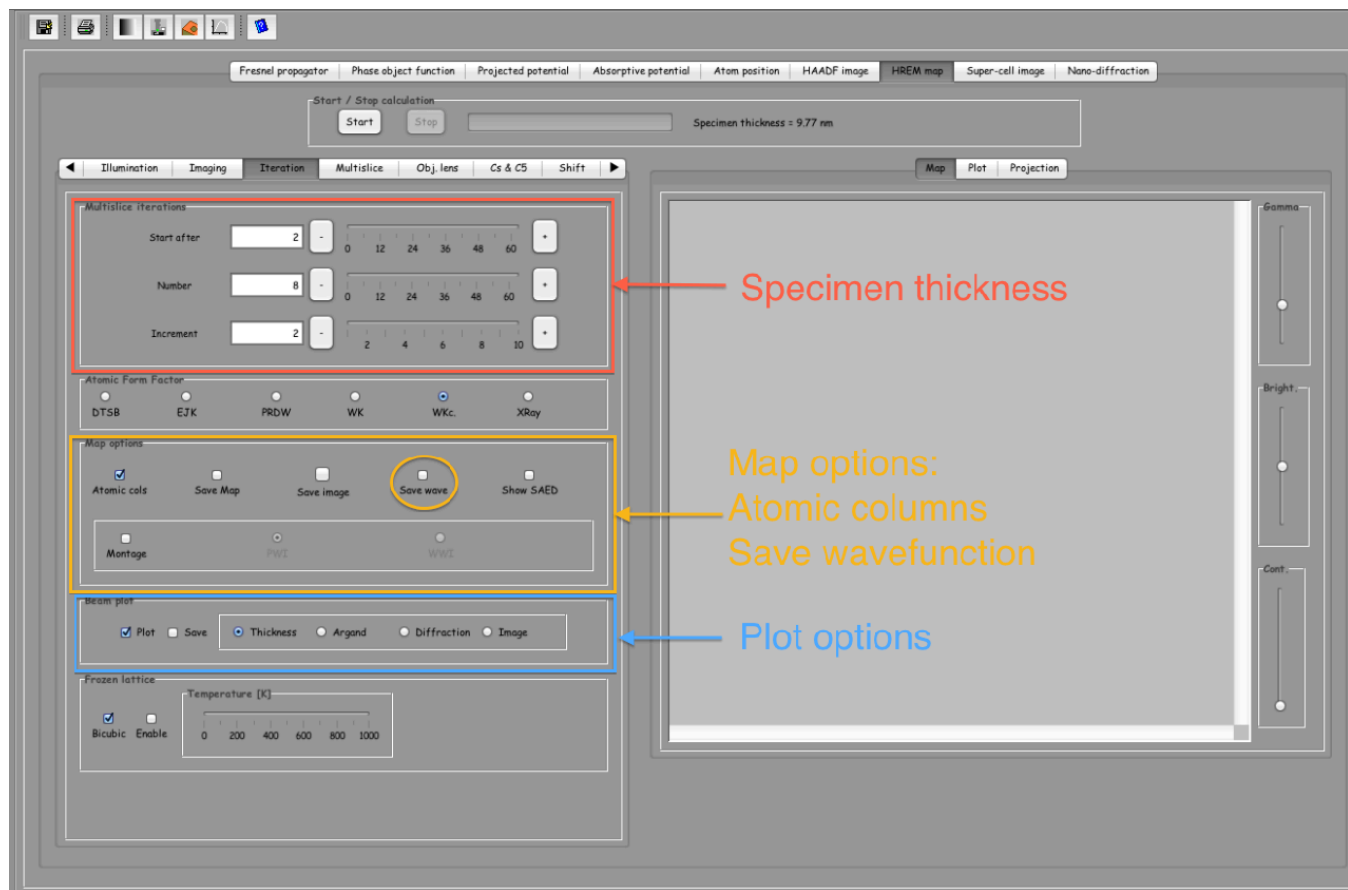


HRTEM image calculation by multislice approach.

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.

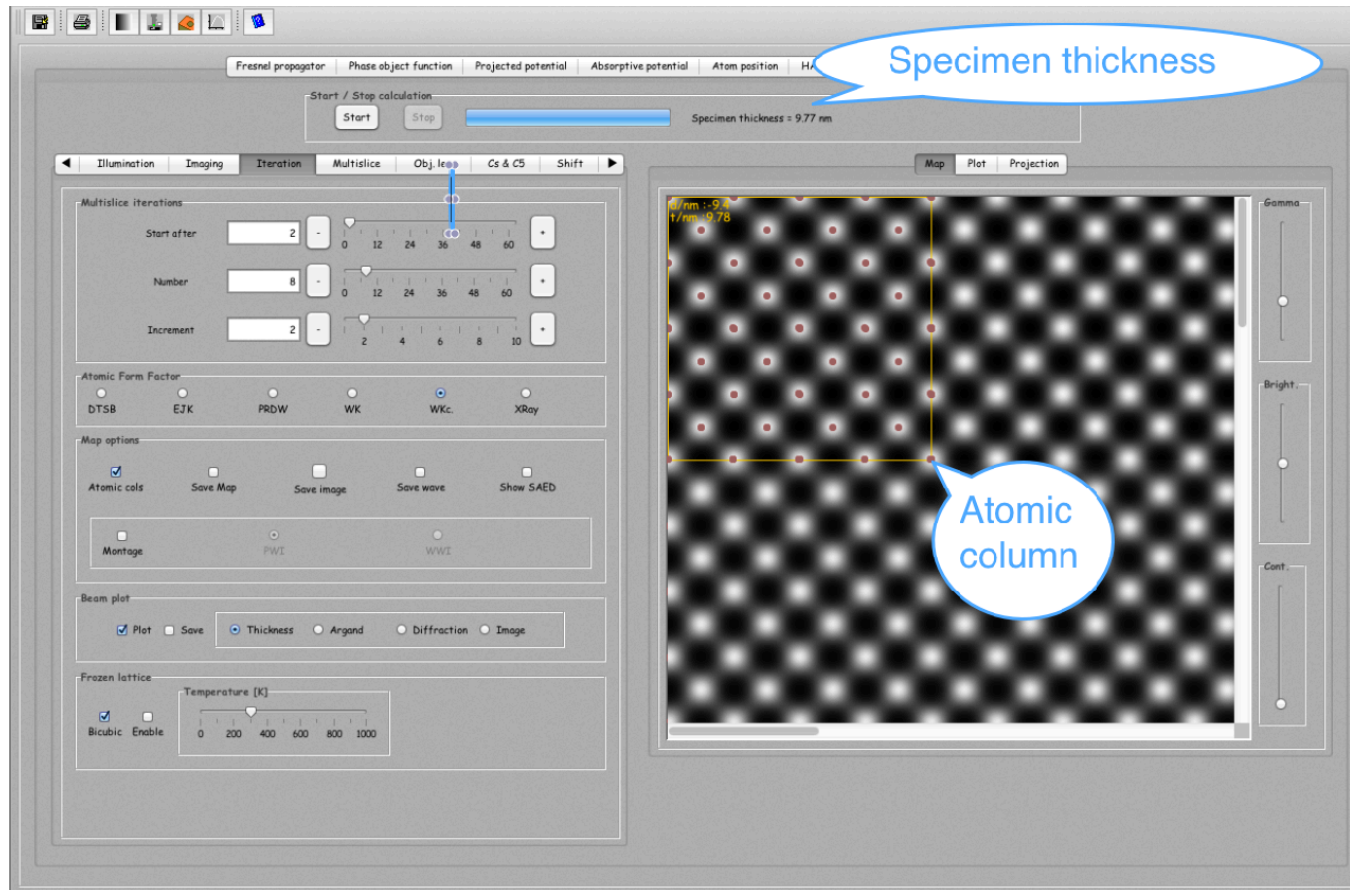
# Select the Iteration tab



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.

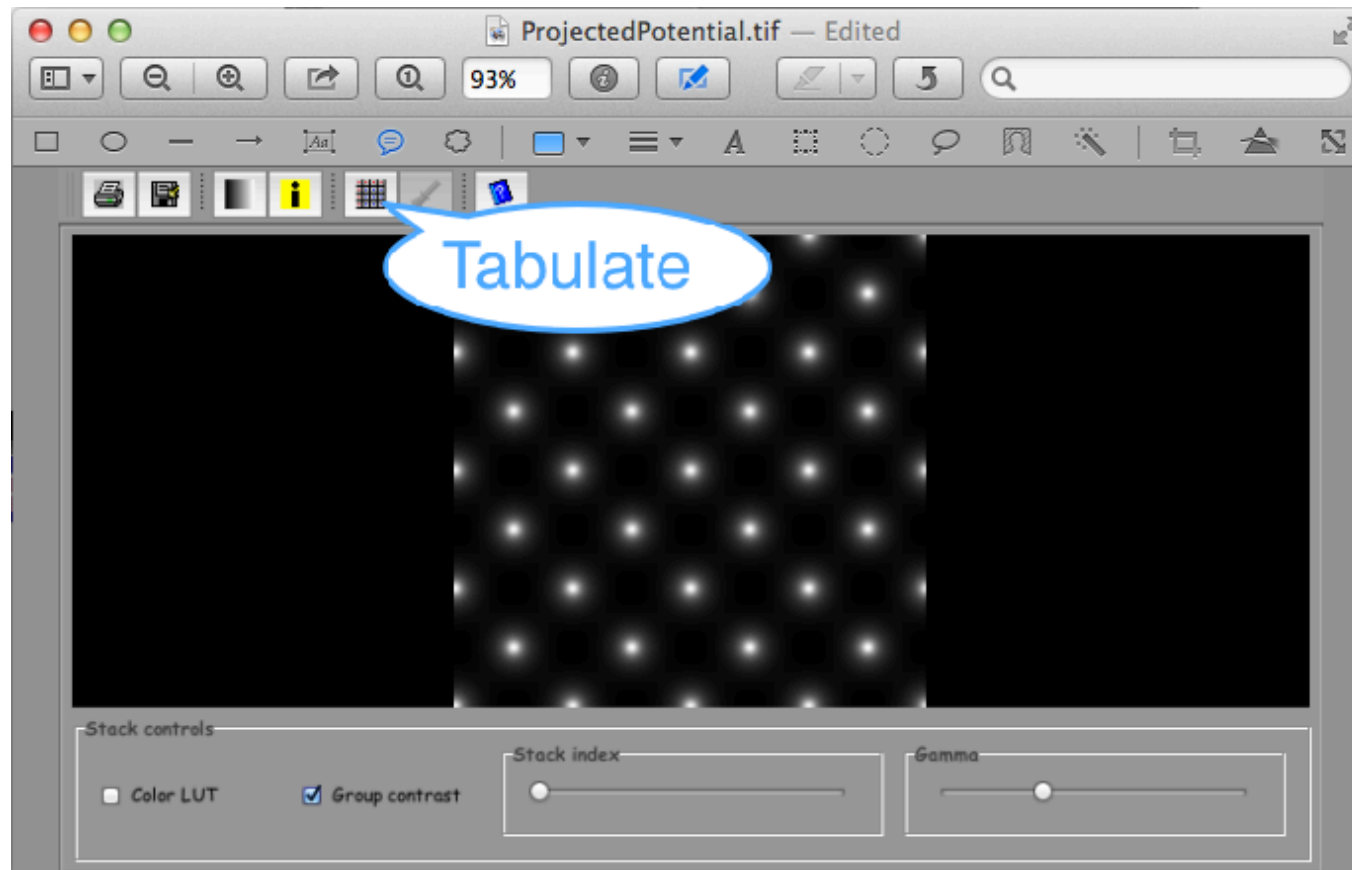


`start` calculates the map.

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

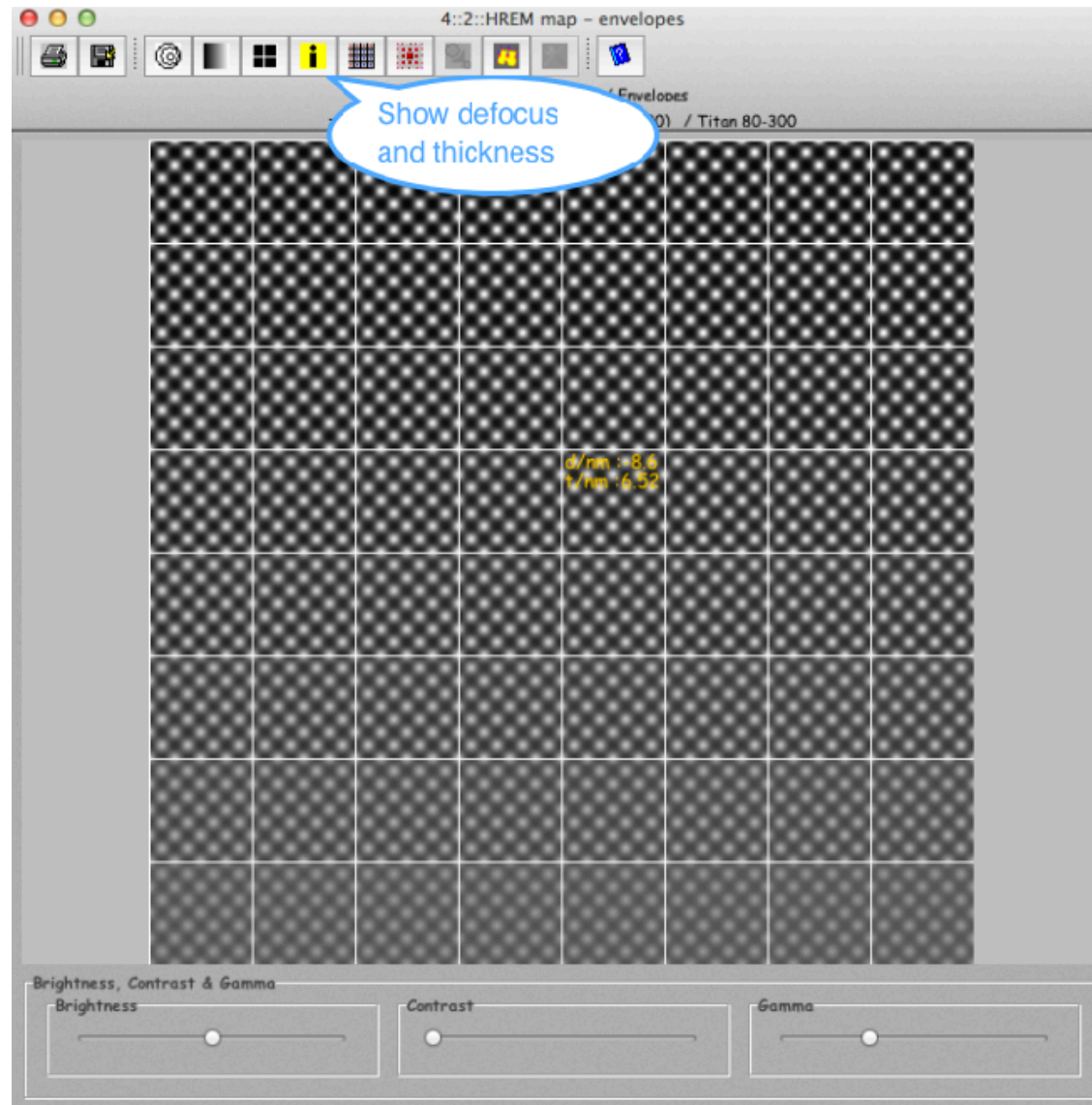


Projected potential of the slice.

Notice that:

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

# HREM map



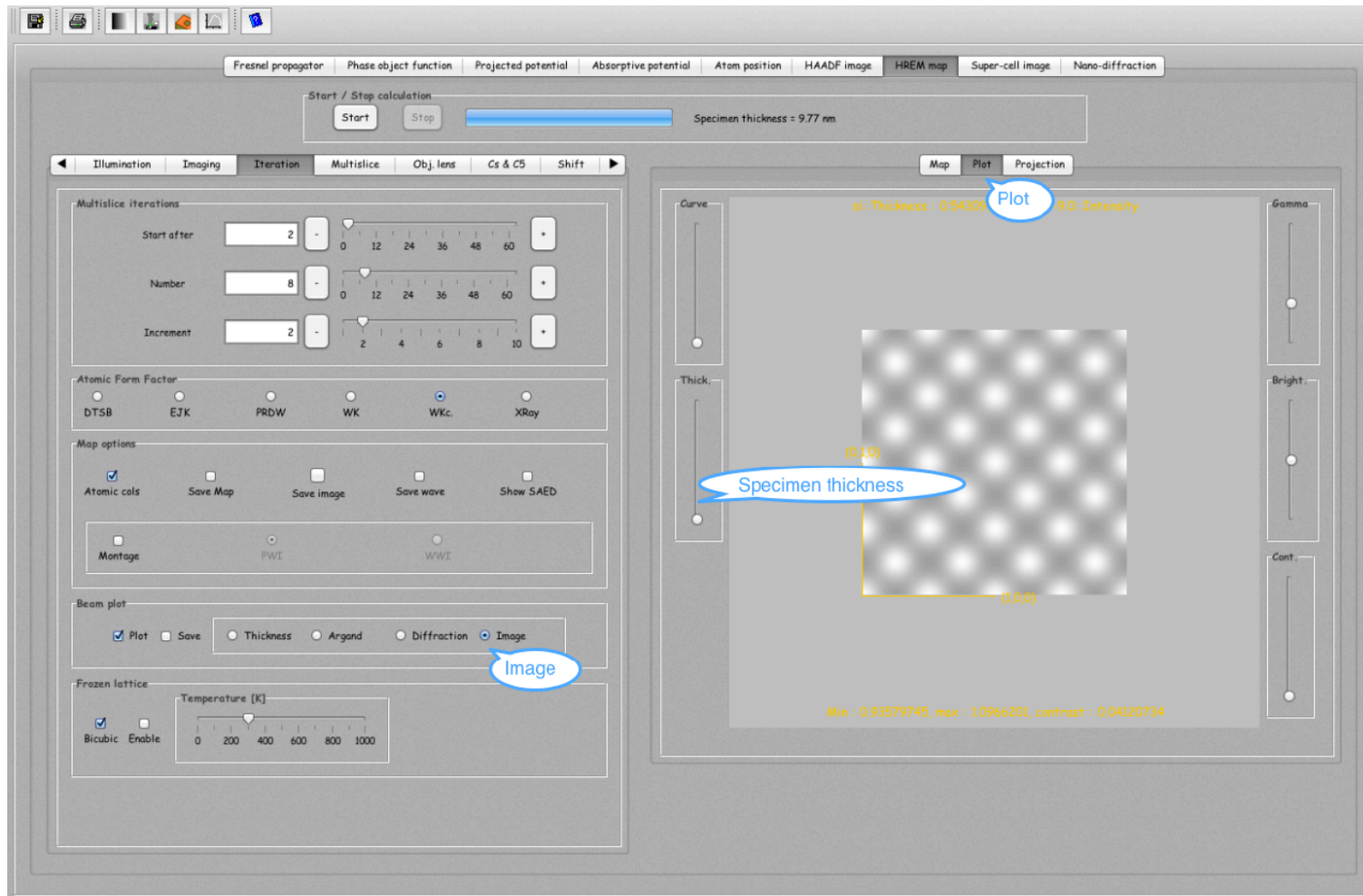
Specimen thickness and defocus are displayed for each image.

Notice that:

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





# Interactive image calculation and display




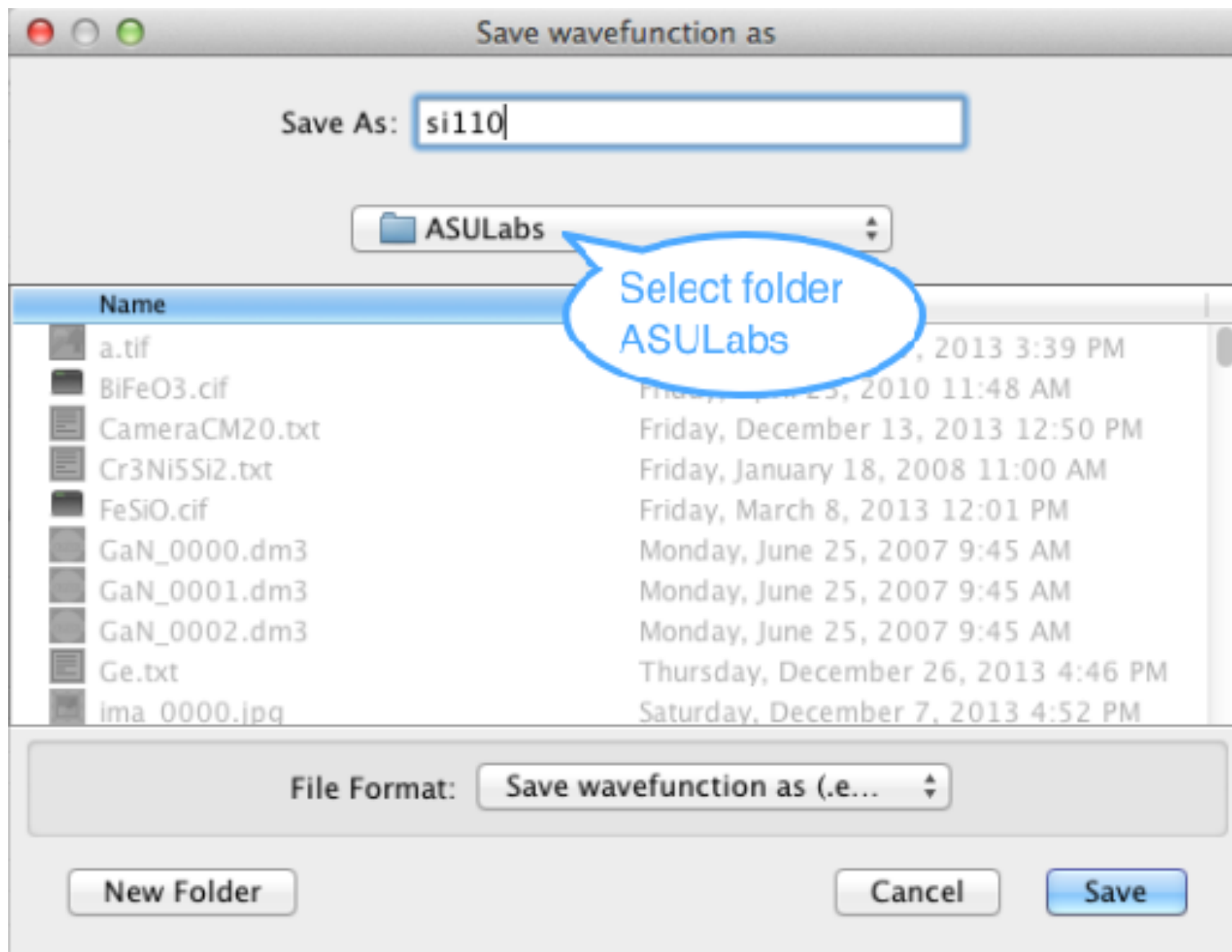
Select  Image and  Plot and change specimen thickness.

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

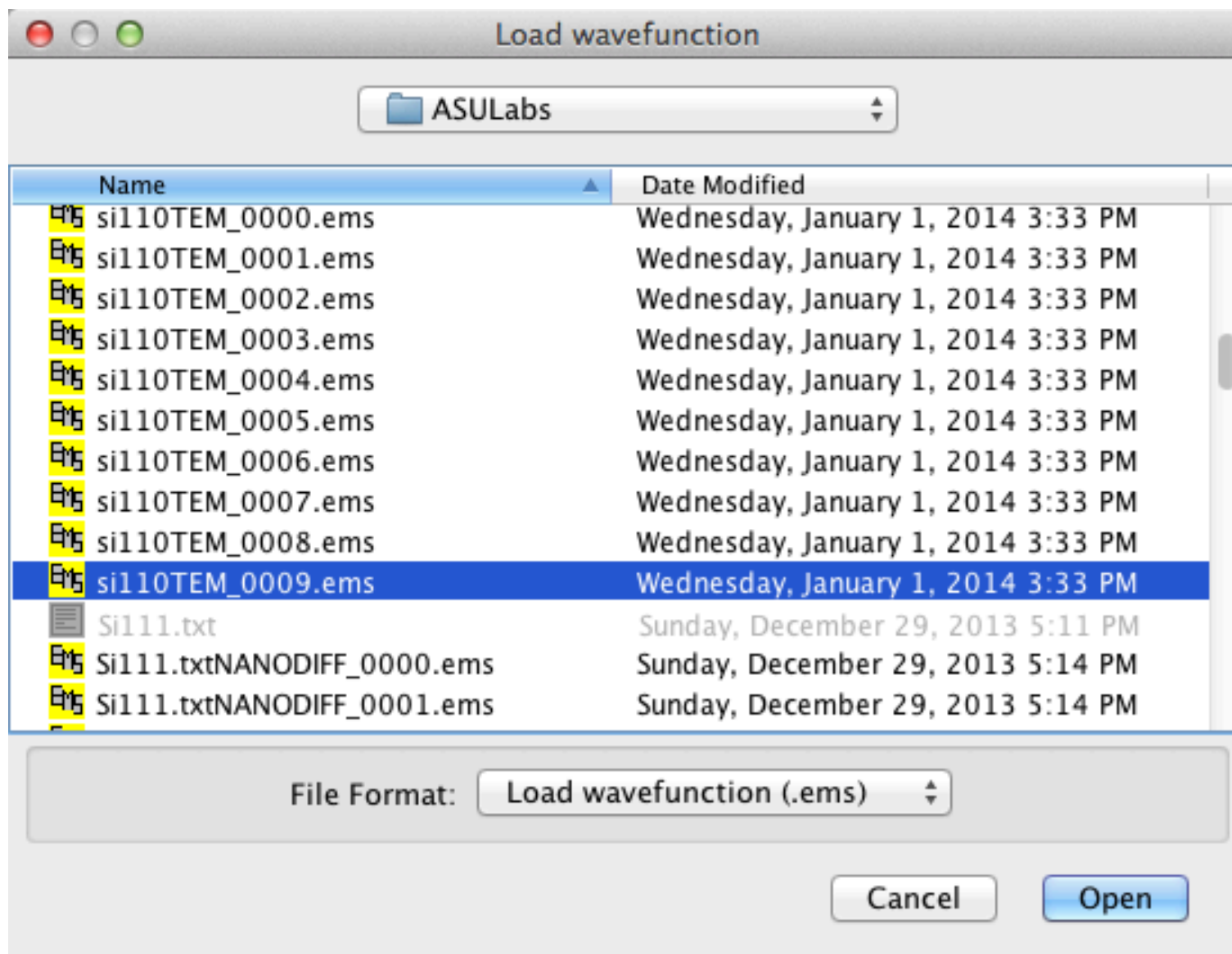
Redo the map calculation with the  Save wave radio button selected. You will be asked to name the wavefunctions.



Saving the wave functions for further imaging.

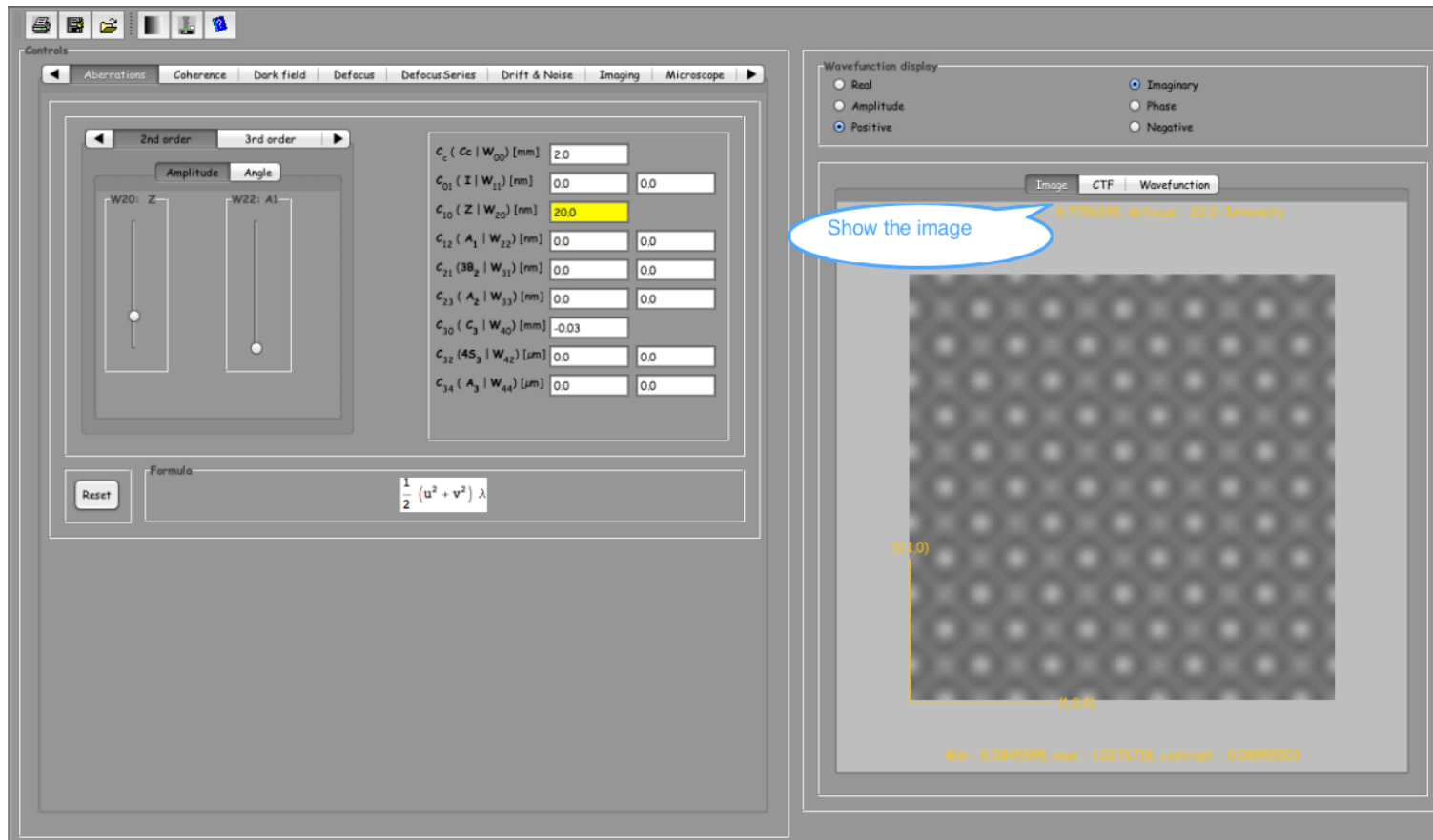


# Select Imaging $\implies$ HRTEM



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

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

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

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

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

Wavefunction display

Real  Imaginary

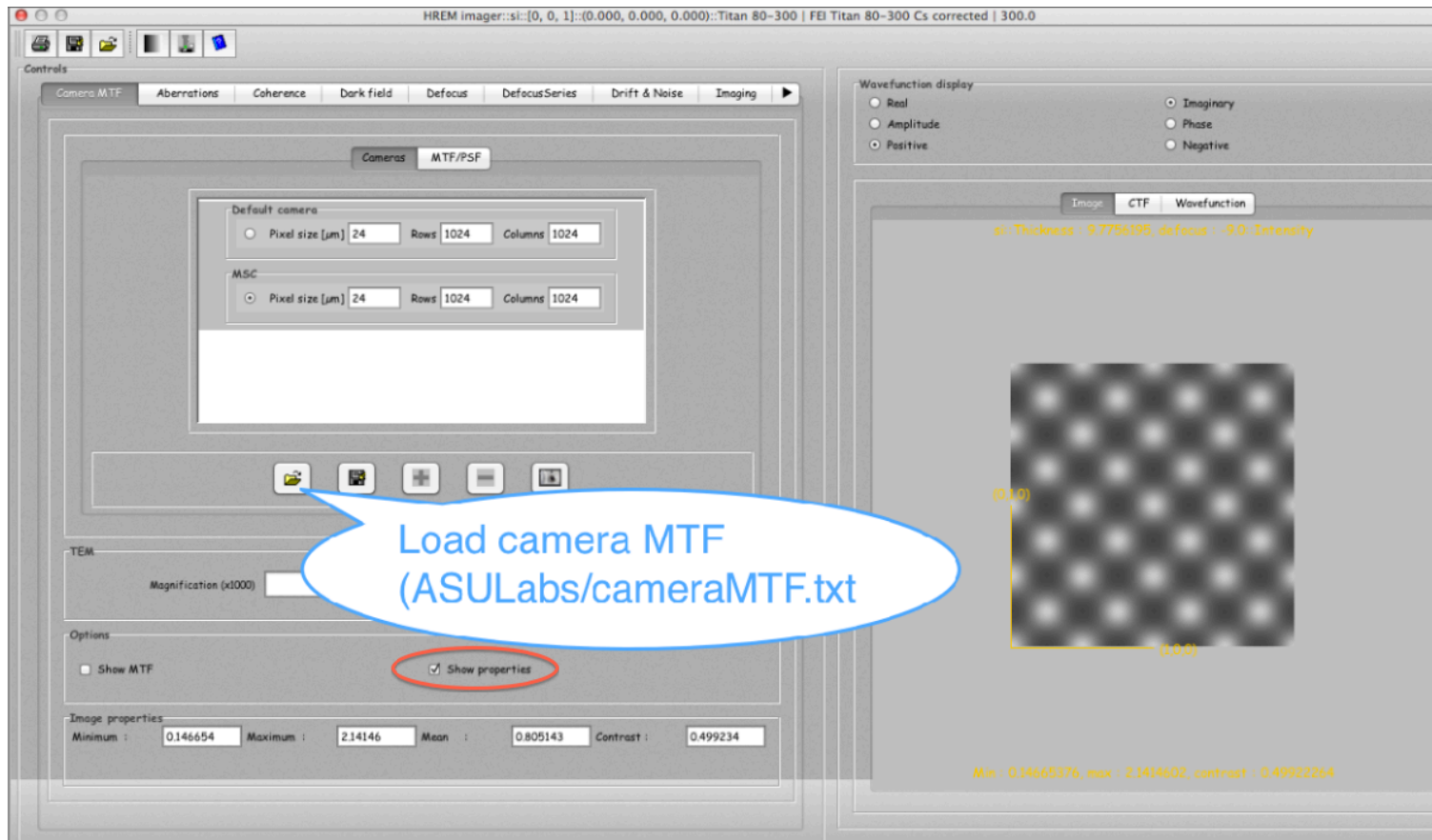
Amplitude  Phase

Positive  Negative

Image CTF Wavefunction

Imager: wavefunction.

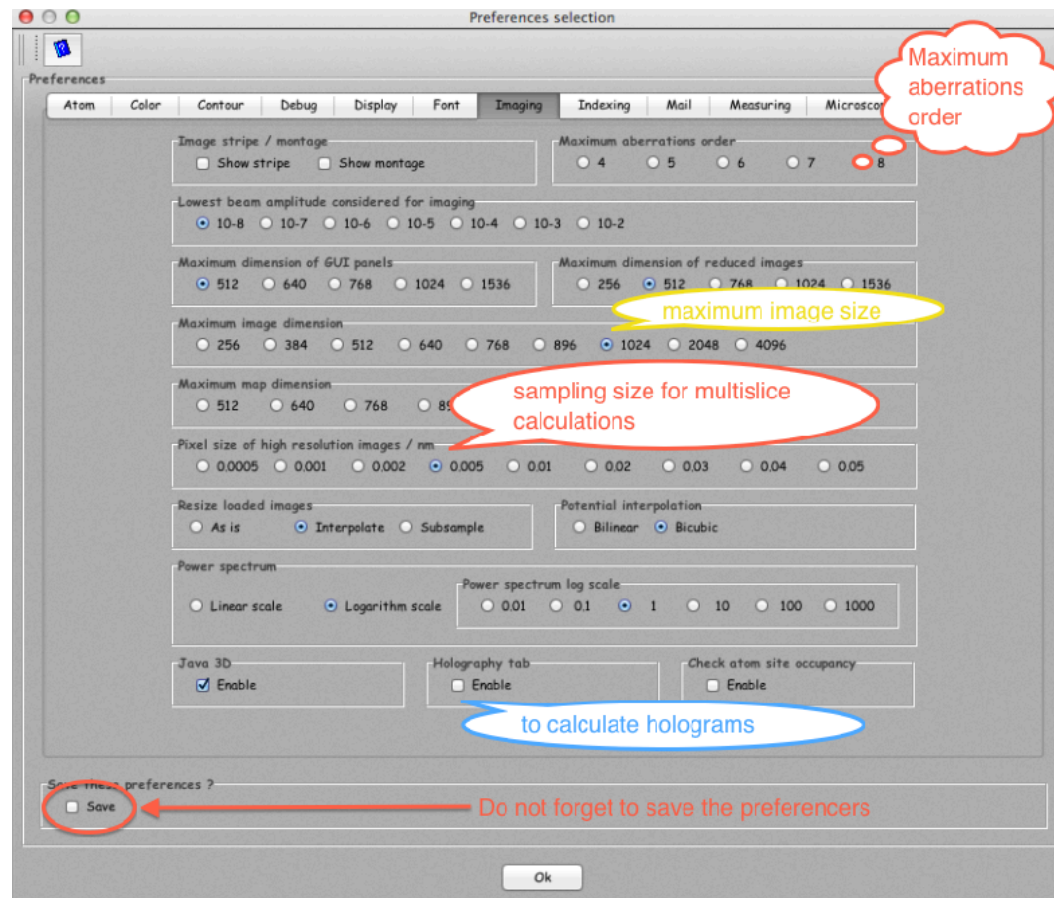
# Interactive imaging: Stobbs factor



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  $\leq 0.01$  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

Transfer Function::Microscope::Titan 80-300 | FEI Titan 80-300 Cs corrected | 300.0

Gamma

Aberations CTF profile CTF Diffractogram OTF

Wavefront aberrations

5 nm<sup>-1</sup>

Transfer function controls

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

5th order 6th order 7th order 8th order

Amplitude Angle

W51:5B4 W53:5B4 W55:A4

Krivanek notation (geometric)  
Haider notation  
Wavefront notation

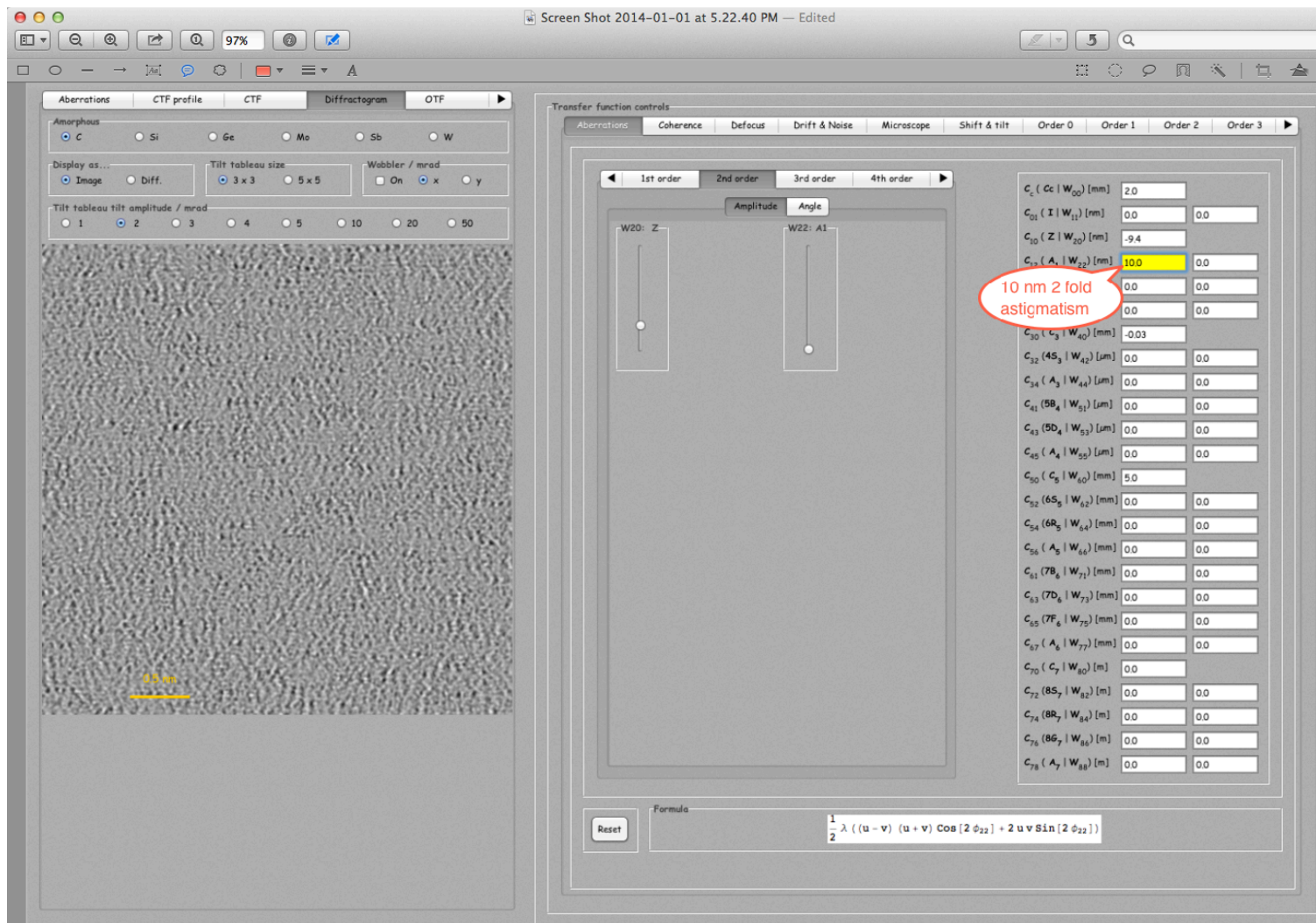
$C_c$ ( $C_c$   $W_{00}$ ) [mm]	2.0	
$C_{01}$ ( $I$   $W_{11}$ ) [nm]	0.0	0.0
$C_{10}$ ( $Z$   $W_{20}$ ) [nm]	-9.4	
$C_{12}$ ( $A_1$   $W_{22}$ ) [nm]	0.0	0.0
$C_{21}$ ( $3B_2$   $W_{31}$ ) [nm]	0.0	0.0
$C_{23}$ ( $A_2$   $W_{33}$ ) [nm]	0.0	0.0
$C_{30}$ ( $C_3$   $W_{40}$ ) [mm]	-0.03	
$C_{32}$ ( $4S_3$   $W_{42}$ ) [ $\mu$ 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

Reset Formula

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

**10 nm 2 fold astigmatism**

$C_c (C_c   W_{00})$ [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
$C_{13} (A_2   W_{22})$ [nm]	0.0	0.0
$C_{14} (A_3   W_{22})$ [nm]	0.0	0.0
$C_{15} (A_4   W_{22})$ [nm]	0.0	0.0
$C_{16} (A_5   W_{22})$ [nm]	0.0	0.0
$C_{17} (A_6   W_{22})$ [nm]	0.0	0.0
$C_{18} (A_7   W_{22})$ [nm]	0.0	0.0
$C_{19} (A_8   W_{22})$ [nm]	0.0	0.0
$C_{20} (C_9   W_{60})$ [mm]	5.0	
$C_{32} (4S_3   W_{42})$ [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
$C_{50} (C_9   W_{60})$ [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
$C_{56} (A_6   W_{66})$ [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
$C_{67} (A_7   W_{77})$ [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

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

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

# Diffractogram: 2-fold astigmatism

Aberrations CTF profile CTF Diffractogram OTF

Amorphous: C Si Ge Mo Sb W

Display as: Image Diff. Tilt tableau size: 3x3 5x5 Wobbler / mrad: On x y

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

5 nm-1

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

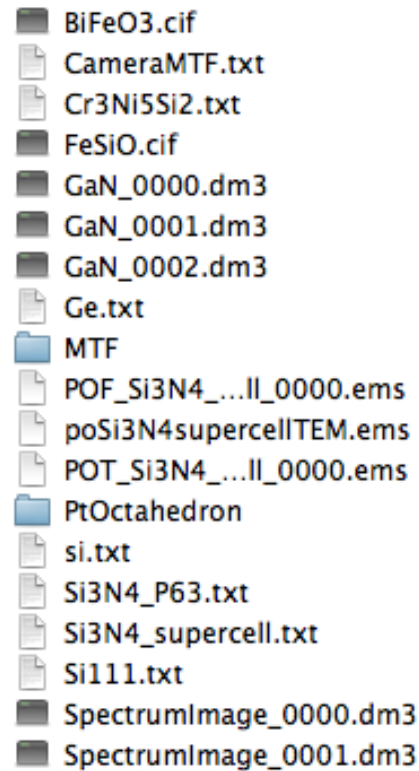
$C_c$ (Cc   $W_{00}$ ) [mm]	2.0	
$C_{01}$ (I   $W_{11}$ ) [nm]	0.0	0.0
$C_{10}$ (Z   $W_{20}$ ) [nm]	-9.4	
$C_{12}$ ( $A_1$   $W_{22}$ ) [nm]	10.0	0.0
$C_{21}$ ( $3B_2$   $W_{31}$ ) [nm]	0.0	0.0
$C_{23}$ ( $A_2$   $W_{33}$ ) [nm]	0.0	0.0
$C_{30}$ ( $C_3$   $W_{40}$ ) [mm]	-0.03	
$C_{32}$ ( $4S_3$   $W_{42}$ ) [ $\mu$ m]	0.0	0.0
$C_{34}$ ( $A_3$   $W_{44}$ ) [ $\mu$ m]	0.0	0.0
$C_{41}$ ( $5B_4$   $W_{51}$ ) [ $\mu$ 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

Aberration formula is given:

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

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  $\approx 0.2$  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  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.

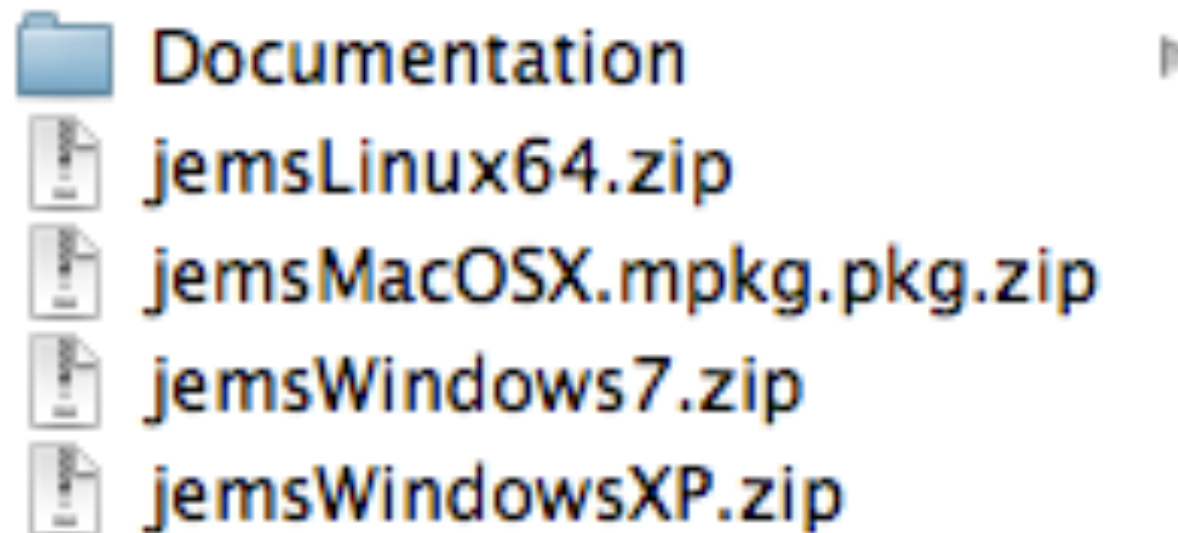
# Suggestions 2

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 .
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  is selected. To see an image after each slice have the  Show image <sup>2</sup> of tab  selected.
5. Select the first slice of the table (PtOct\_0000.txt). Start the calculation (). 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.

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<sup>2</sup>You 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

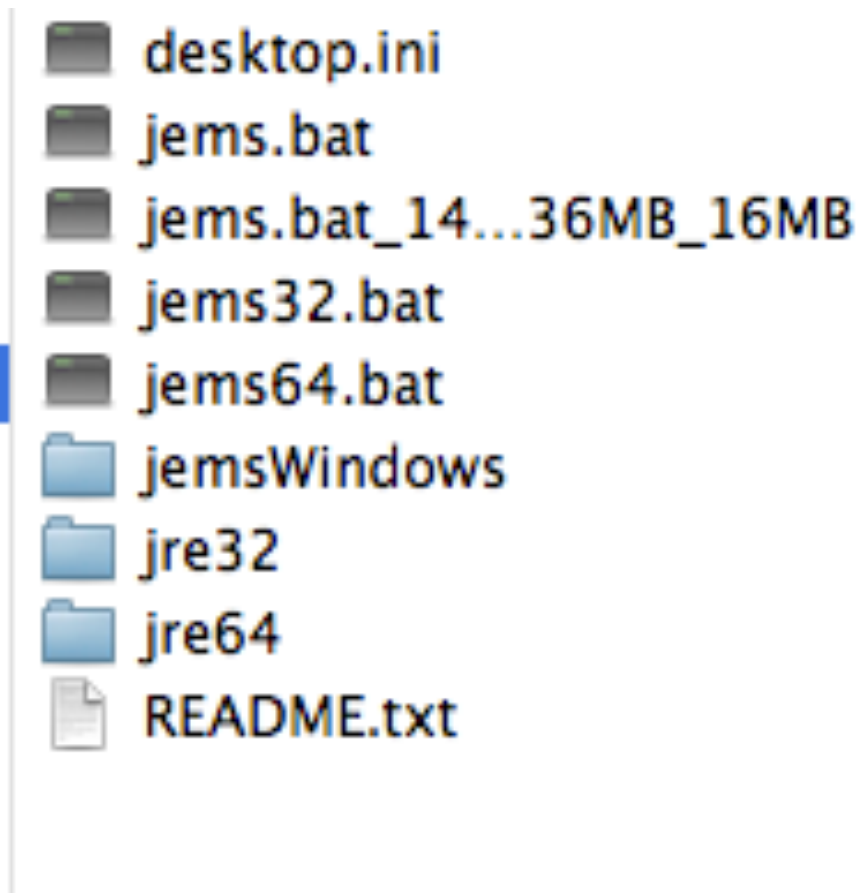


Figure: Windows 7 or 8 version: jems started either using jems32.bat or jems64.bat depending on Windows being 32 or 64 bits.

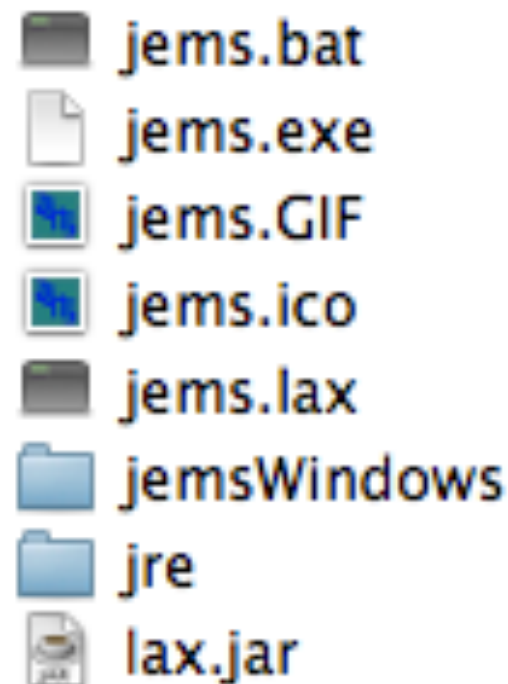


Figure: Windows XP (only 32 bits).

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