

# Modelling particles using jems

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February 5, 2024

## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Generating the particle model</b>	<b>3</b>
<b>3</b>	<b>Suggested steps to create the faceted particle</b>	<b>5</b>
3.1	Generating a parallel projection (Figure ??) . . . . .	8
3.2	Setting the model size (Figure ??) . . . . .	9
3.3	Making the model comparable to the HAADF, PP or WPOA images (Figure ??) . . . . .	10
3.4	Hiding the model cell frame (Figure ??) . . . . .	11
3.5	Changing the size and color of the atoms (Figure ??) . . . . .	12
3.6	Facetting the crystal (Figure ??) . . . . .	13
3.7	Making a single (0, 1, 3) facet (Figure ??) . . . . .	14
3.8	(Figure ??) . . . . .	15
3.9	Amorphous supporting film (Figure ??) . . . . .	16
3.10	Generating images for different zone axis (Figure ??) . . . . .	17
3.11	Setting the maximum size of calculated images and models (Figure ??) . . . . .	18
3.12	Pop-up menu attached to the 3-D drawing (Figure ??) . . . . .	19
3.13	Displaying atoms bonds (Figure ??) . . . . .	20
3.14	Saving the facets (h,k,l) indices and distances (Figure ??) . . . . .	21

3.15	Tool buttons of the <i>Toolbar</i> and stereographic projection (Figure ??)	22
3.16	Slicing the model (Figure ??)	23
3.17	Saving the model slices (Figure ??)	24
3.18	Doing a standard multislice calculation (Figure ??)	25
3.19	Starting the multislice calculation (Figure ??)	26
3.20	Loading slices xxxx_0001 to xxxx_nnnn (Figure ??)	27
3.21	Displaying the whole model (Figure ??)	28
3.22	3-D drawing of the model (Figure ??)	29
3.23	Multislice calculation result (Figure ??)	30
3.24	WPOA calculation result (Figure ??)	31
3.25	HAADF example (Figure ??)	33
3.26	Projected potential example (Figure ??)	34
3.27	SAED example (Figure ??)	35
3.28	WPOA example (Figure ??)	36
3.29	WPOA images and models example (Figure ??)	37
3.30	WPOA images of particles deposited on amorphous carbon film (Figure ??)	38
3.31	Model particles (Figure ??)	39
<b>4</b>	<b>Final remarks</b>	<b>40</b>

# 1 Introduction

Particles of sizes up to 10-15 nm can be modelled using the *To particle*, menu *Miscellany*. Using the generated particle models, HAADF (High Angle Annular Dark Field), PP (projected potential), SAED (Selected Area Electron Diffraction) and WPOA (Weak Phase Object Approximation) images and patterns calculated (Figure 1).

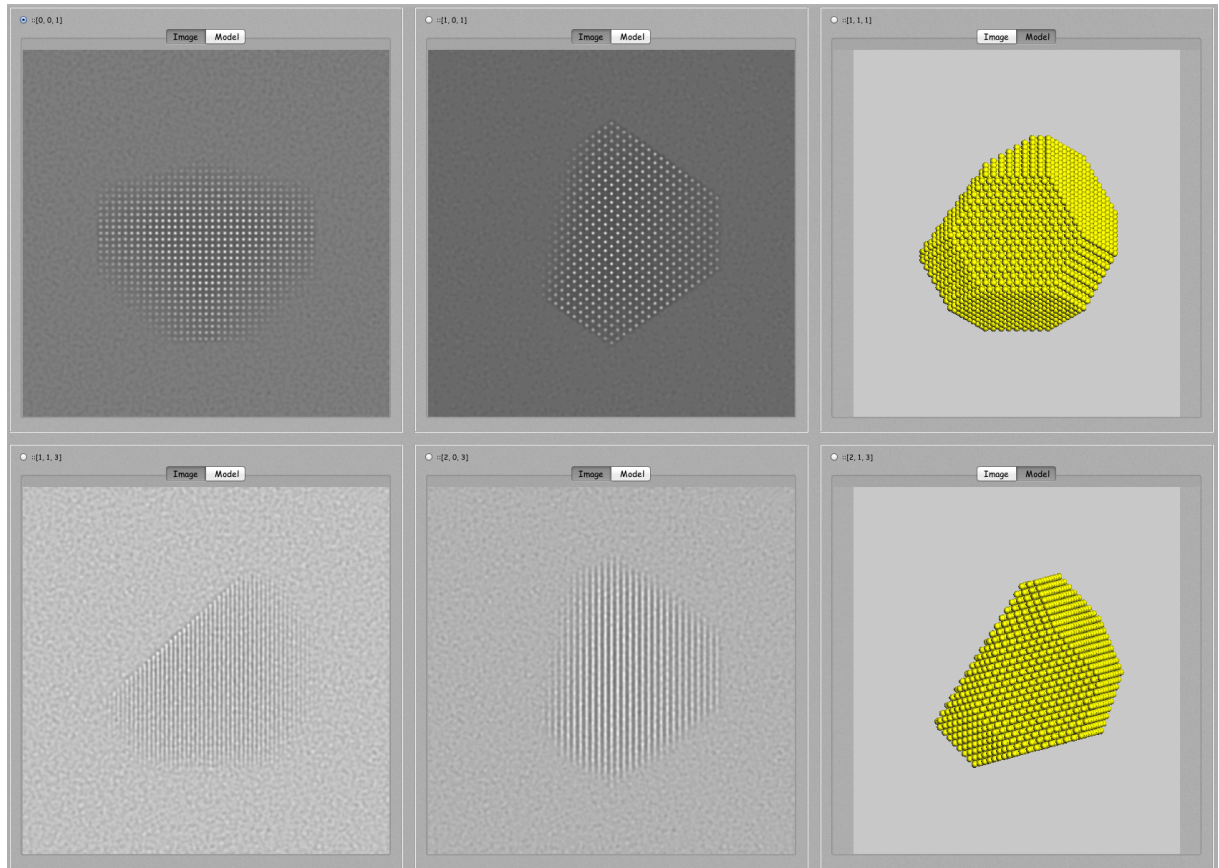


Figure 1: Example of WPOA images and models arranged on a grid map.

The *Image* and *Model* tabs display either the calculated image or its model. A possible rotation between the image and the model can be compensated for (see section 4).

## 2 Generating the particle model

To generate the Au particle shown in (Figure 2).

Particle modelling is started selecting the ***To particle*** menu item of the ***Miscel-lany*** menu. The *To particle* dialogue is shown in Fig. 3.

The Au unit cell is duplicated in  $\vec{a}, \vec{b}, \vec{c}$  using the *Duplicate x, y, z*. The *Show spherical* checkbox will generate a spherical particle. The *3-D icon* displays the 10x10x10 unit cells model (Figure 4).

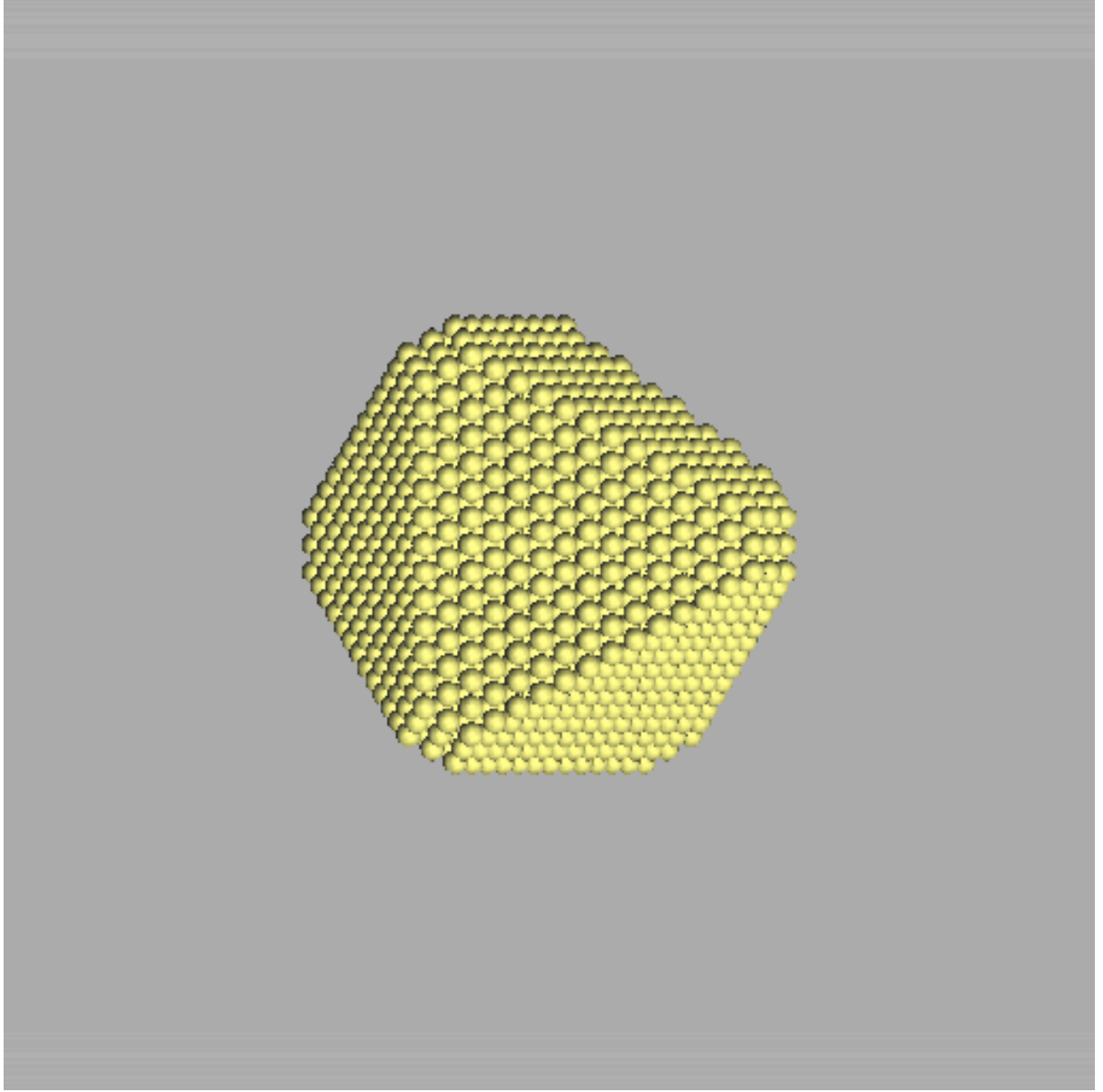


Figure 2: Facetted Au particle.

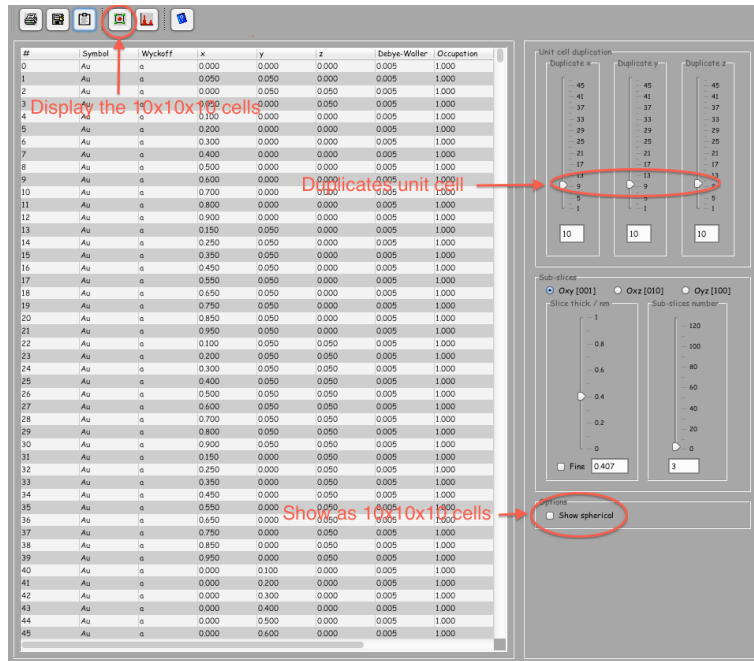


Figure 3: To particle dialogue.

### 3 Suggested steps to create the facettted particle

The model is made of atoms placed at  $(x, y, z)$  coordinates in an orthogonal box of sides  $a, b, c$  with  $0 \leq x, y, z \leq 1$ . Note that the model is projected along the  $Oz$  direction and can be rotated around the box center  $(x = 0.5, y = 0.5, z = 0.5)$ .  $[0,0,1]$  direction is parallel to  $Oz$  ( $c$ ) where  $[u,v,w]$  is a direction of the Bravais lattice of the original crystal (i.e. before duplication).

1. Select the *Options* tab and select the *Parallel* to generate a parallel projection (Fig. 5).
2. Select the *Slices* tab and use the *Box size* slider to increase the unit cell size (box size) (Fig. 6).
3. Select the *Zoom* slider to make the box as large as the 3-D display area (Fig. 7).
4. Select the *Options* tab and the *Frame* checkbox to hide the model frame (optional) (Fig. 8).
5. Select the *Au* tab to increase the atom size and/or color (Fig. 9).

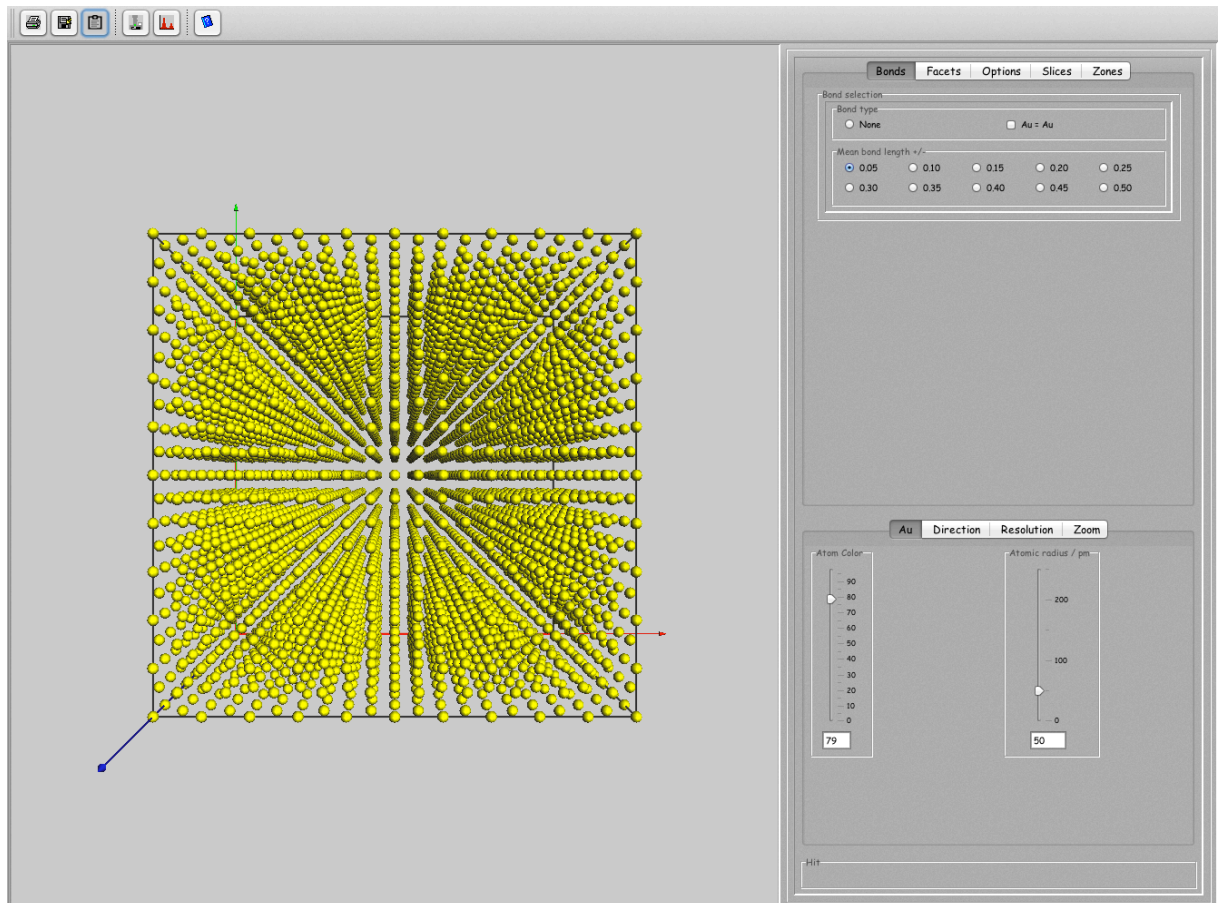


Figure 4: Display the 10x10x10 unit cells model.

6. Select the *Facets* tab and the hkl indices of the facets. Use the *Facet distance* slider to facet the 10x10x10 unit cells model (Fig. 10).

More details are provided in Figures 11 - 39.



### 3.1 Generating a parallel projection (Figure 5)

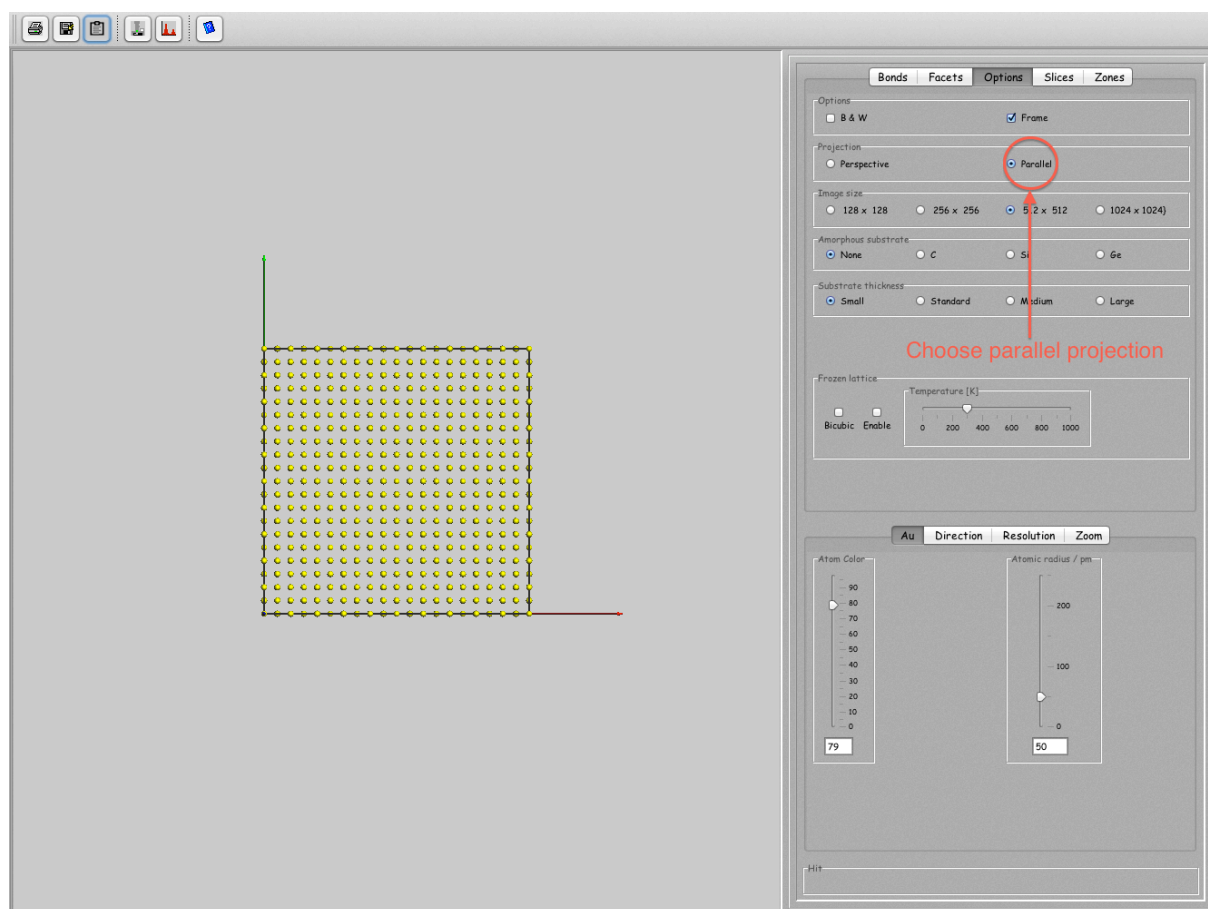


Figure 5: Generate a parallel projection (depending on the number of atoms it may necessary to *Zoom* the model to observe the parallel projection).

Note that the 3-D display is made asynchronously and the parallel projection is not always immediately displayed.

### 3.2 Setting the model size (Figure 6)

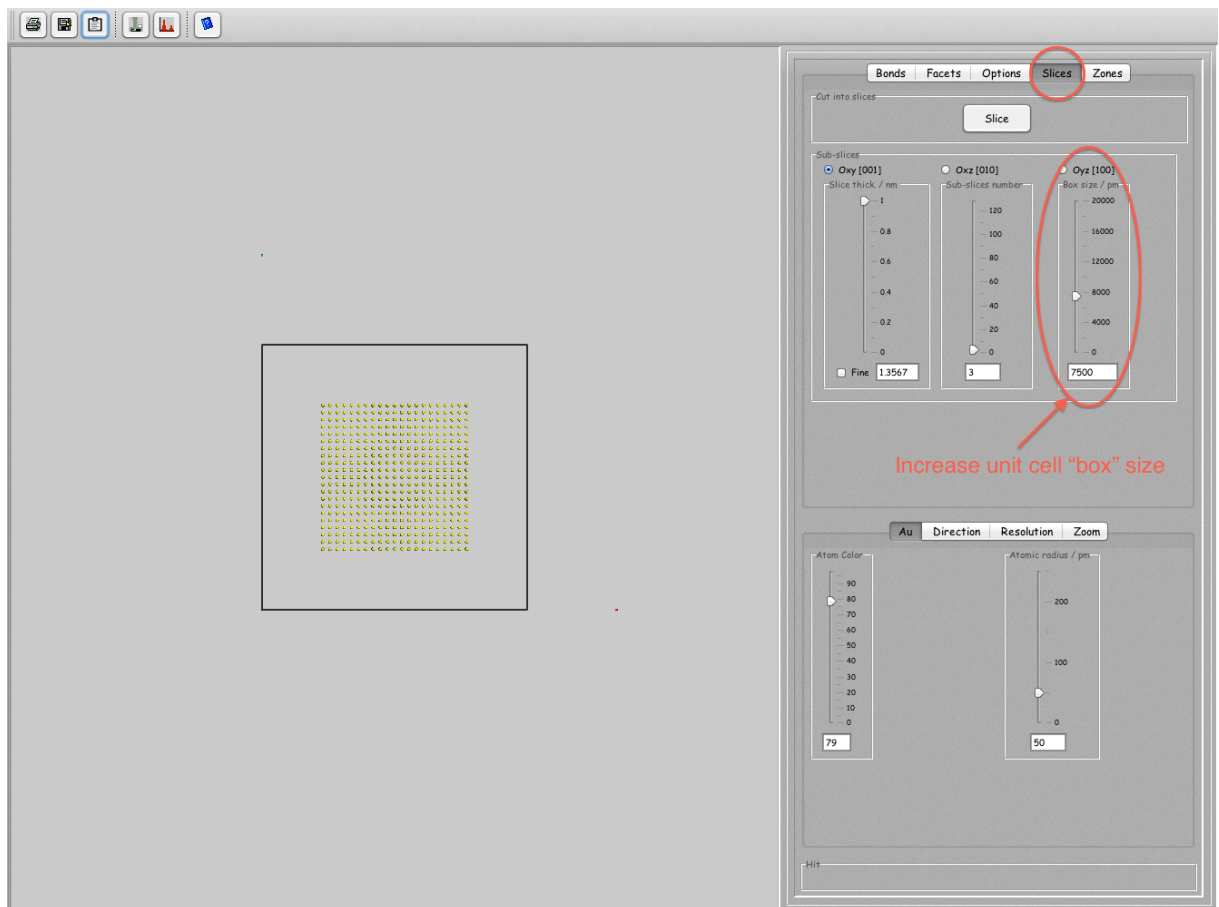


Figure 6: Change the box size, in order to be able to rotate the particle inside the box (without having atoms positioned outside the box).

### 3.3 Making the model comparable to the HAADF, PP or WPOA images (Figure 7)

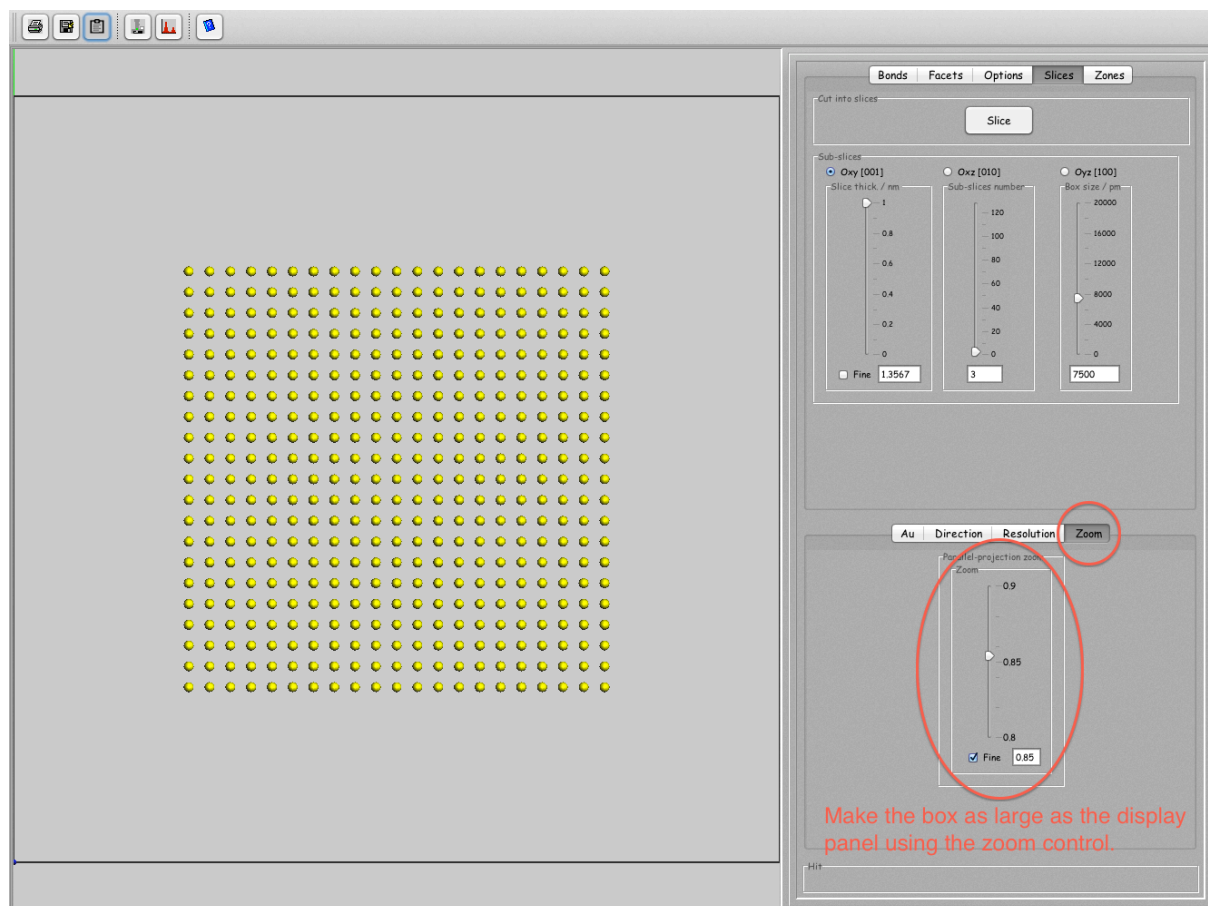


Figure 7: Use the *Zoom* slider to increase the model size until the model box is as large as the 3-D display area.

### 3.4 Hiding the model cell frame (Figure 8)

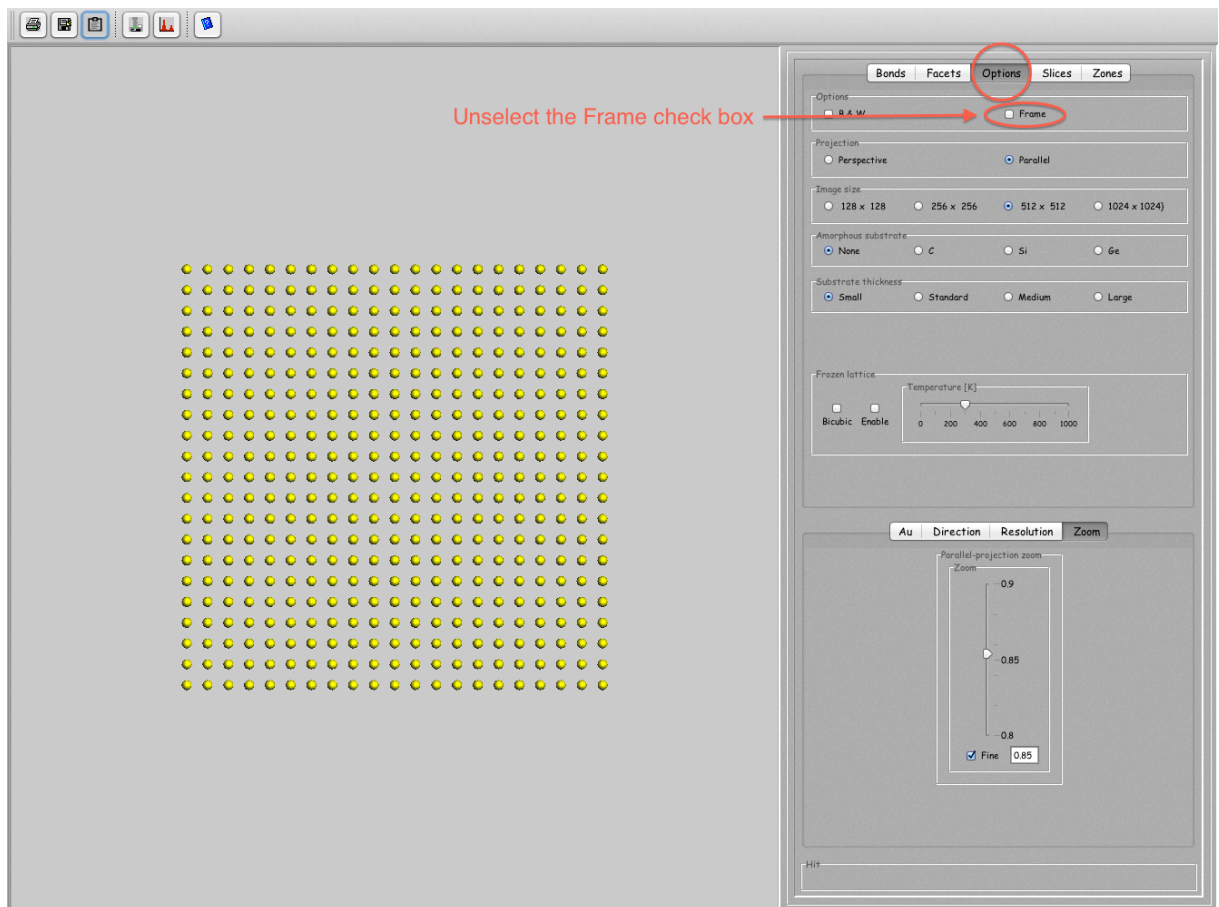


Figure 8: The unit cell frame can be hidden.

### 3.5 Changing the size and color of the atoms (Figure 9)

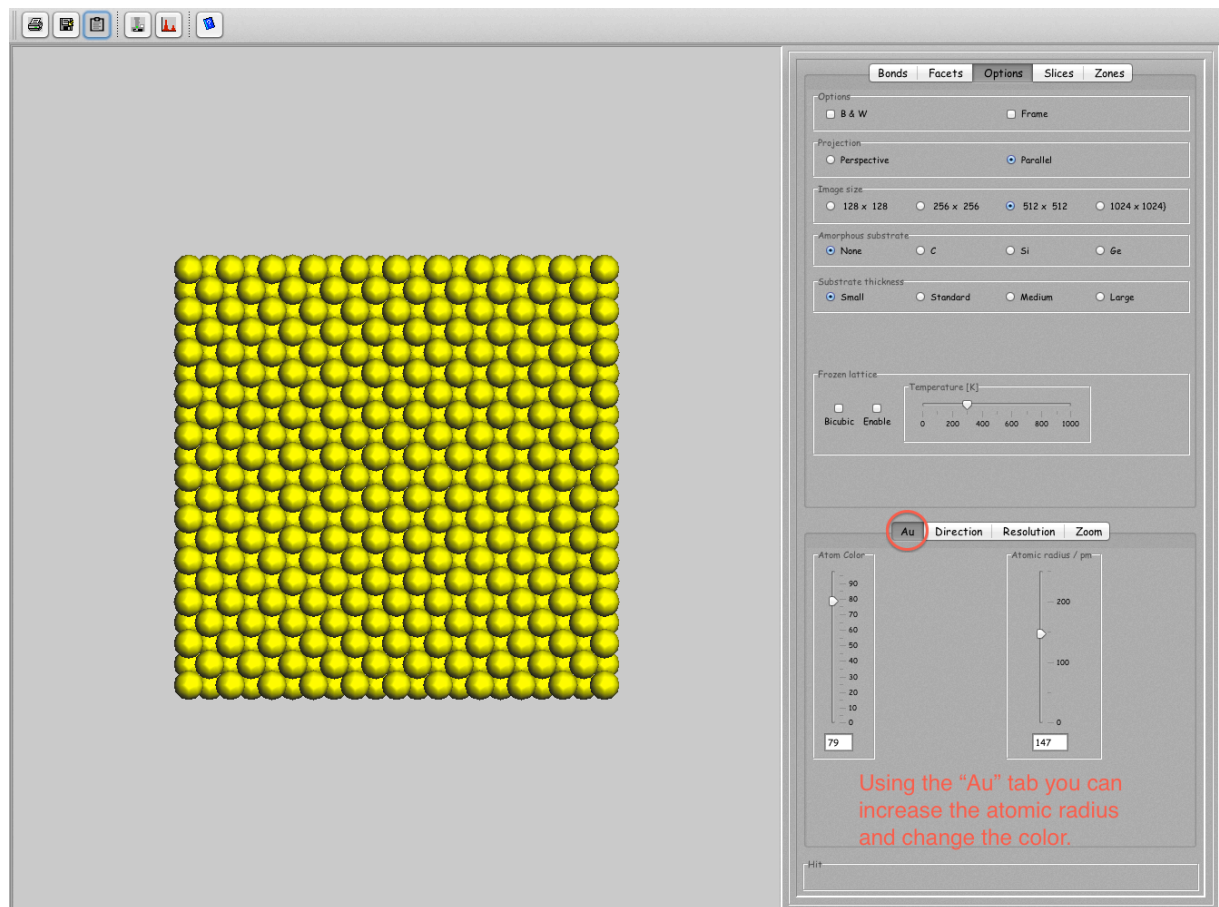


Figure 9: Select the *Au* tab (or atomic symbol tab) to change both atomic radius and atom color.

Note that the atoms sphere resolution is set very low by default in order accelerate the 3-D display. The sliders of the *Resolution* tab set both the sphere resolution and the bond resolution.

### 3.6 Facetting the crystal (Figure 10)

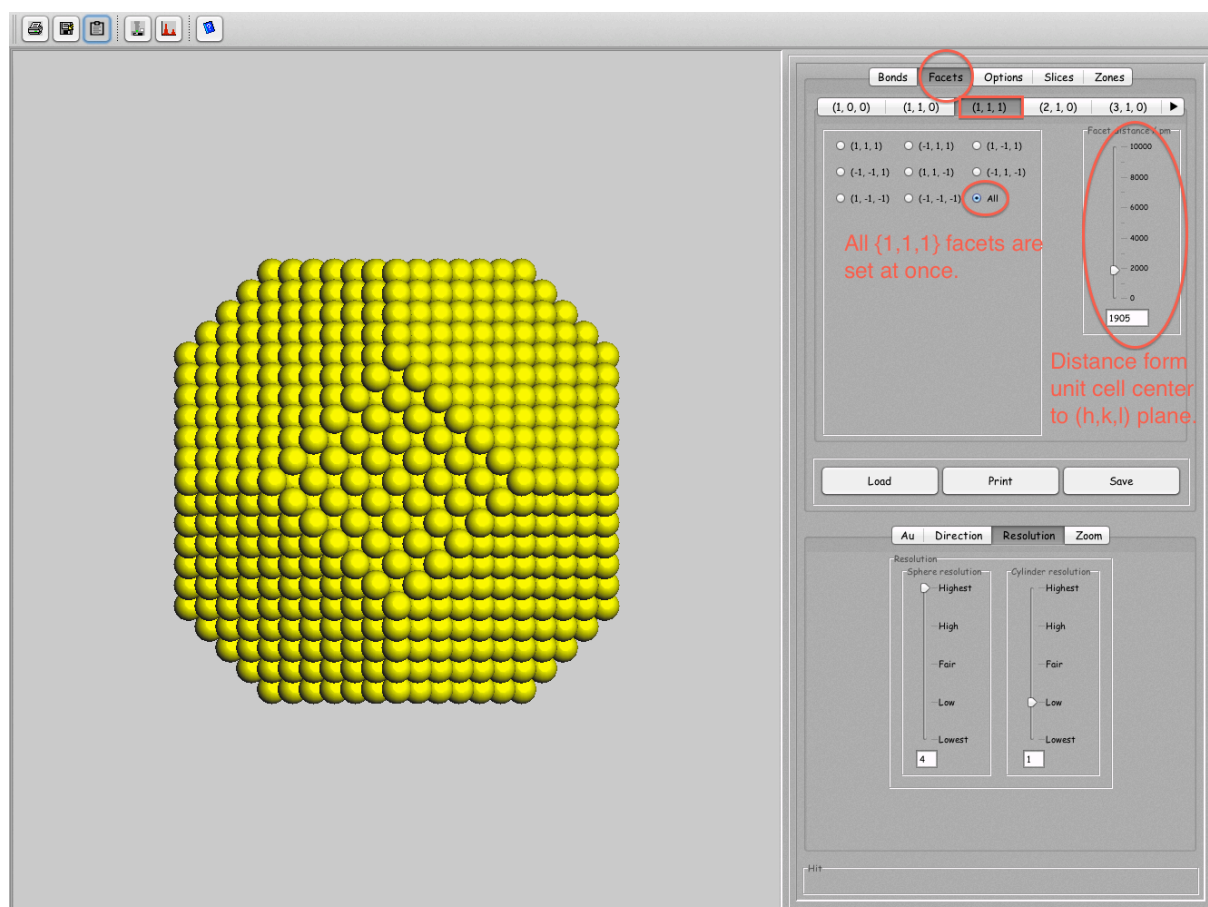


Figure 10: Select the *Facets* tab and the (h,k,l) crystal plane's indices as well as its distance to the model center to facet the model. The *All* radio button sets the distance for the whole set of equivalent (h,k,l) planes.

### 3.7 Making a single (0, 1, 3) facet (Figure 11)

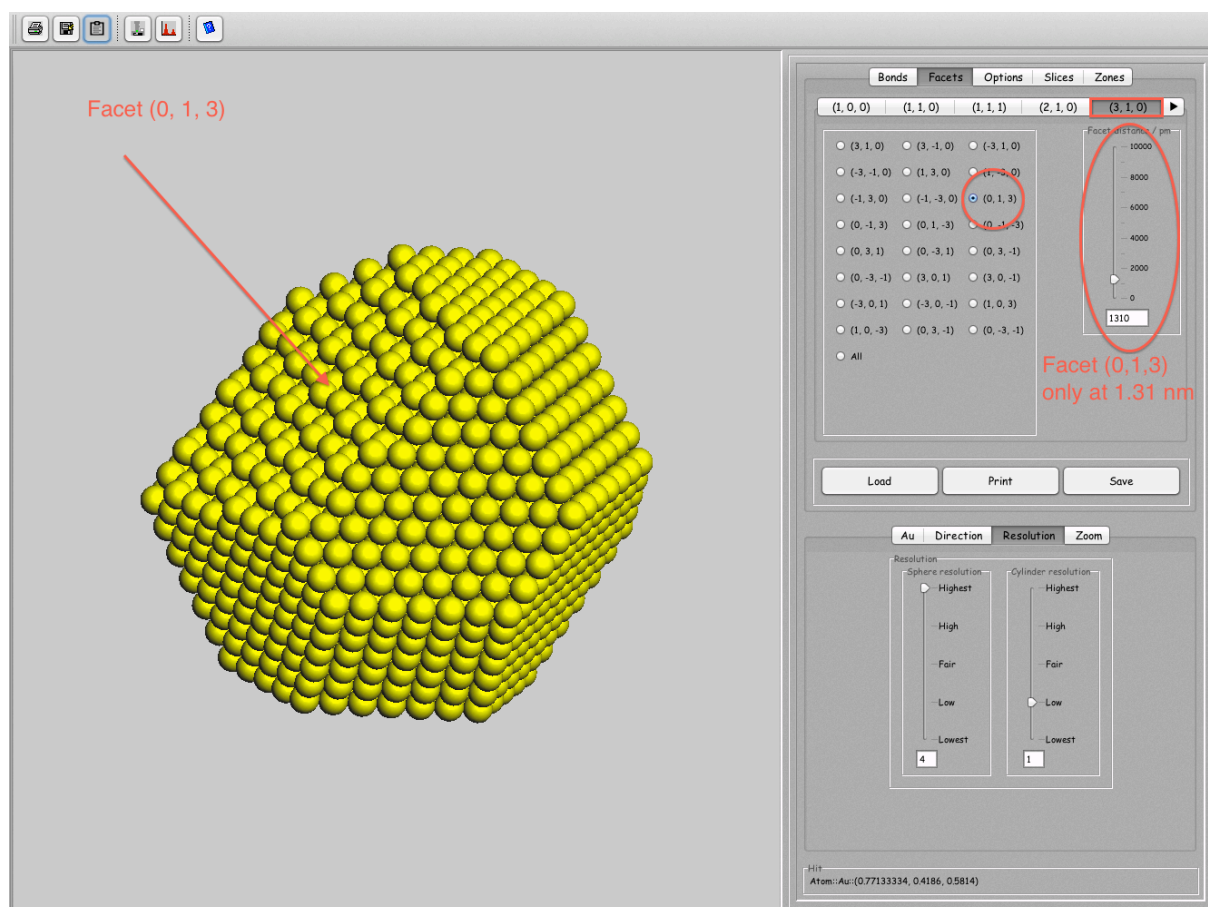


Figure 11: Facets of different kinds can be created. Facets not provided in the predefined (h,k,l) sets can be defined with the *Selected* tab.

For user selected facets enter the (h,k,l) indices of the facet, then select them and use the slider to set the distance<sup>1</sup>.

<sup>1</sup>It is necessary to hit the carriage return/enter key

### 3.8 (Figure 12)

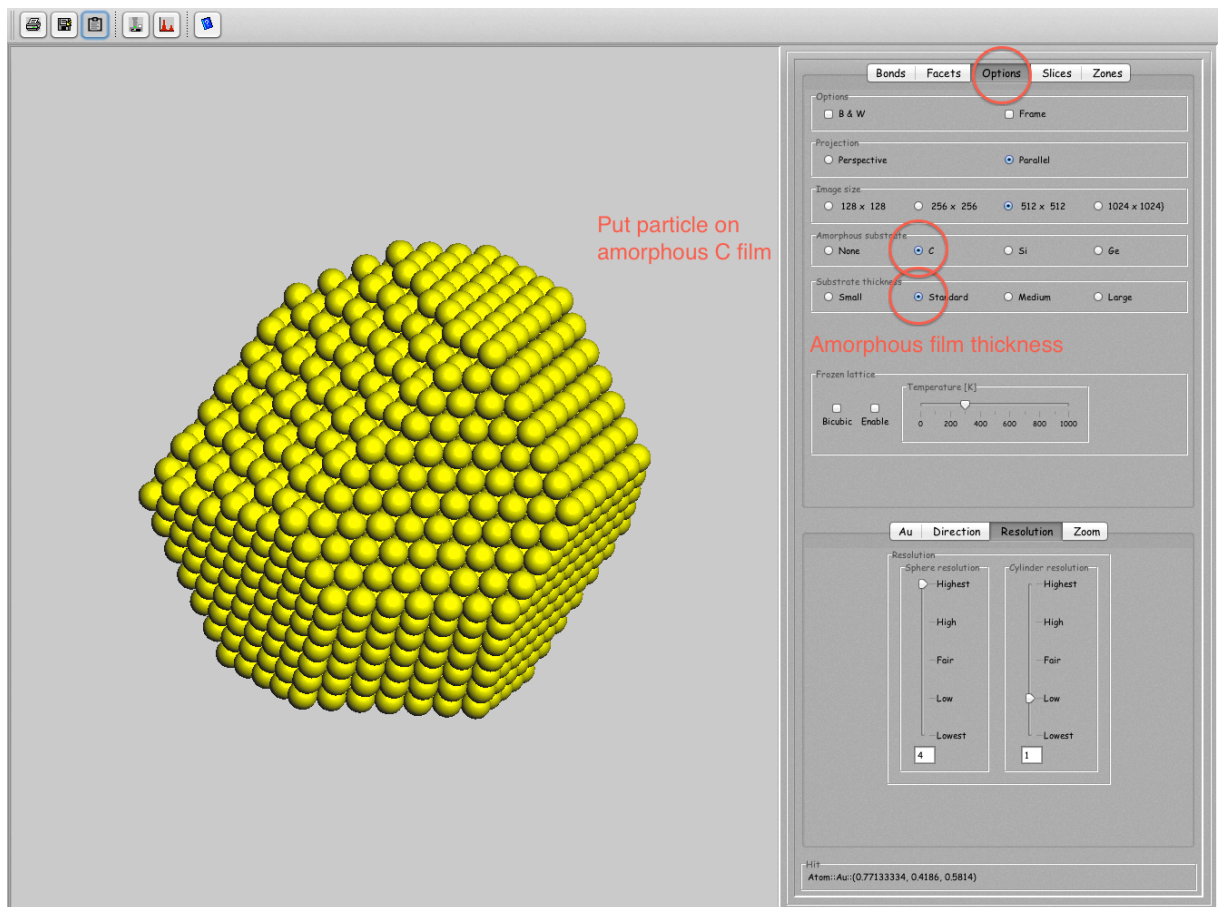


Figure 12: .



### 3.9 Amorphous supporting film (Figure 13)

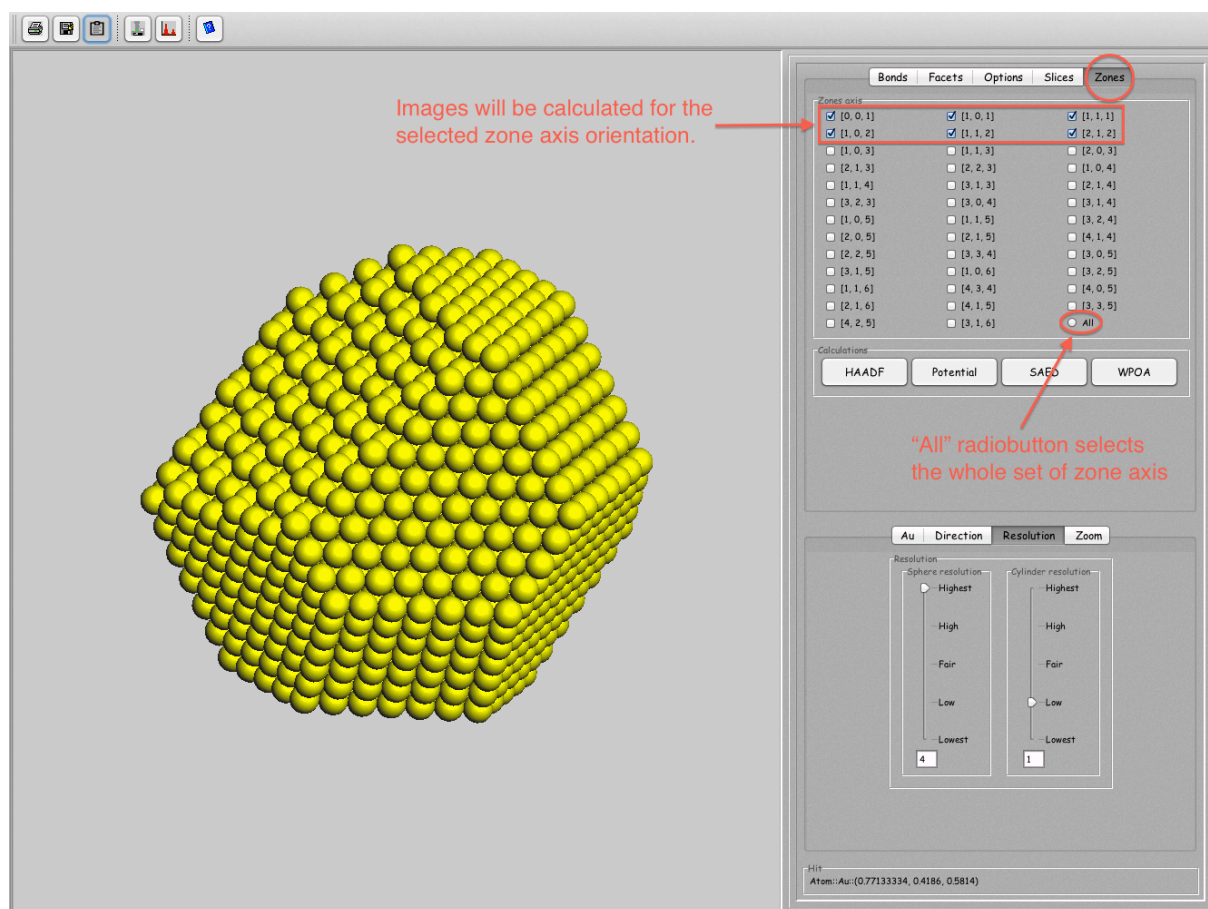


Figure 13: WPOA images can be generated with the model particles supported by an amorphous thin film (*Options* tab).

### 3.10 Generating images for different zone axis (Figure 14)

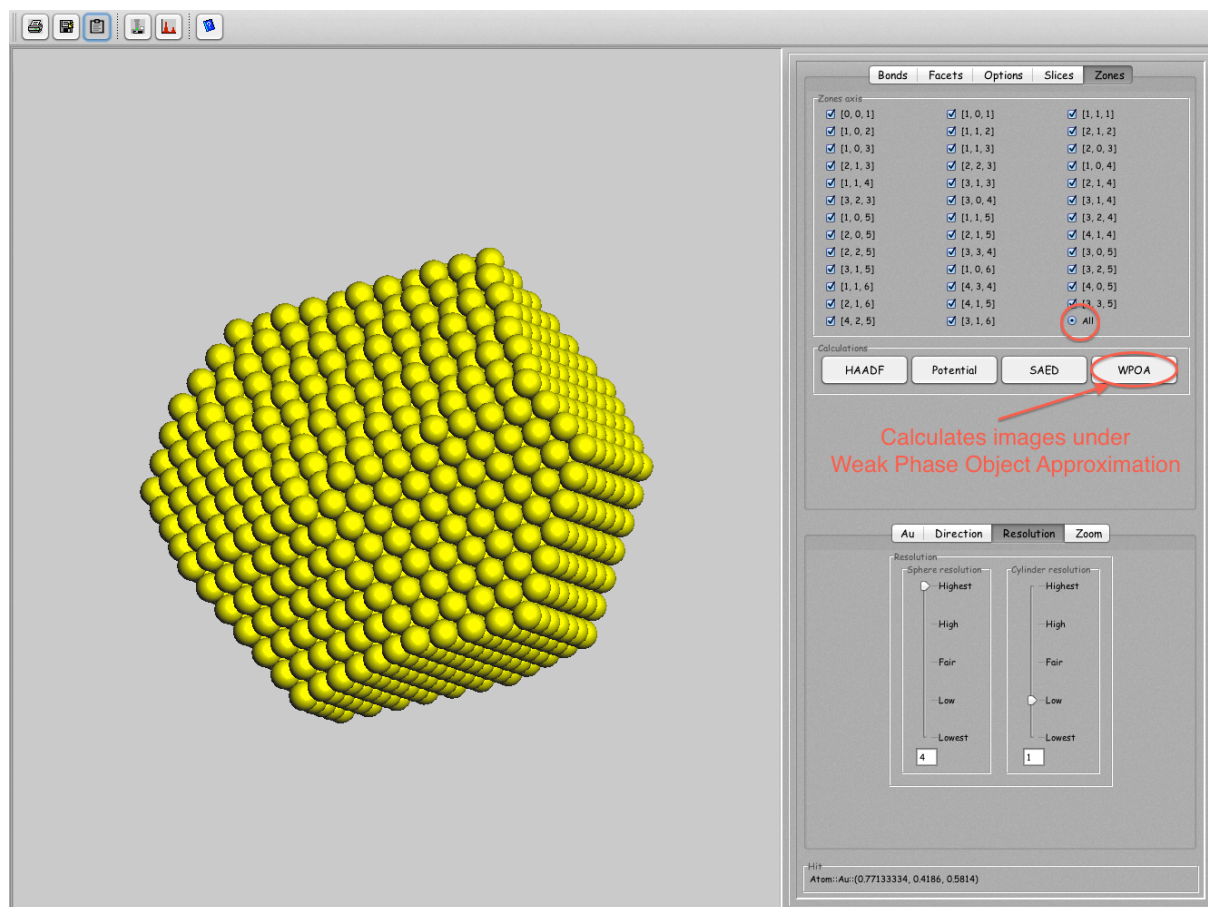


Figure 14: The text `itZones` tab displays a number of  $[u,v,w]$  zone axes for images calculation.

The *All* radio button selects/unselects the whole set of zone axes. To calculate HRTEM images under the WPOA approximation push the *WPOA* button.

### 3.11 Setting the maximum size of calculated images and models (Figure 15)

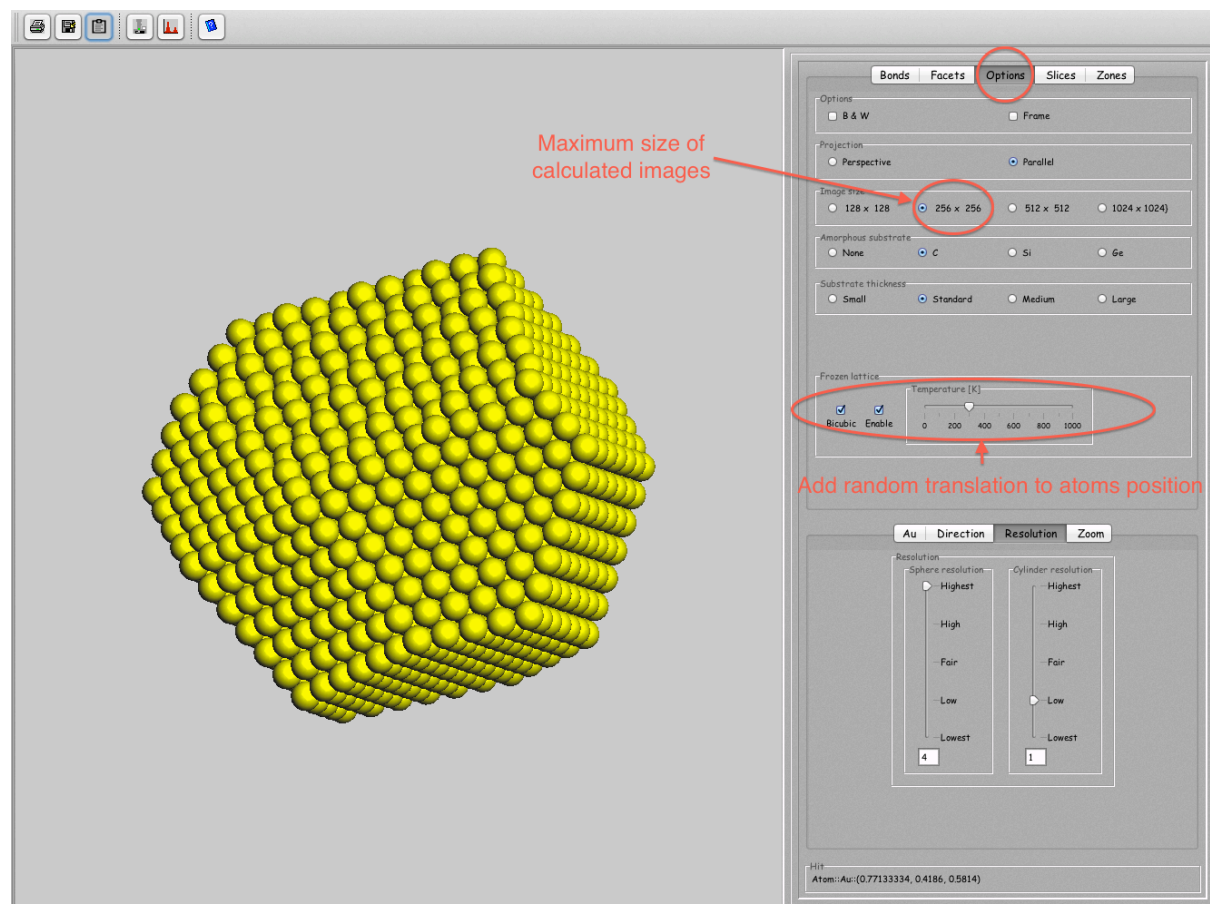


Figure 15: Select the *Options* tab to select the maximum size of the images of the grid map.

The radio buttons and slider grouped in the *Frozen lattice* box allows to add a small random displacement to the atoms position.

### 3.12 Popup menu attached to the 3-D drawing (Figure 16)

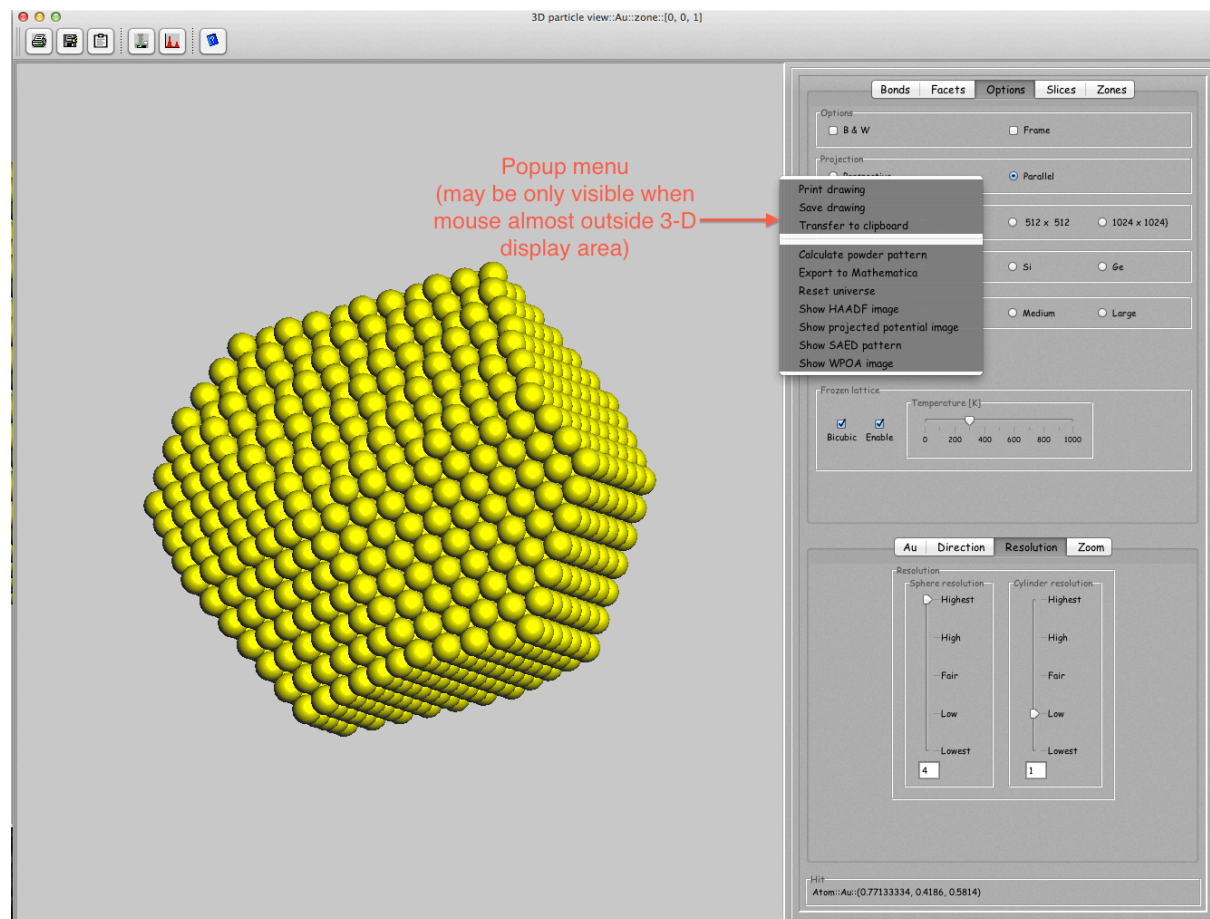


Figure 16: Popup menu attached to the 3-D drawing.

Most jems drawings, tables, controls, etc have an attached popup menu<sup>2</sup> that offers menu items to save, print, transfer the drawing to the clipboard or to do various image calculations.

<sup>2</sup>Mouse right click or two mouse clicks to pop it up

### 3.13 Displaying atoms bonds (Figure 17)

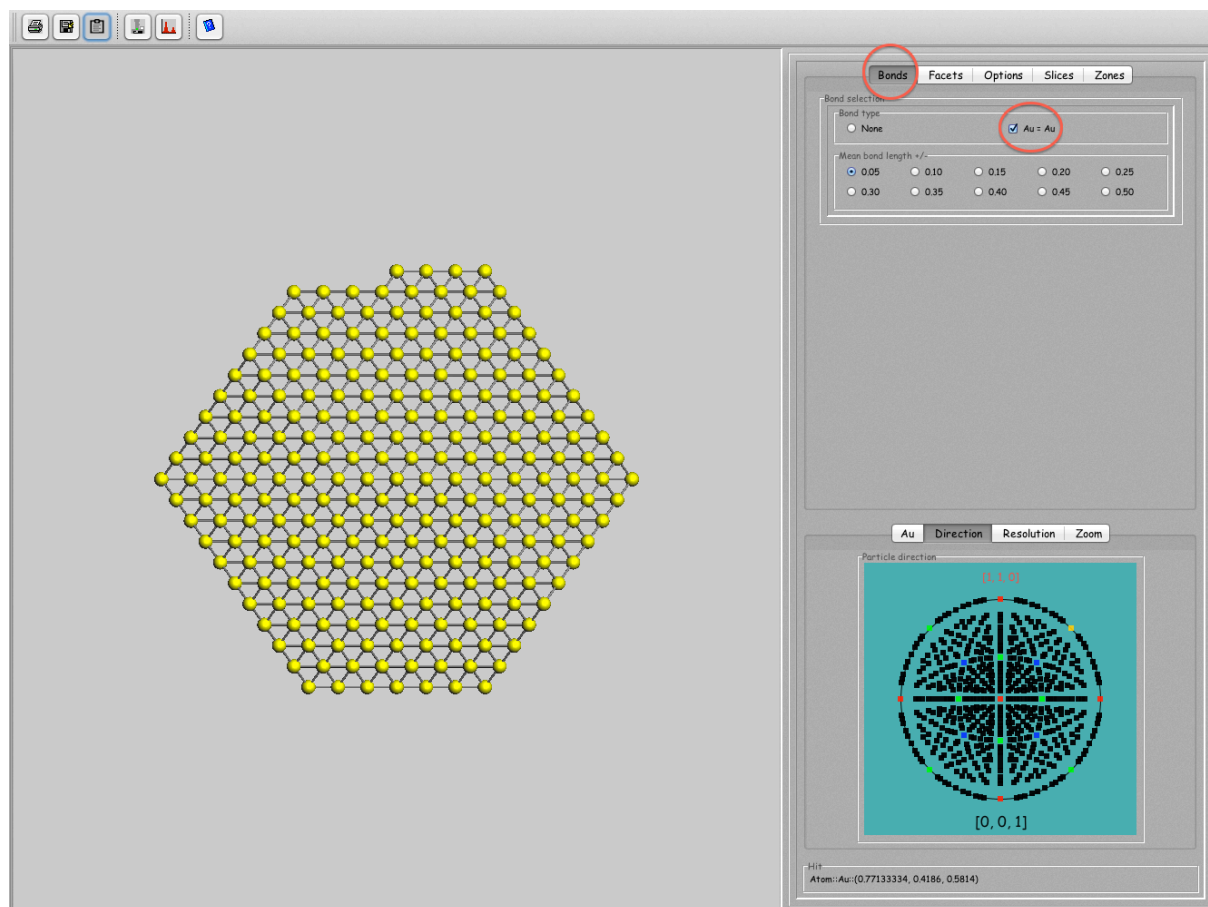


Figure 17: Atoms bonds can be added to the model.

Note that the time needed to refresh the drawing increases largely when bonds are added.

### 3.14 Saving the facets (h,k,l) indices and distances (Figure 18)

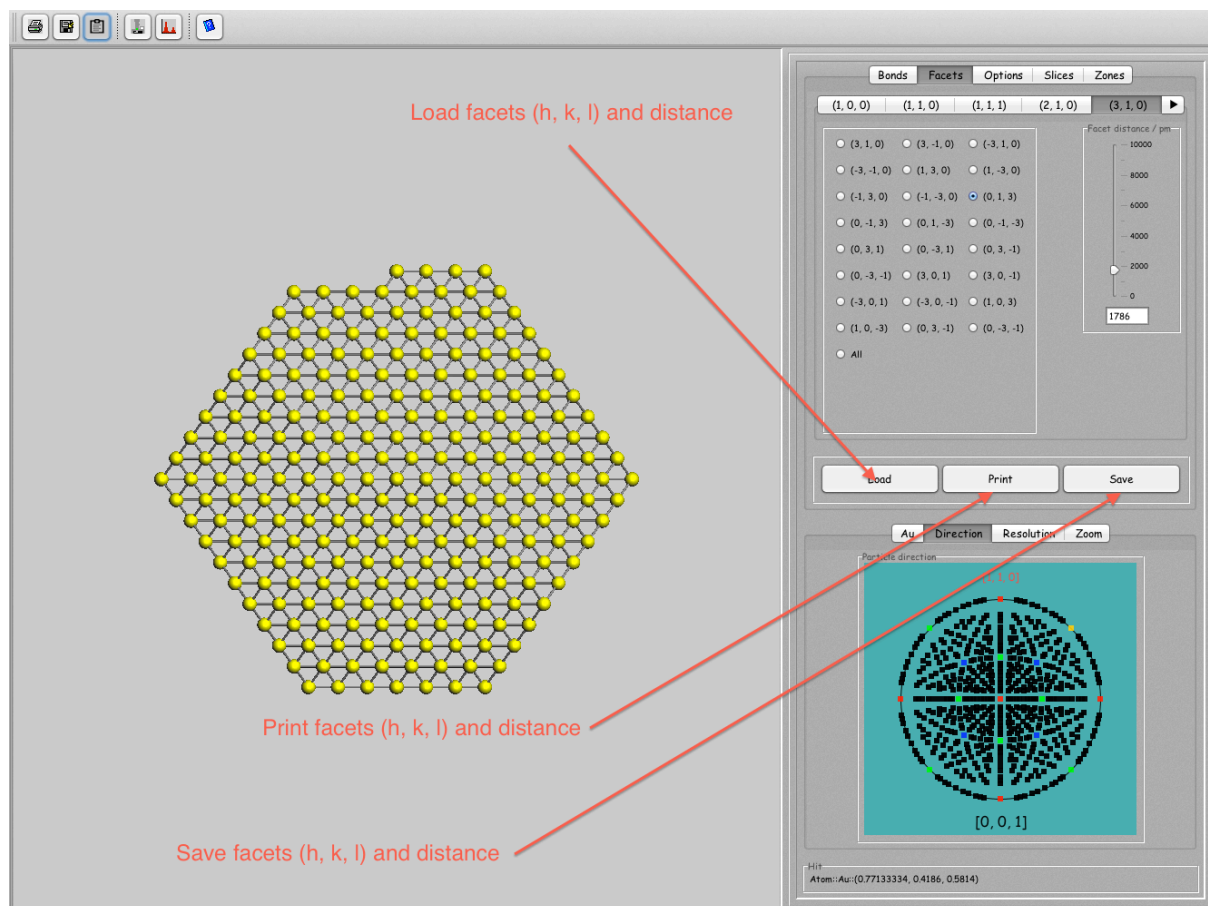


Figure 18: The *Load*, *Print* and *Save* buttons loads, prints and saves the facets data.

### 3.15 Tool buttons of the *Toolbar* and stereographic projection (Figure 19)

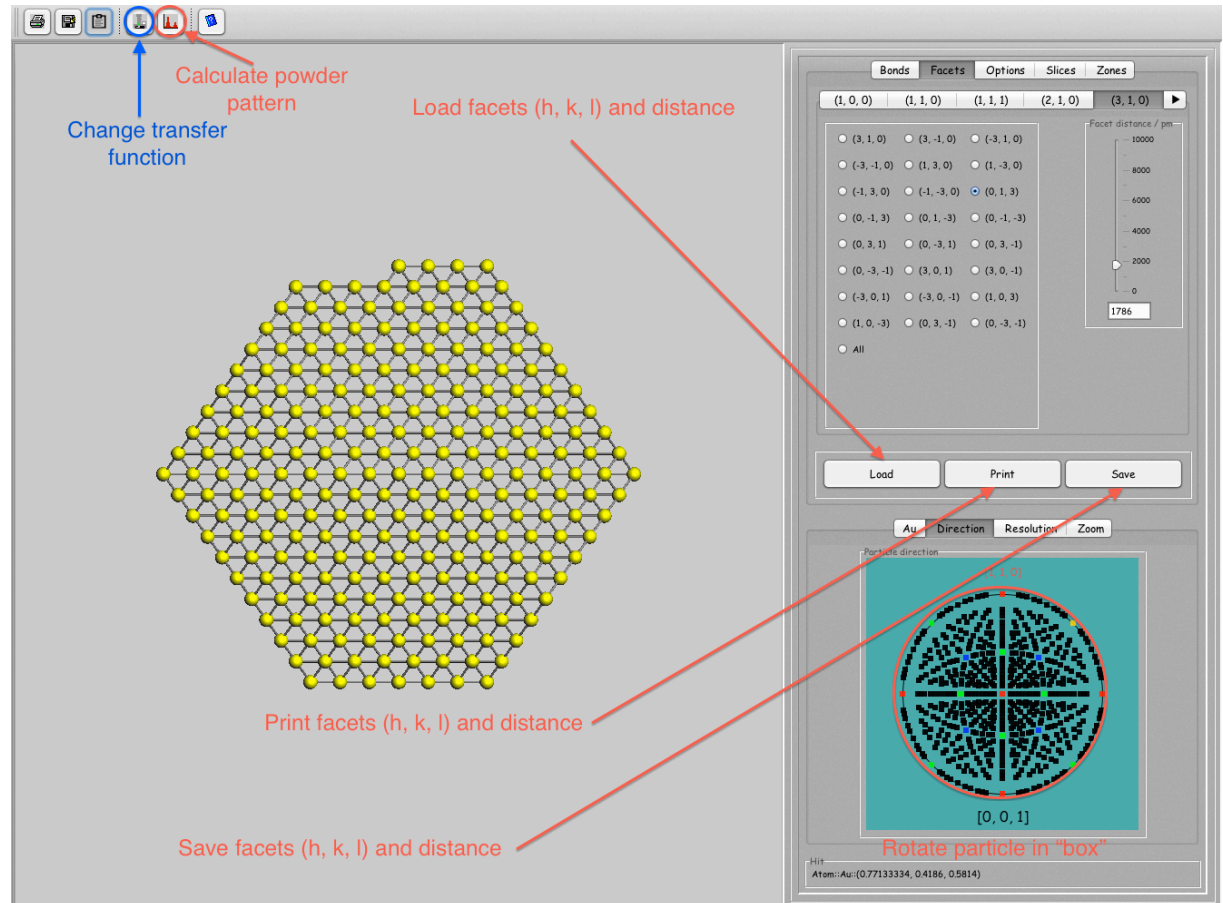


Figure 19: Tool buttons allows to change the microscope settings and to calculate ab-initio powder patterns.

### 3.16 Slicing the model (Figure 20)

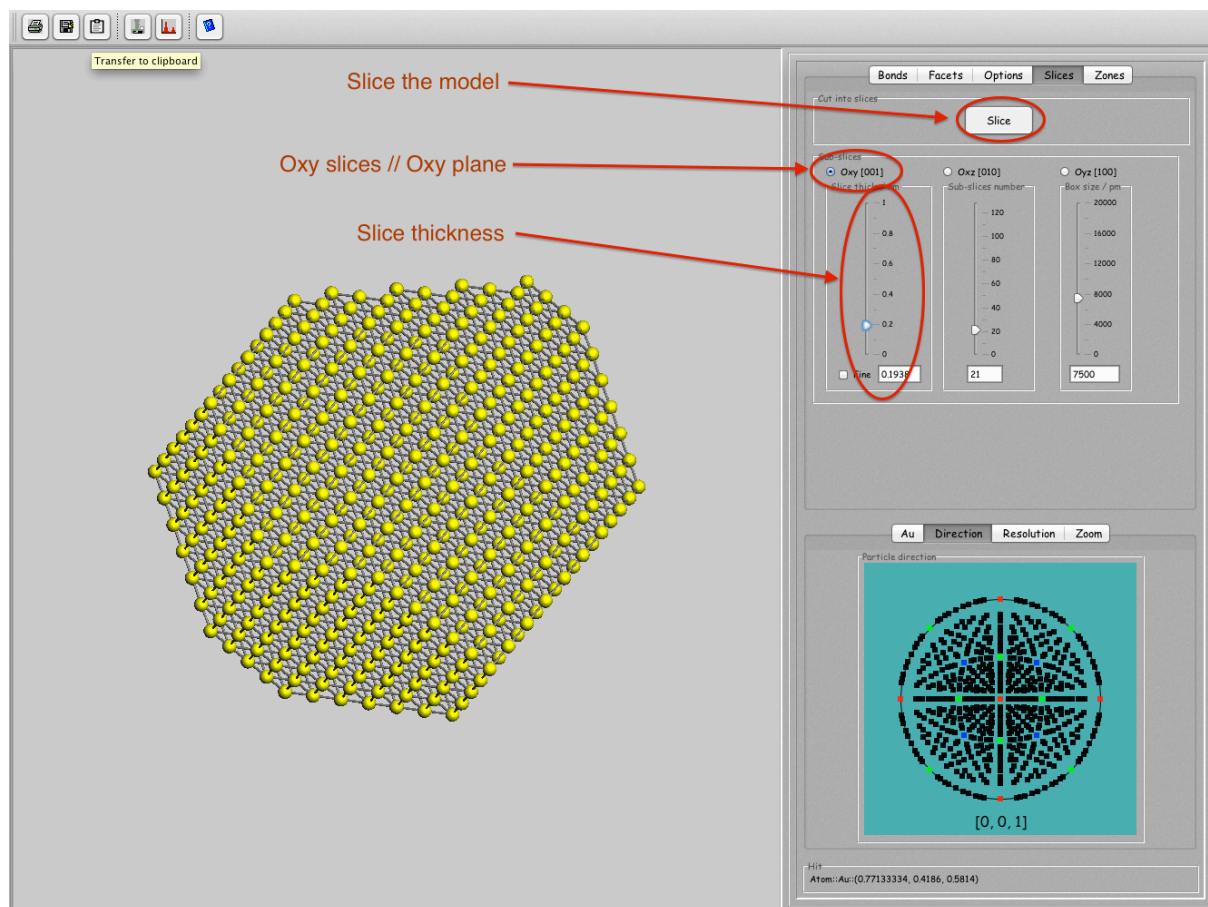


Figure 20: The model can be sliced into thin slices for standard multislice calculation.



### 3.17 Saving the model slices (Figure 21)

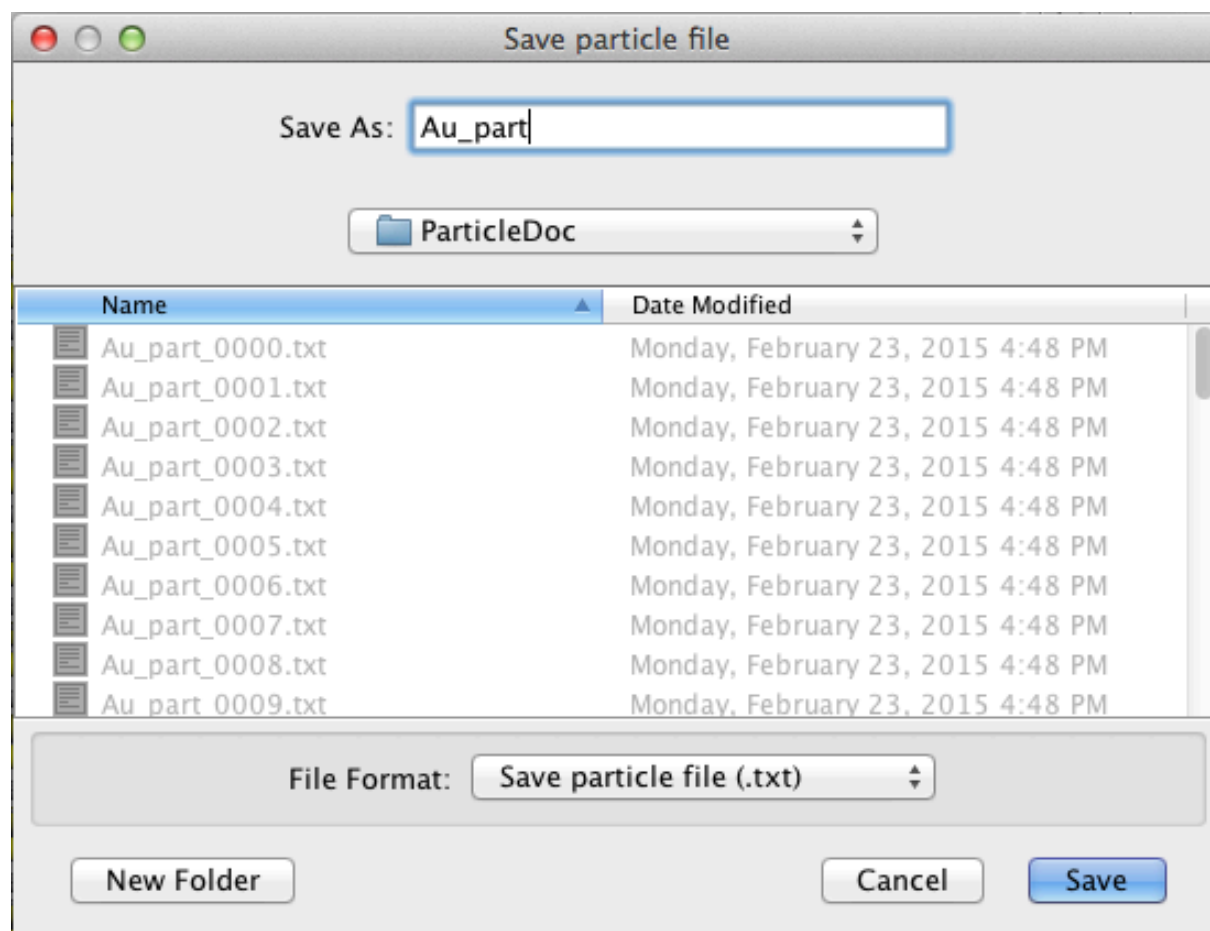


Figure 21: The slices are numbered xxxx\_0000 to xxxx.nnnn.

Note that xxxx\_particle.txt provides the lattice parameters and atoms position of the full model.

### 3.18 Doing a standard multislice calculation (Figure 22)

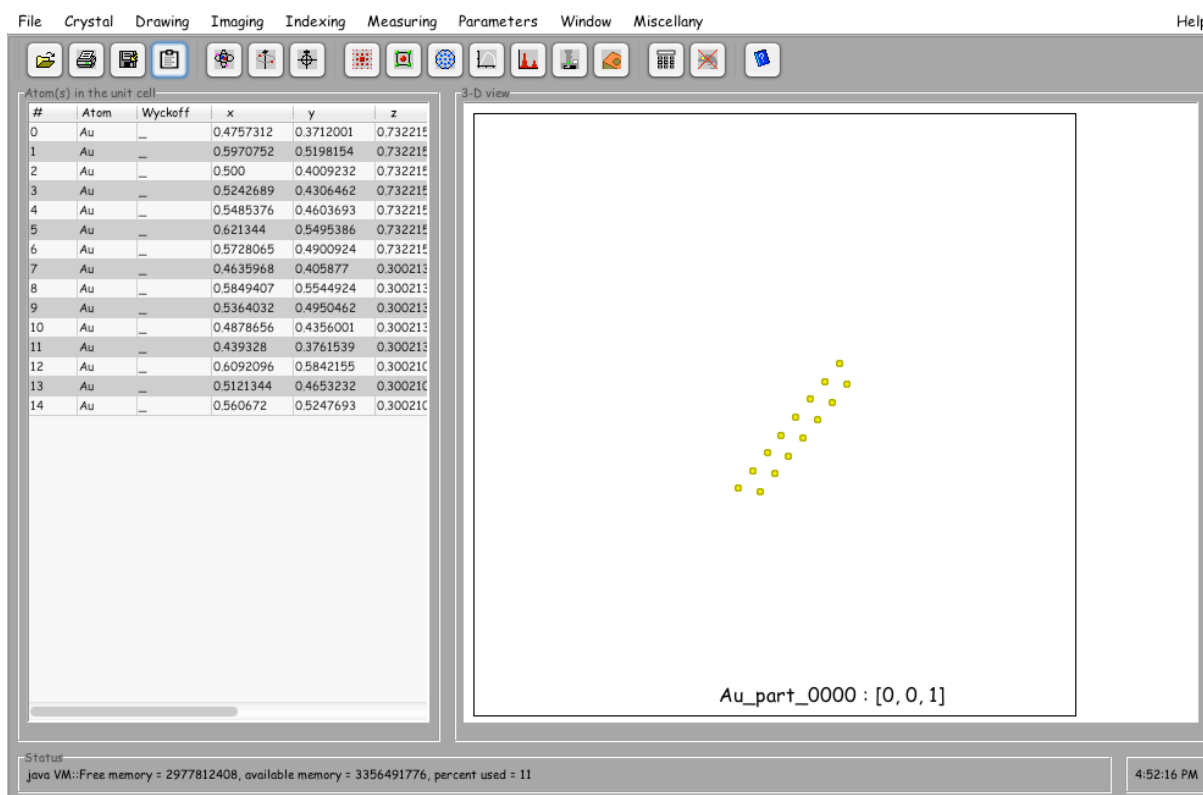


Figure 22: To perform a multislice calculation using the slices, first have slice xxxxx\_0000.txt loaded.

### 3.19 Starting the multislice calculation (Figure 23)

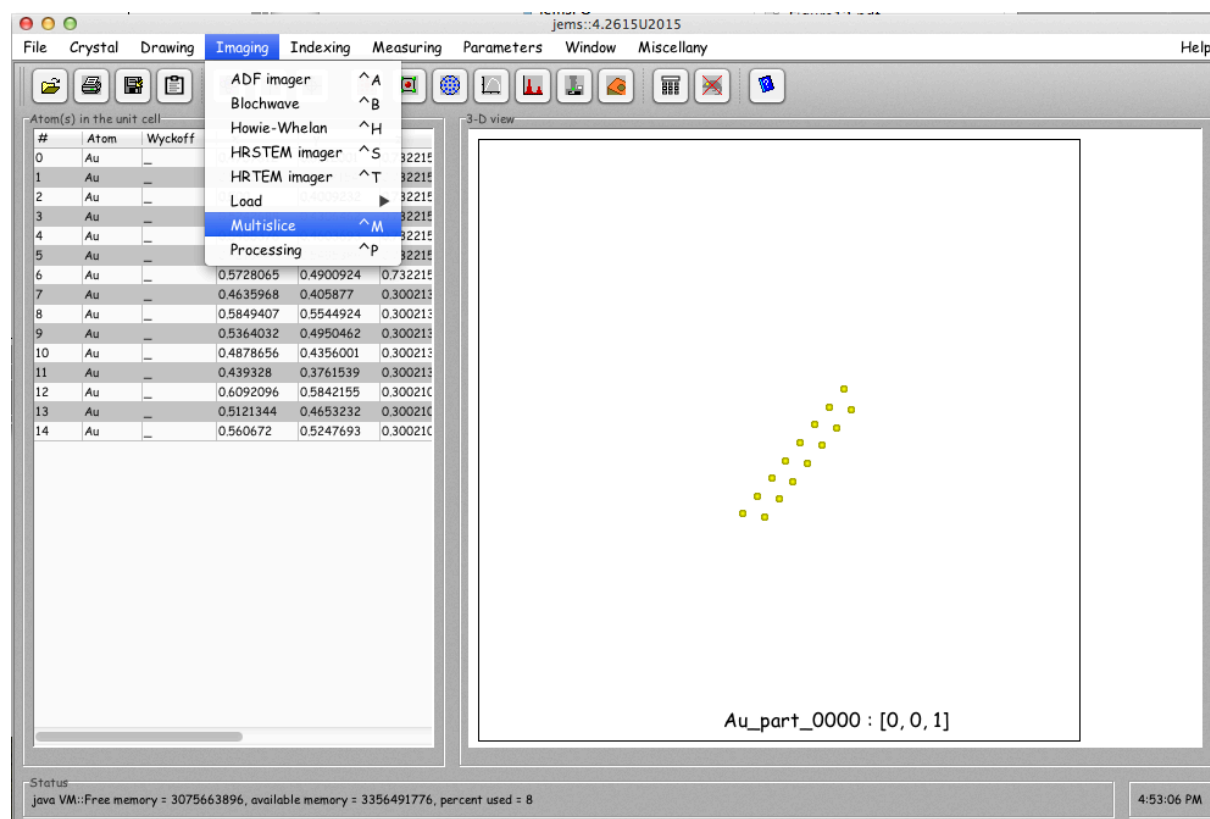


Figure 23: Select the *Multislice* menu item of menu *Imaging*.

### 3.20 Loading slices xxxx\_0001 to xxxx\_nnnn (Figure 24)

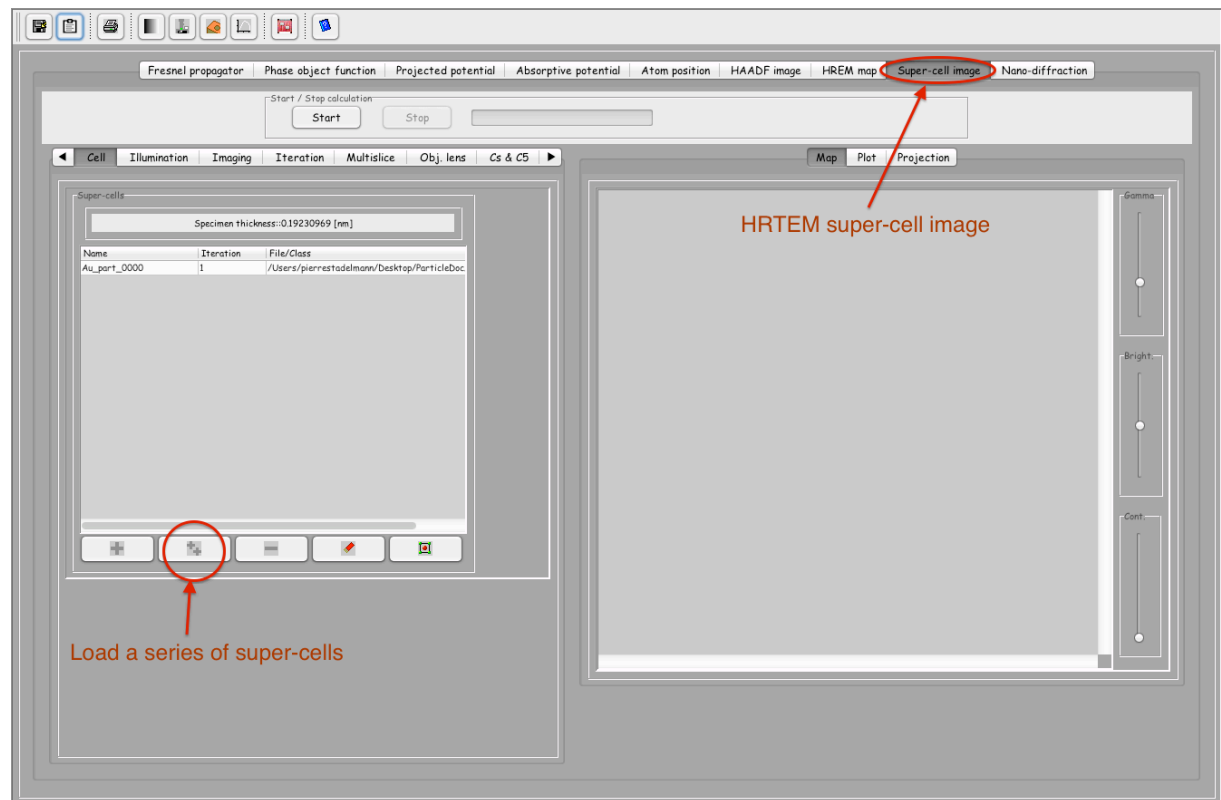


Figure 24: Select tab Super-cell image and load a series of super-cells.

### 3.21 Displaying the whole model (Figure 25)

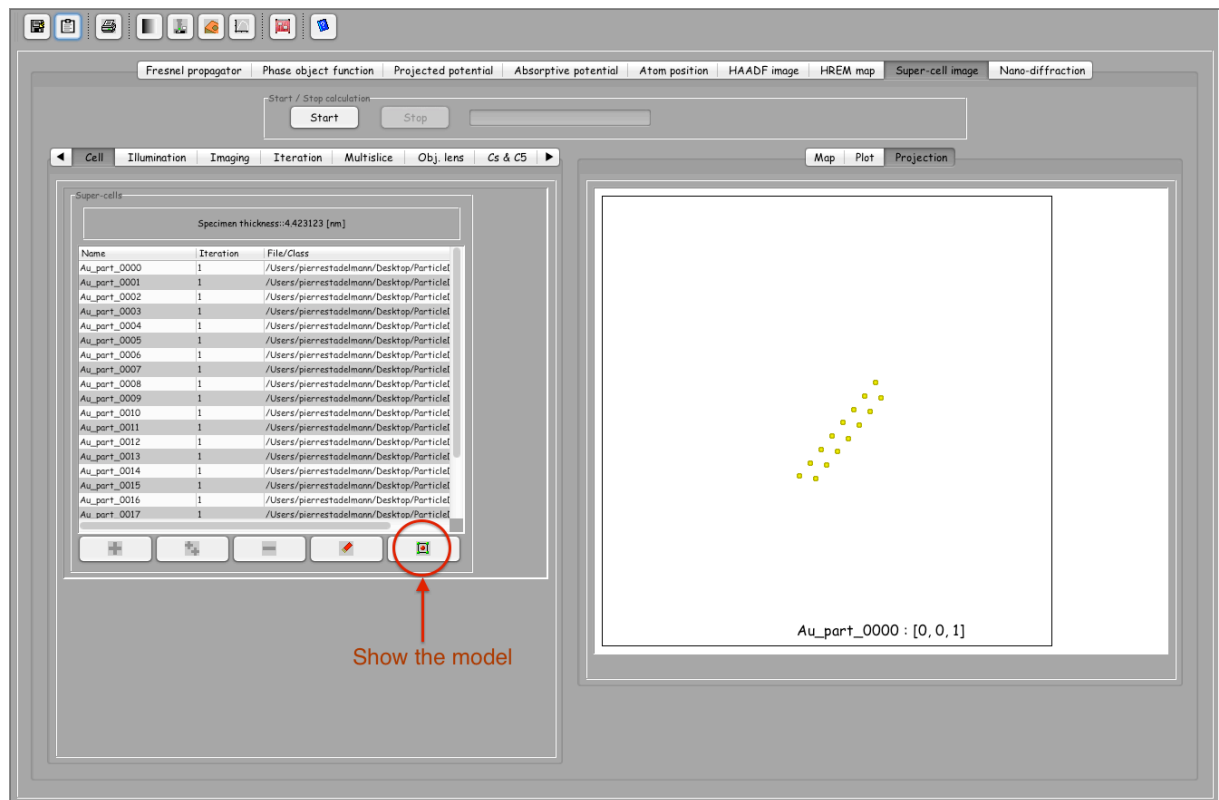


Figure 25: Show the model as a 3-D drawing.

### 3.22 3-D drawing of the model (Figure 26)

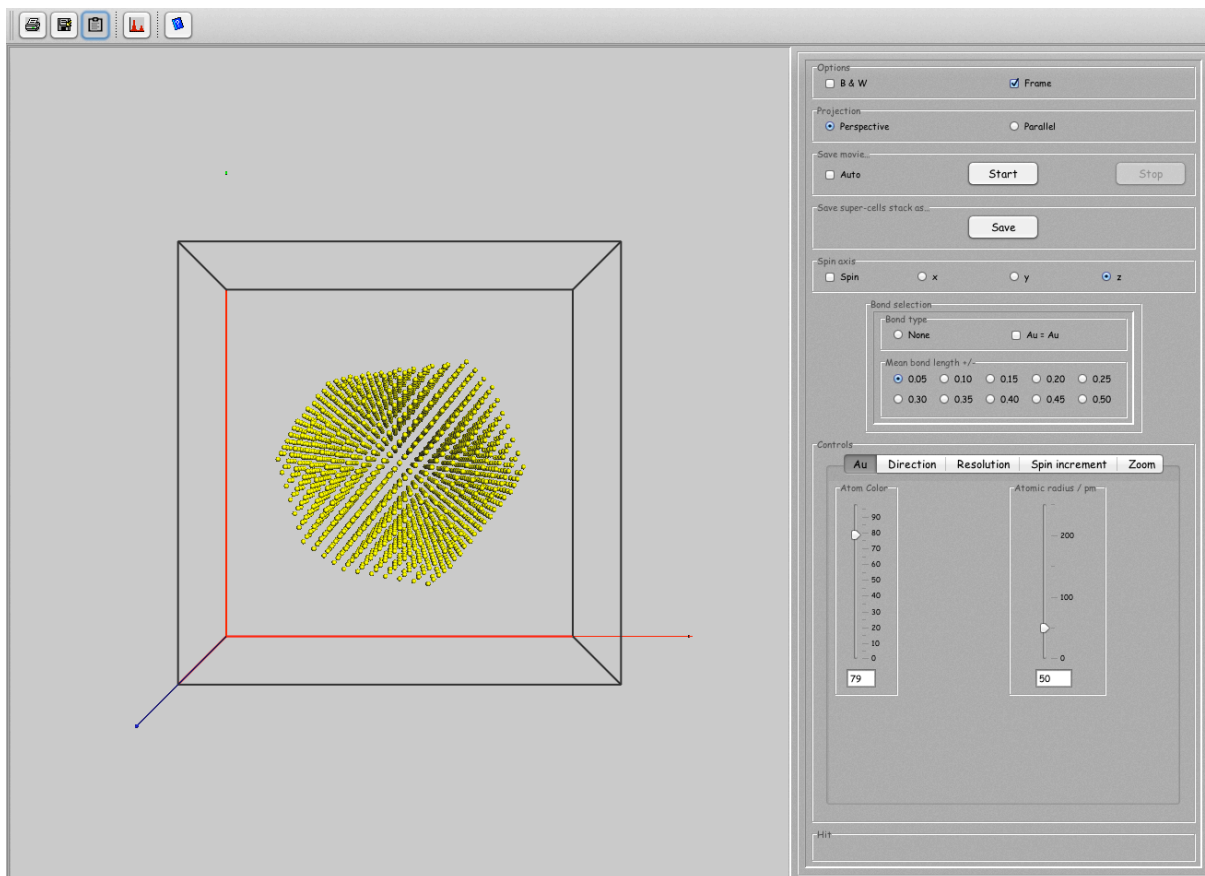


Figure 26: The 3-D model is show in its enclosing box.

Verify that the model is completely enclosed in the box before performing the multislice calculation.

### 3.23 Multislice calculation result (Figure 27)

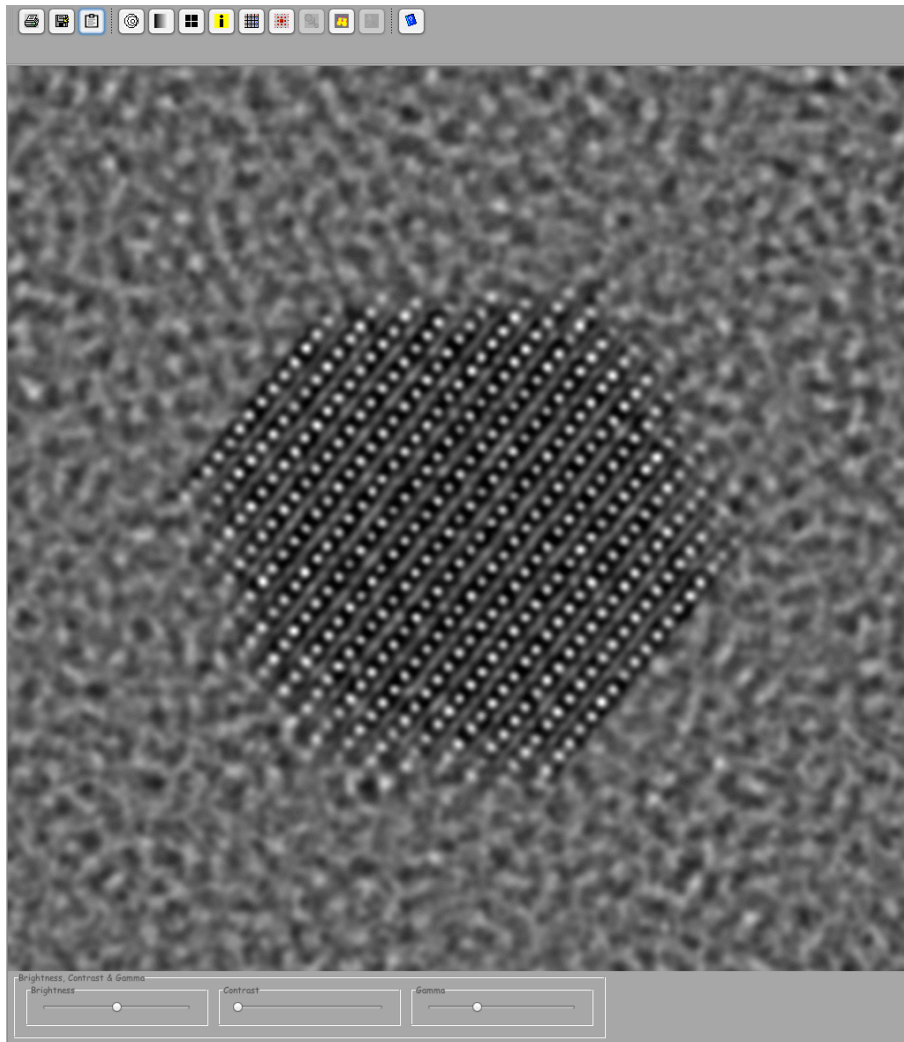


Figure 27: Multislice calculated HRTEM image.

Note the the contrast appears more important here (different contrast scale). The calculated values can be checked using tables of pixels. A more or less important difference should be expected since the WPOA calculation is only an approximation of the full image calculation.

### 3.24 WPOA calculation result (Figure 28)



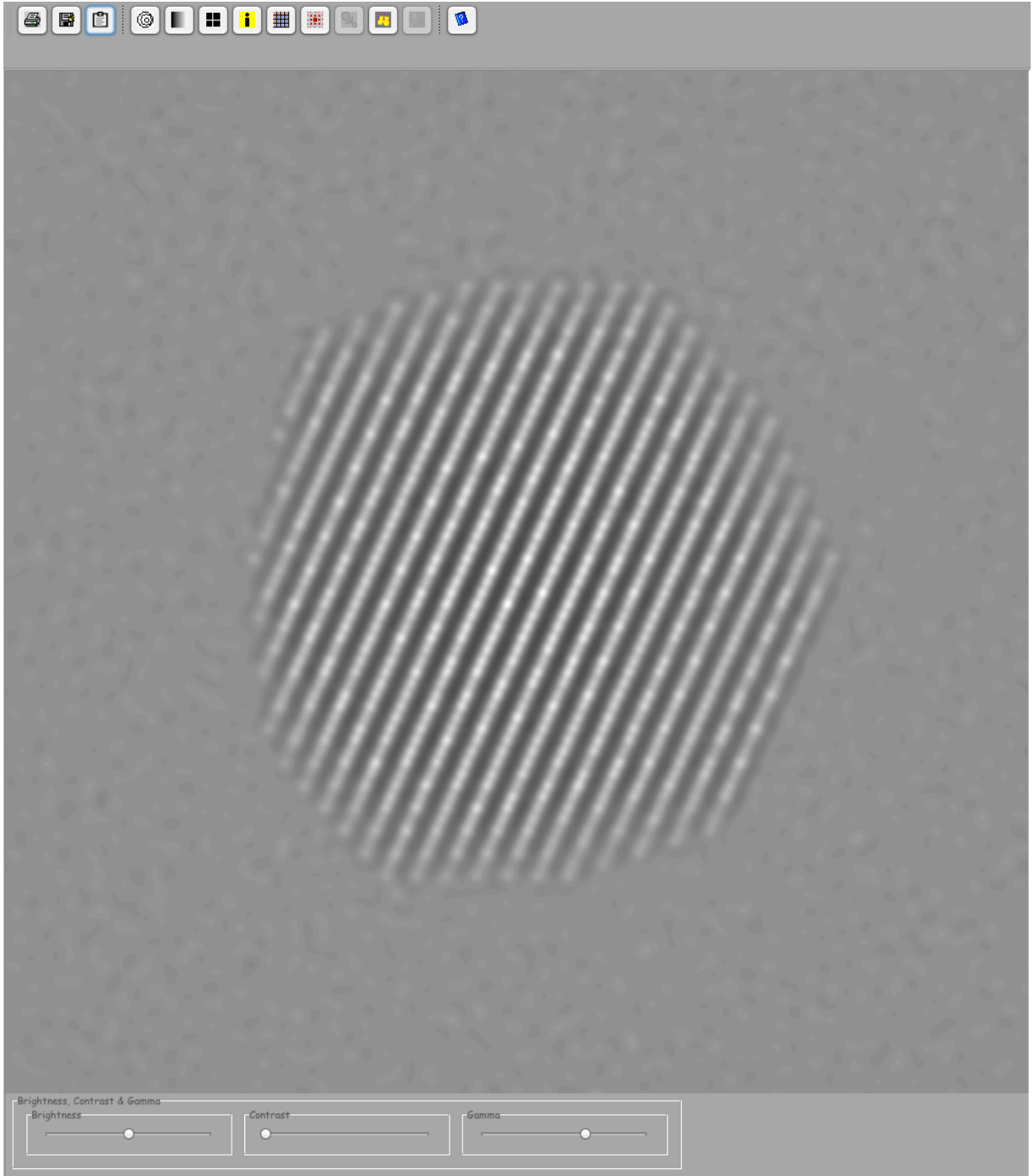


Figure 28: WPOA calculated image.

### 3.25 HAADF example (Figure 29)

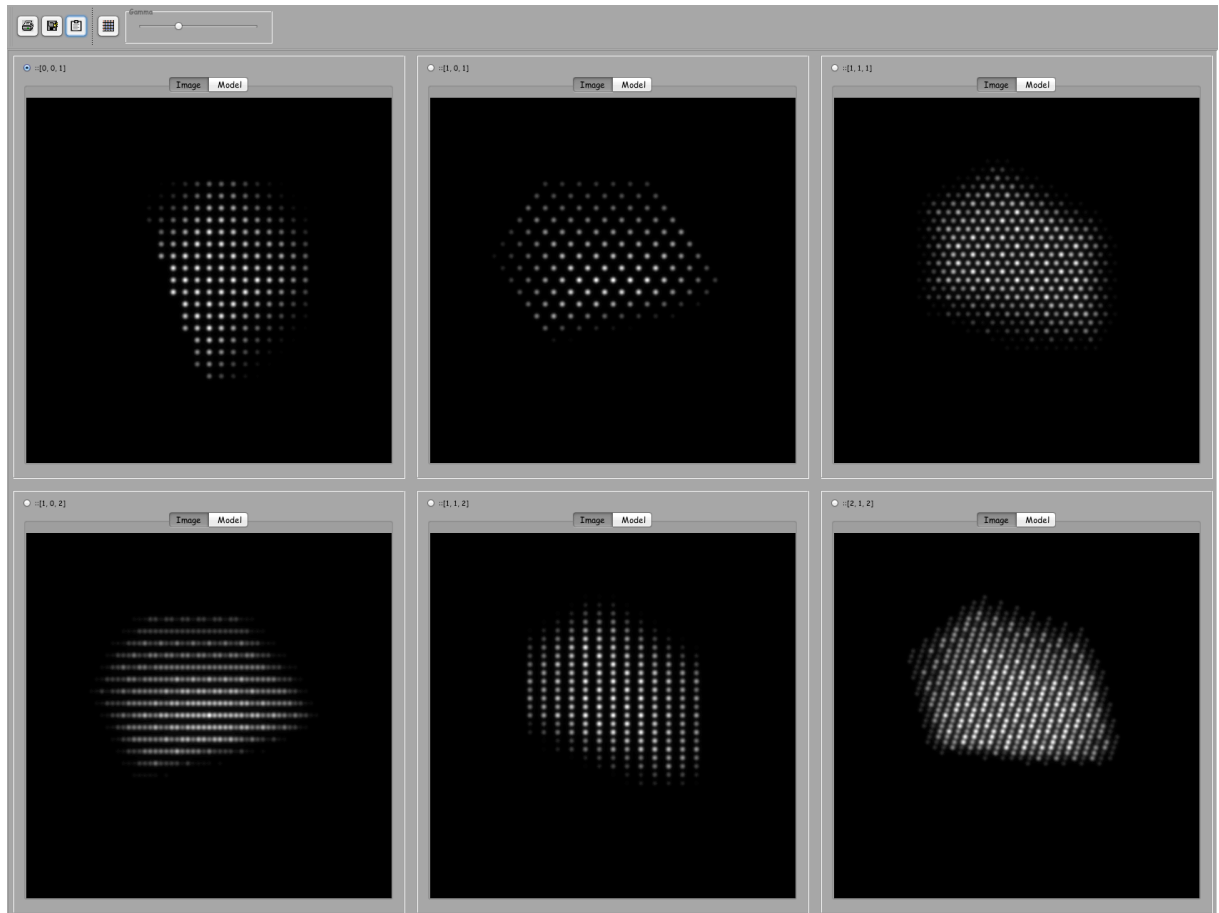


Figure 29: HAADF images.

### 3.26 Projected potential example (Figure 30)

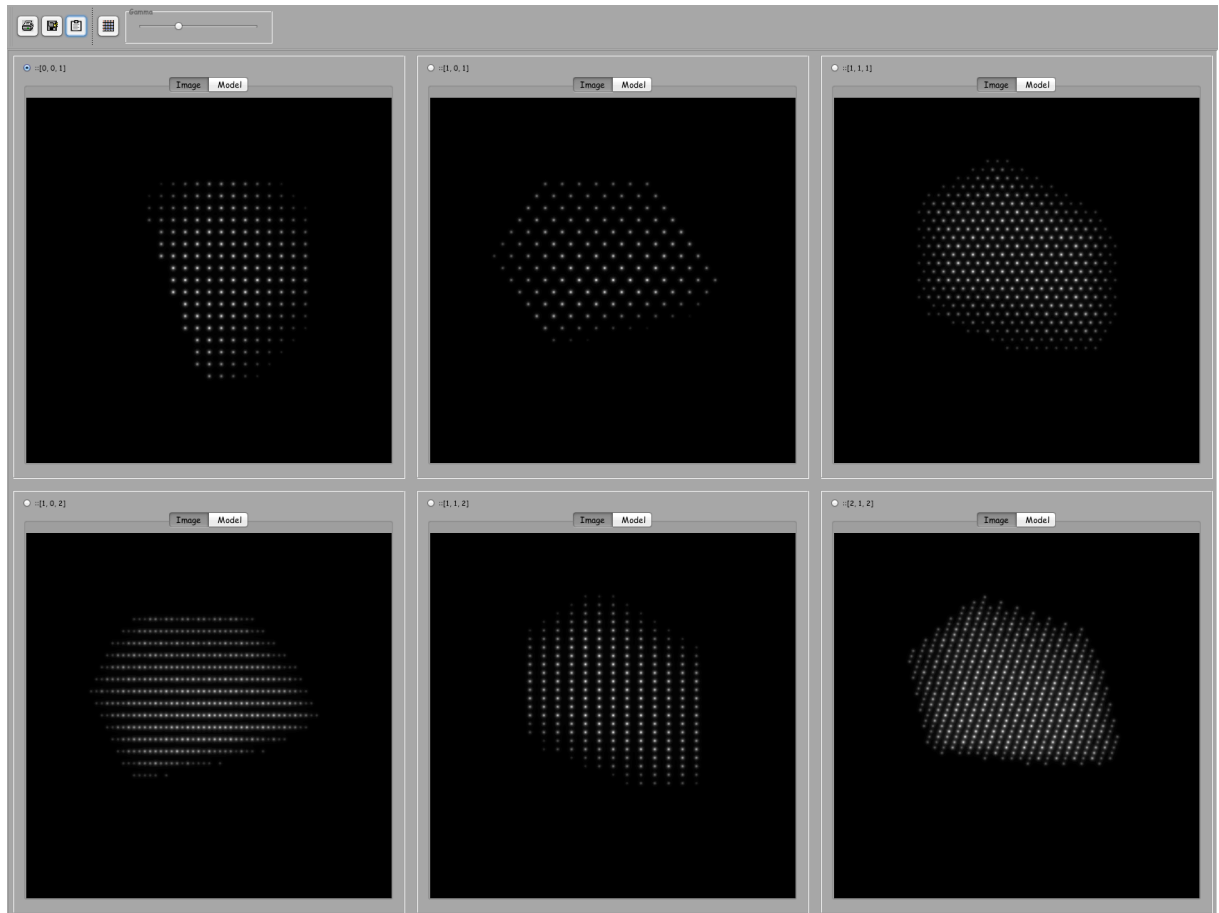


Figure 30: Projected potential images.

### 3.27 SAED example (Figure 31)

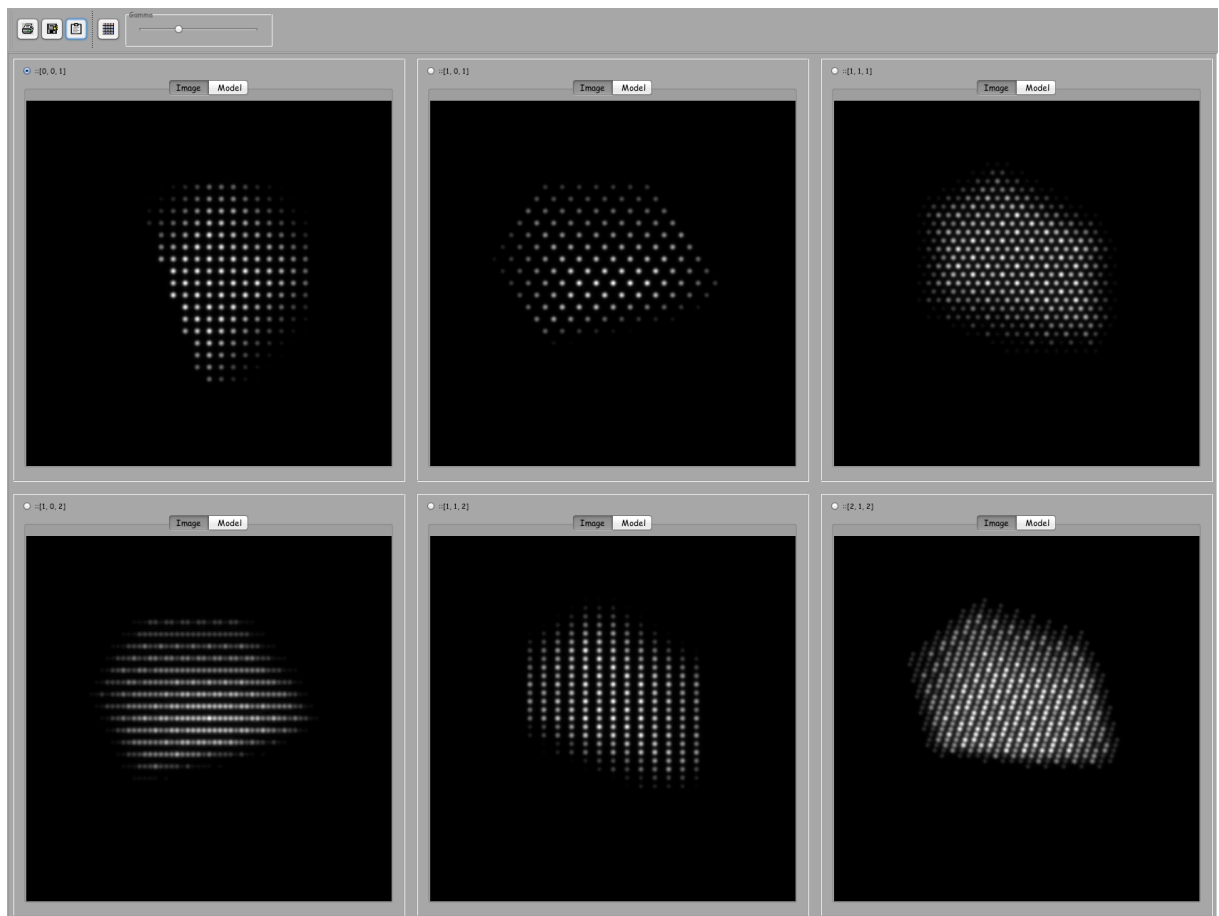


Figure 31: SAED patterns.

### 3.28 WPOA example (Figure 32)

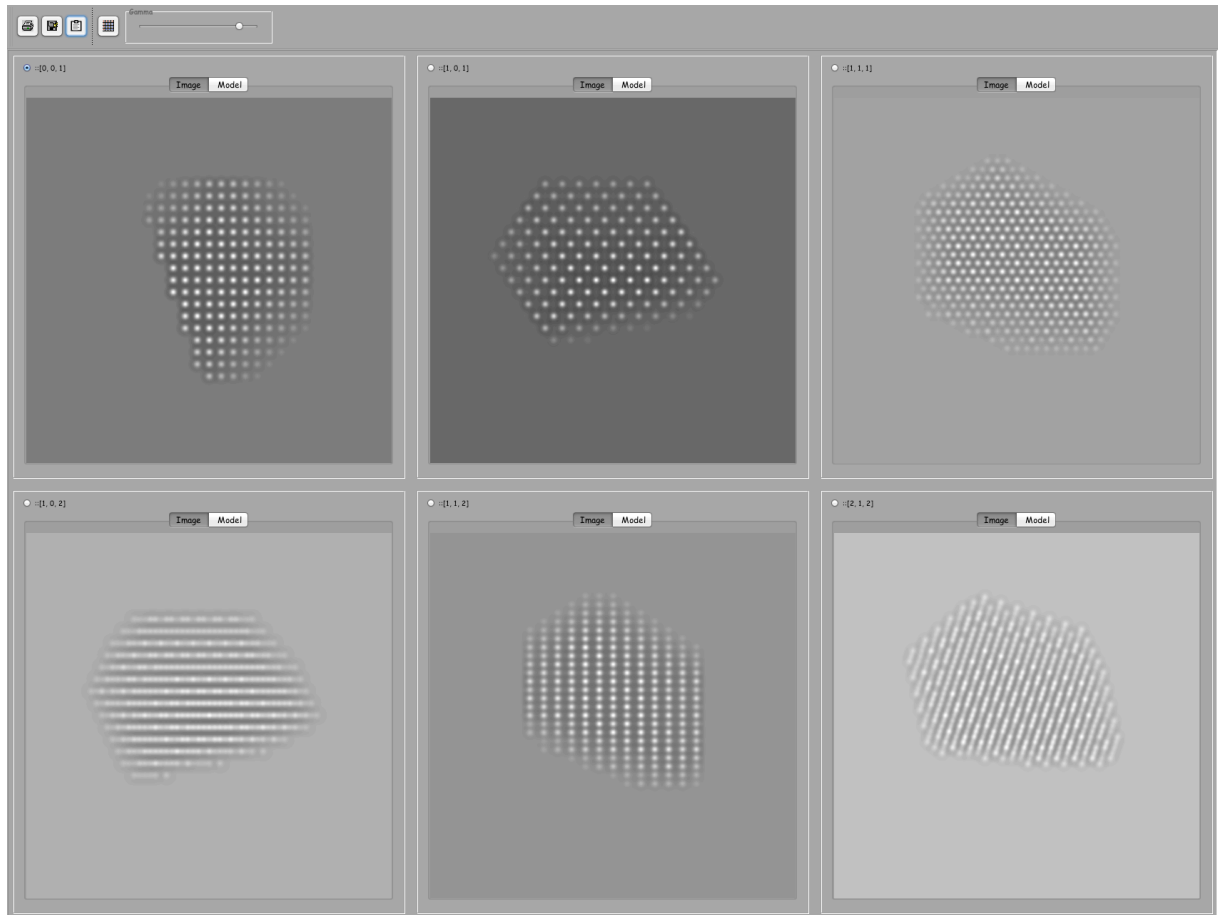


Figure 32: WPOA images.

### 3.29 WPOA images and models example (Figure 33)

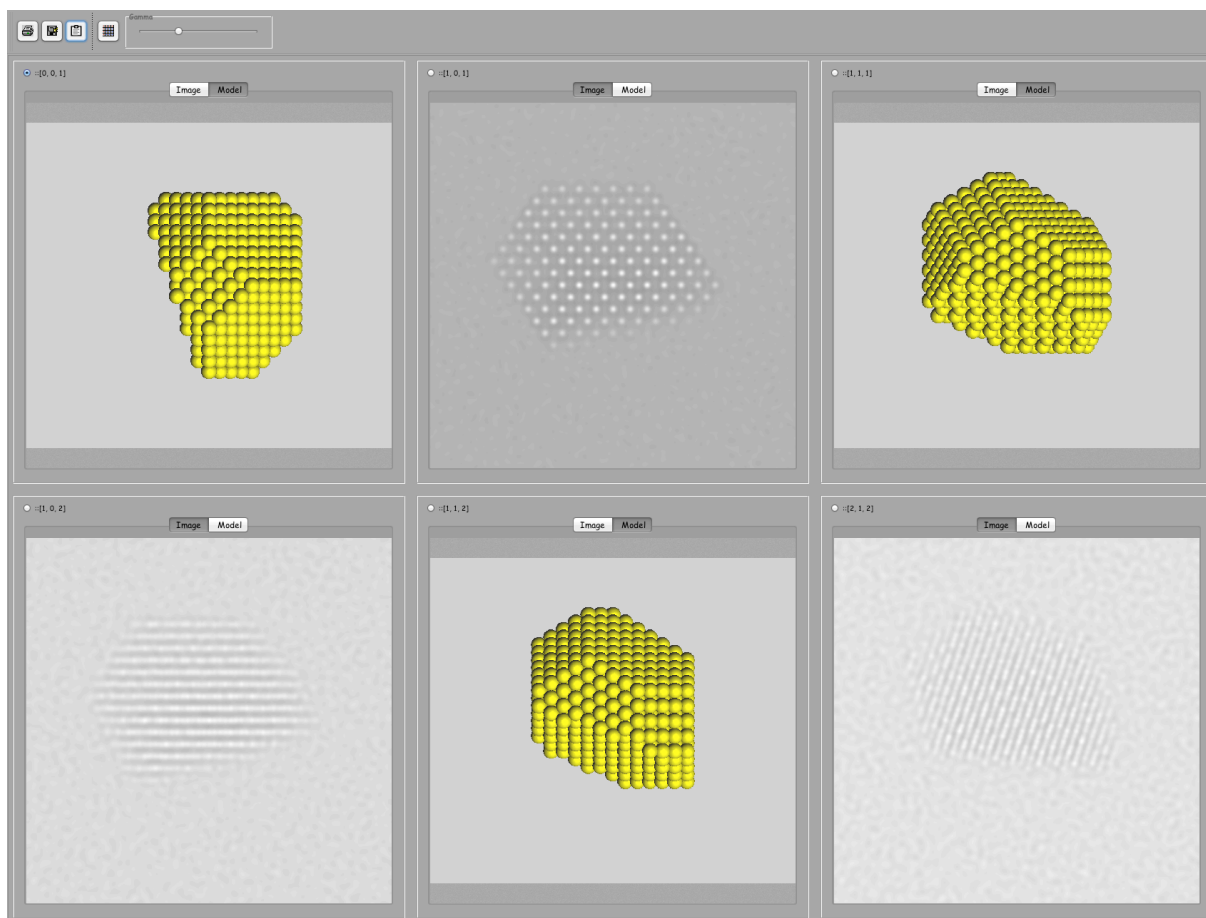


Figure 33: Each image is provided with its crystal model.

### 3.30 WPOA images of particles deposited on amorphous carbon film (Figure 34)

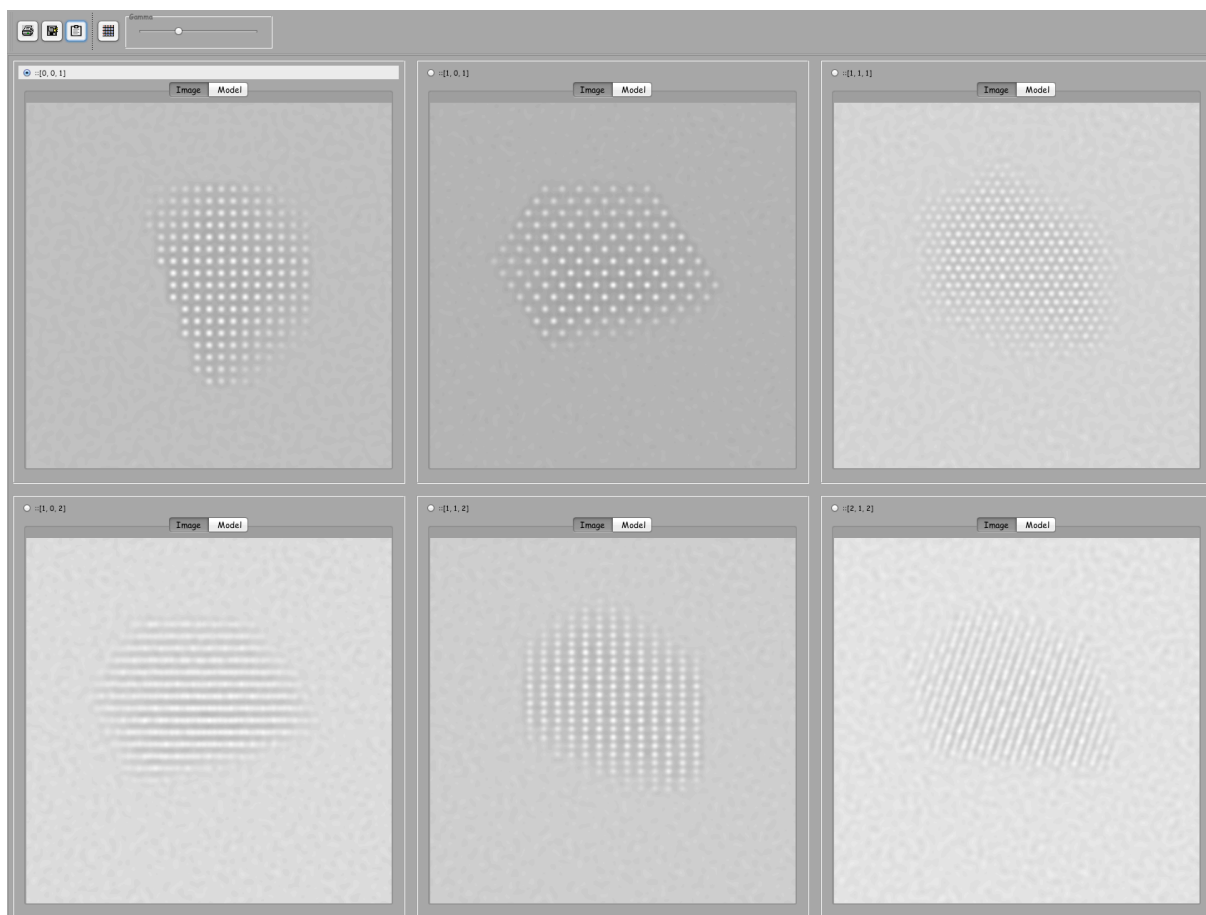


Figure 34: WPOA images of particles deposited on an amorphous carbon film.

### 3.31 Model particles (Figure 35)

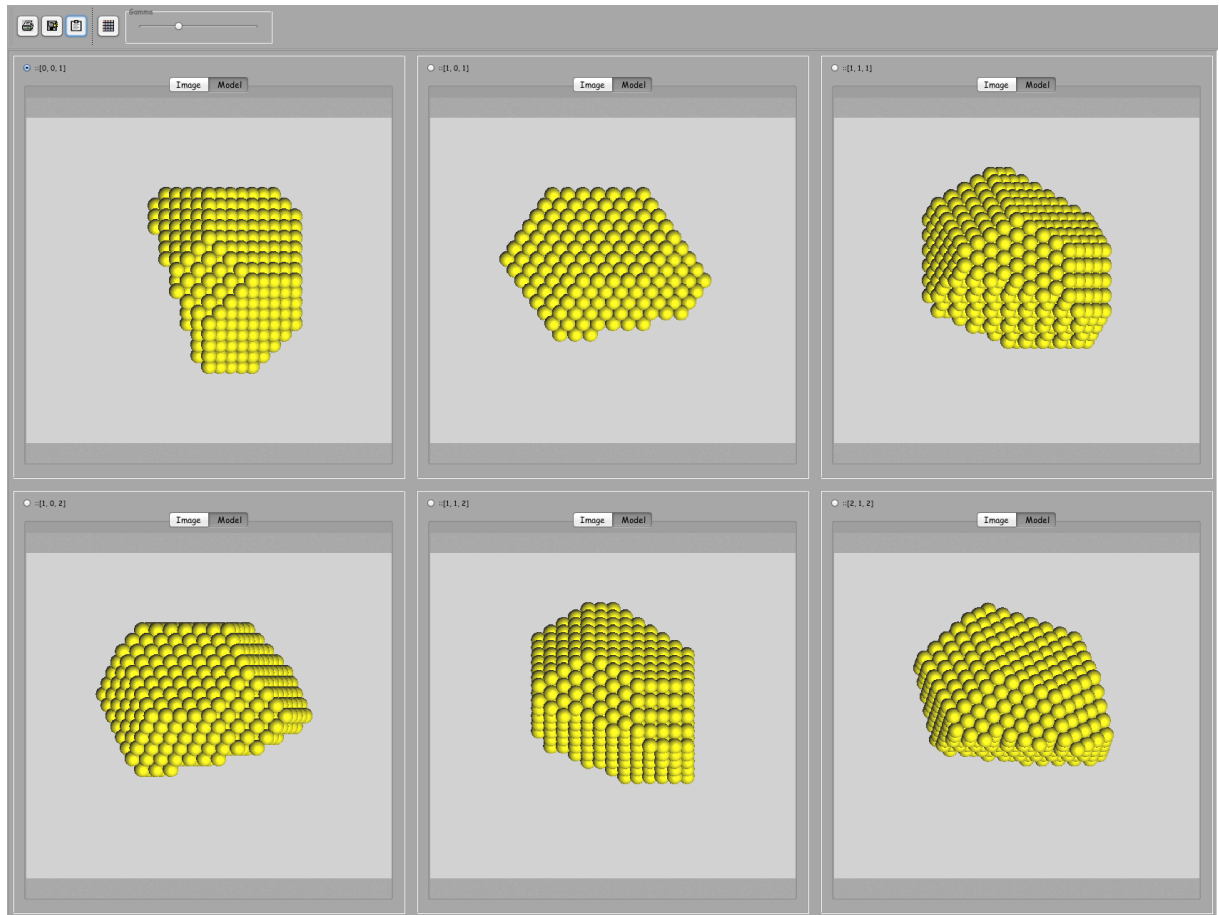


Figure 35: Grid of particle model.



## 4 Final remarks

Images and models can be rotated with respect to each other. This rotation depends on the model size. It can be compensated for each model using a popup menu (Figure 38) or for all models using the *Model rotation* controls of the *Options* tab (Figure 39) .



Figure 36: WPOA image.

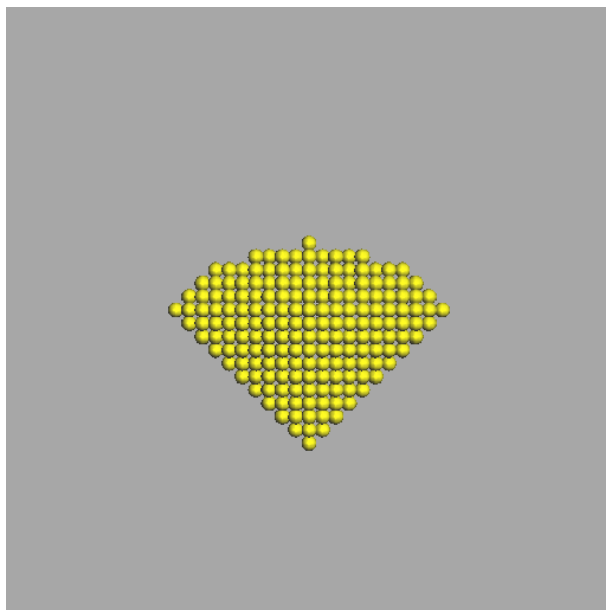


Figure 37: Model rotated with respect to the WPOA image.

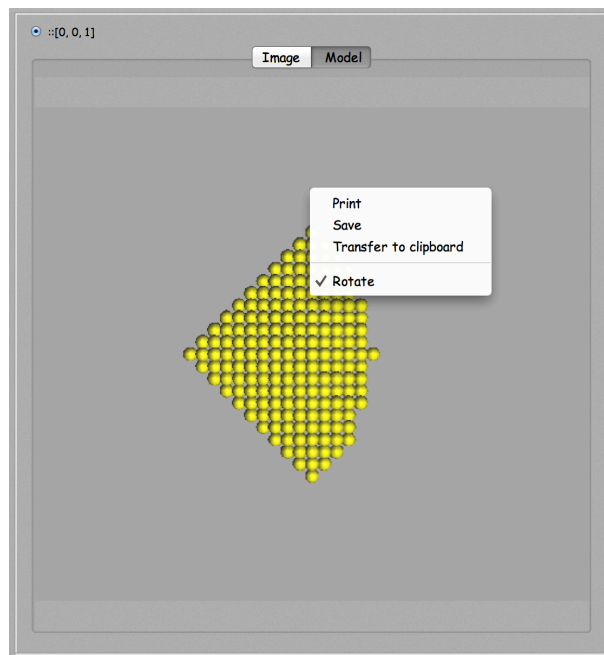


Figure 38: Using the model popup menu a rotation is applied to the model (default rotation is 90 deg.).

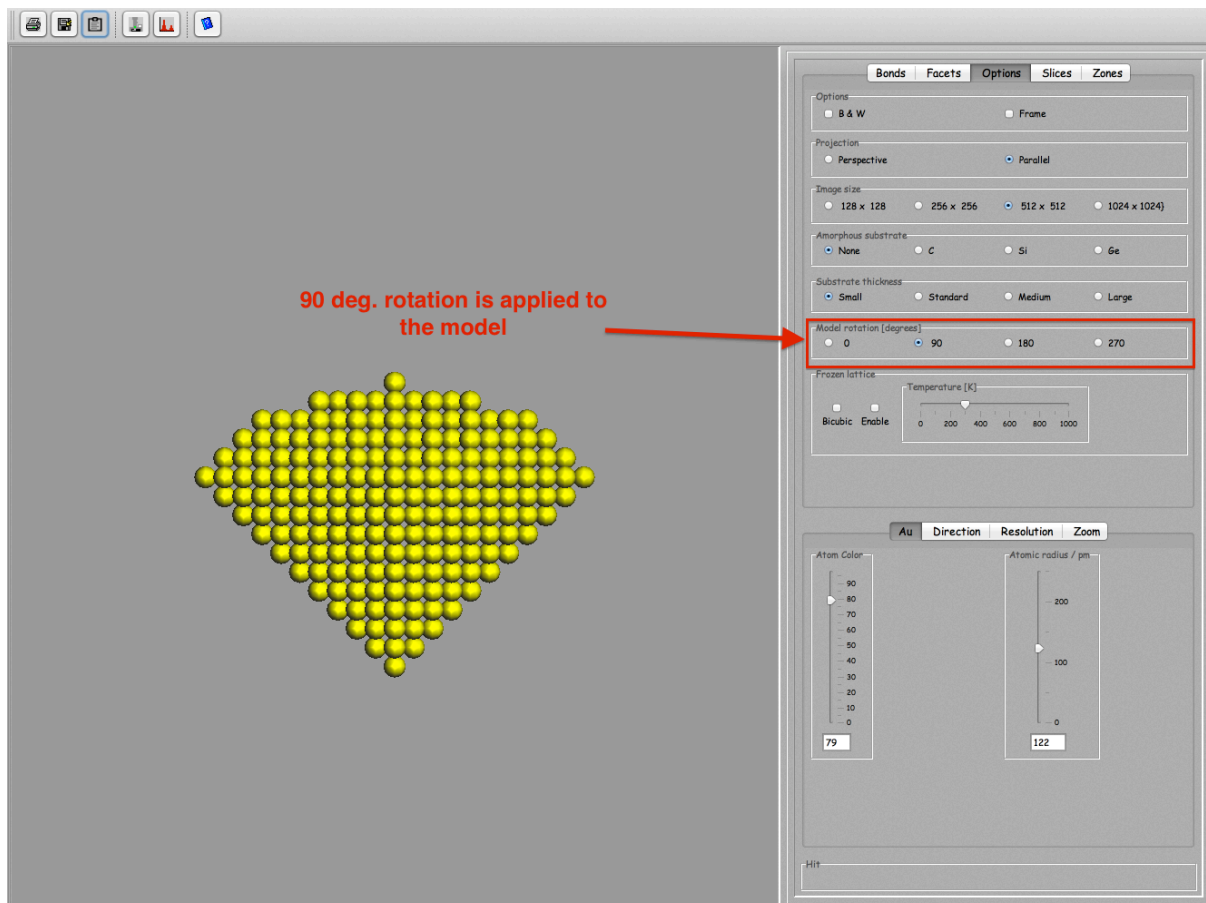


Figure 39: A rotation of 90 deg. is applied to all models.