Precession Electron Diffraction calculations using jems

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1 Introduction

Jems offers both kinematical and dynamical calculations of precession electron diffraction patterns (PED). These PED are calculated using the following scheme:

1. A zone axis pattern (ZAP) is selected (Fig. 1).
2. The crystal is tilted a few degrees out of perfect ZAP orientation (Fig. 2).
3. For each precession orientation a kinematical or dynamical ZAP electron diffraction pattern (up to 100 different crystal thickness) is calculated and the reflections' intensity are accumulated in an square array or in a stack of square arrays.
4. Finally the PED is displayed (Fig. 3).

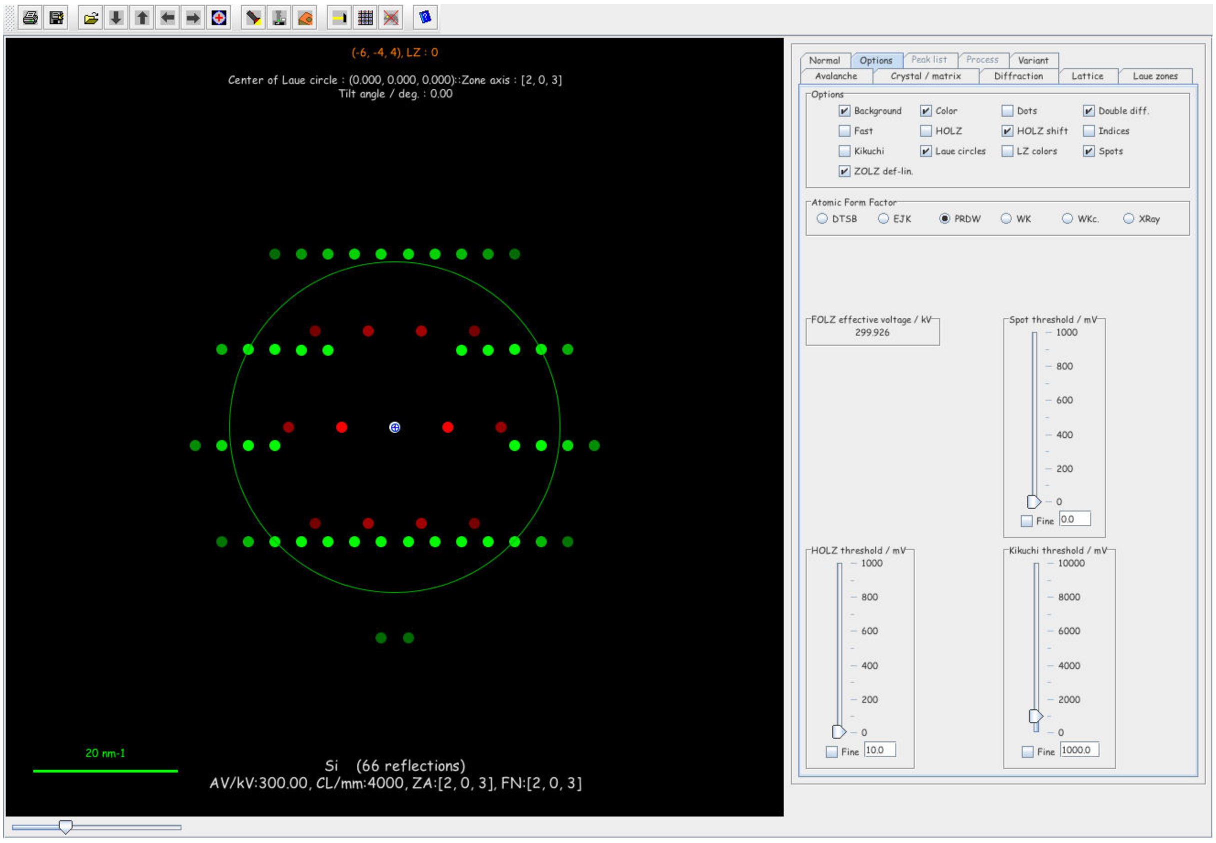


Figure 1: Zone axis electron diffraction pattern.

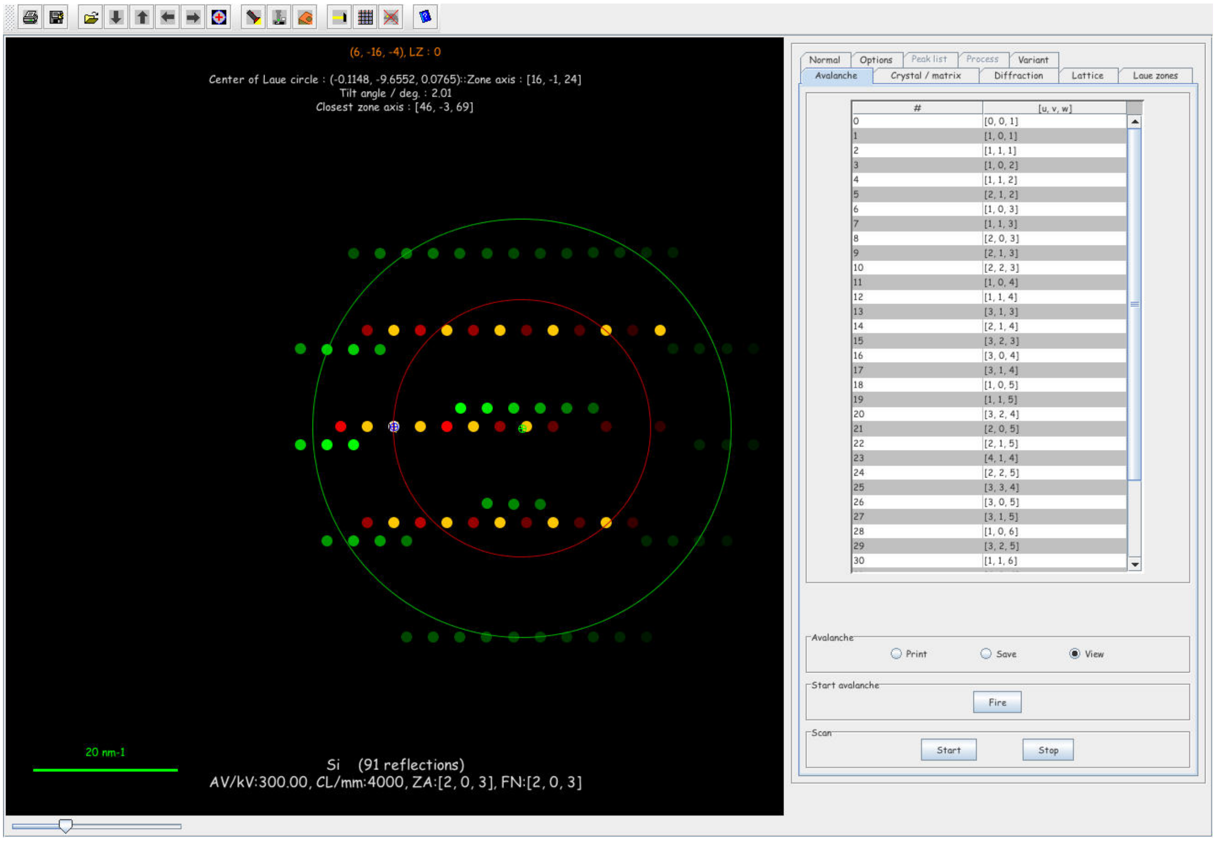


Figure 2: Tilted ZAP diffraction pattern. The red spots mark the zero order Laue zone (ZOLZ) reflections, the green ones the first order Laue (FOLZ) reflections and the yellow ones the double diffraction spots. These later spots are not included in the PED (see section 3).

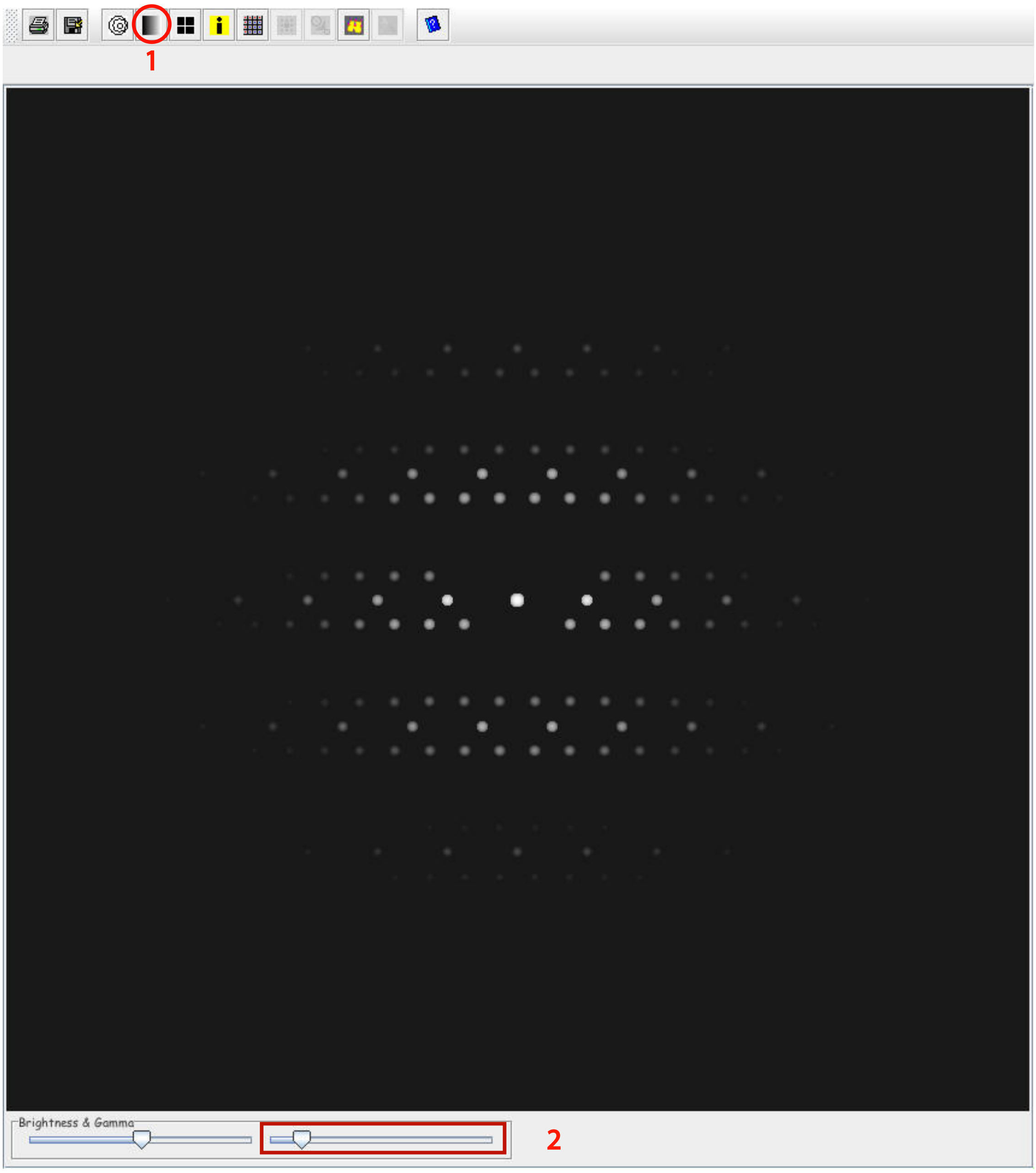


Figure 3: A kinematical Si [230] PED pattern (note that double diffraction spots are not calculated). The icon 1 resets the default gray lookup table (LUT), while slider 2 adds a gamma correction to the gray LUT.

2 Kinematical PED: details

The kinematical PED calculations can be started either using *Drawing* → *Diffraction* (Fig. 4) or the *Diffraction* icon (Fig. 5). A ZAP of default orientation is displayed (Fig. 6).

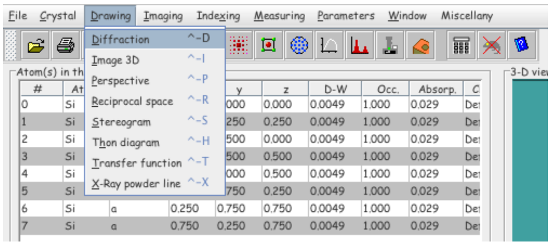


Figure 4: Drawing diffraction patterns using the *Drawing* menu.

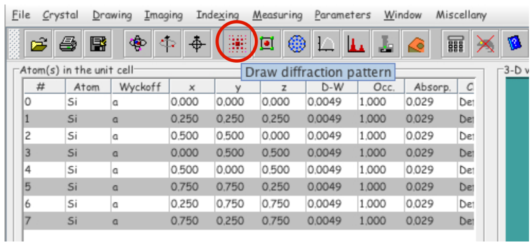


Figure 5: Drawing diffraction patterns using the *Diffraction* icon.

The ZAP controls are grouped in a *toolbar* placed at the top of the frame and in several tabs at its right. The icons 1, 2, 3 allow to select the ZAP orientation (when not directly available in the *Avalanche* tab [1]), to start the precession calculation and to tabulate the reflections (Fig. 7) respectively. After selecting the crystal orientation, here [230], the *Crystal / matrix* tab allows to plot several Laue zones (Fig. 8).

The following tabs allow to control the plot of the ZAP:

1. **Avalanche** (Fig. 9).
2. **Crystal / matrix** (Fig. 10).
3. **Diffraction** (Fig. 11).
4. **Lattice** (Fig. 13).
5. **Laue zones** (Fig. 14).
6. **Normal** (Fig. 15).
7. **Options** (Fig. 12).

The ZAP plot uses default values like the camera length, the acceptance angle, the maximum deviation, etc that are defined at startup time when the crystal is

[1]The list of [uvw] ZAP indices provided in this tab does not include equivalent directions (see Fig. 9).

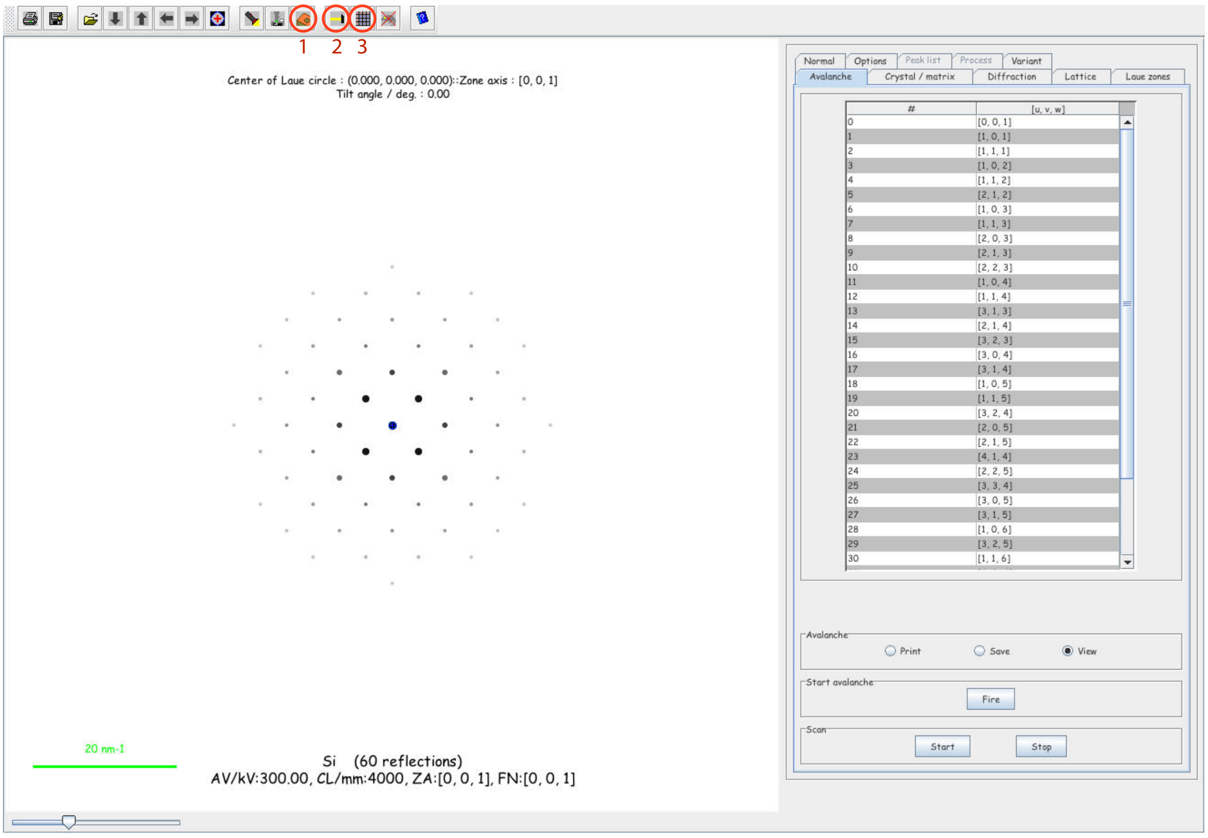


Figure 6: The default kinematical Si [001] ZAP pattern.

g	Vr Volt	Vi Volt	Amplitude	Phase deg.	||g|| nm-1	||g|| nm	g / g0	<(g, g0)	Laue zone	Devia. nm-1	Selected
(2, 2, 0)	6.86822	0.19918	6.87111	1.66111	5.20803	0.19201	1.000	0.000000	0	-0.0267	true
(-2, 2, 0)	6.86822	0.19918	6.87111	1.66111	5.20803	0.19201	1.000	90.000	0	-0.0267	true
(2, -2, 0)	6.86822	0.19918	6.87111	1.66111	5.20803	0.19201	1.000	90.000	0	-0.0267	true
(-2, -2, 0)	6.86822	0.19918	6.87111	1.66111	5.20803	0.19201	1.000	180.000	0	-0.0267	true
(4, 0, 0)	4.06232	0.11781	4.06403	1.66111	7.36526	0.13577	1.41421	45.000	0	-0.0534	true
(-4, 0, 0)	4.06232	0.11781	4.06403	1.66111	7.36526	0.13577	1.41421	135.000	0	-0.0534	true
(0, 4, 0)	4.06232	0.11781	4.06403	1.66111	7.36526	0.13577	1.41421	45.000	0	-0.0534	true
(0, -4, 0)	4.06232	0.11781	4.06403	1.66111	7.36526	0.13577	1.41421	135.000	0	-0.0534	true
(4, 4, 0)	2.33338	0.06767	2.33436	1.66111	10.41605	0.09601	2.000	0.000000	0	-0.10681	true
(-4, 4, 0)	2.33338	0.06767	2.33436	1.66111	10.41605	0.09601	2.000	90.000	0	-0.10681	true
(4, -4, 0)	2.33338	0.06767	2.33436	1.66111	10.41605	0.09601	2.000	90.000	0	-0.10681	true
(-4, -4, 0)	2.33338	0.06767	2.33436	1.66111	10.41605	0.09601	2.000	180.000	0	-0.10681	true
(6, 2, 0)	1.94829	0.0565	1.94911	1.66111	11.6455	0.08587	2.23607	26.56505	0	-0.13351	true
(6, -2, 0)	1.94829	0.0565	1.94911	1.66111	11.6455	0.08587	2.23607	63.43495	0	-0.13351	true
(2, 6, 0)	1.94829	0.0565	1.94911	1.66111	11.6455	0.08587	2.23607	26.56505	0	-0.13351	true
(-2, 6, 0)	1.94829	0.0565	1.94911	1.66111	11.6455	0.08587	2.23607	63.43495	0	-0.13351	true
(-6, 2, 0)	1.94829	0.0565	1.94911	1.66111	11.6455	0.08587	2.23607	116.56505	0	-0.13351	true
(-6, -2, 0)	1.94829	0.0565	1.94911	1.66111	11.6455	0.08587	2.23607	153.43495	0	-0.13351	true
(2, -6, 0)	1.94829	0.0565	1.94911	1.66111	11.6455	0.08587	2.23607	116.56505	0	-0.13351	true
(-2, -6, 0)	1.94829	0.0565	1.94911	1.66111	11.6455	0.08587	2.23607	153.43495	0	-0.13351	true
(8, 0, 0)	1.26558	0.0367	1.26611	1.66111	14.73052	0.06789	2.82843	45.000	0	-0.21364	true
(-8, 0, 0)	1.26558	0.0367	1.26611	1.66111	14.73052	0.06789	2.82843	135.000	0	-0.21364	true
(0, -8, 0)	1.26558	0.0367	1.26611	1.66111	14.73052	0.06789	2.82843	135.000	0	-0.21364	true
(0, 8, 0)	1.26558	0.0367	1.26611	1.66111	14.73052	0.06789	2.82843	45.000	0	-0.21364	true
(6, 6, 0)	1.11804	0.03242	1.11851	1.66111	15.62408	0.064	3.000	0.000000	0	-0.24035	true
(-6, 6, 0)	1.11804	0.03242	1.11851	1.66111	15.62408	0.064	3.000	90.000	0	-0.24035	true
(-6, -6, 0)	1.11804	0.03242	1.11851	1.66111	15.62408	0.064	3.000	180.000	0	-0.24035	true
(6, -6, 0)	1.11804	0.03242	1.11851	1.66111	15.62408	0.064	3.000	90.000	0	-0.24035	true
(8, 4, 0)	0.99504	0.02886	0.99546	1.66111	16.46923	0.06072	3.16228	18.43495	0	-0.26706	true
(-8, 4, 0)	0.99504	0.02886	0.99546	1.66111	16.46923	0.06072	3.16228	108.43495	0	-0.26706	true
(4, -8, 0)	0.99504	0.02886	0.99546	1.66111	16.46923	0.06072	3.16228	108.43495	0	-0.26706	true
(-4, 8, 0)	0.99504	0.02886	0.99546	1.66111	16.46923	0.06072	3.16228	71.56505	0	-0.26706	true
(4, 8, 0)	0.99504	0.02886	0.99546	1.66111	16.46923	0.06072	3.16228	18.43495	0	-0.26706	true
(8, -4, 0)	0.99504	0.02886	0.99546	1.66111	16.46923	0.06072	3.16228	71.56505	0	-0.26706	true
(-8, -4, 0)	0.99504	0.02886	0.99546	1.66111	16.46923	0.06072	3.16228	161.56505	0	-0.26706	true
(-4, -8, 0)	0.99504	0.02886	0.99546	1.66111	16.46923	0.06072	3.16228	161.56505	0	-0.26706	true
(-2, 10, 0)	0.7282	0.02112	0.72851	1.66111	18.77781	0.05325	3.60555	56.30993	0	-0.34721	true
(2, 10, 0)	0.7282	0.02112	0.72851	1.66111	18.77781	0.05325	3.60555	33.69007	0	-0.34721	true
(10, 2, 0)	0.7282	0.02112	0.72851	1.66111	18.77781	0.05325	3.60555	33.69007	0	-0.34721	true
(10, -2, 0)	0.7282	0.02112	0.72851	1.66111	18.77781	0.05325	3.60555	56.30993	0	-0.34721	true
(-10, -2, 0)	0.7282	0.02112	0.72851	1.66111	18.77781	0.05325	3.60555	146.30993	0	-0.34721	true
(2, -10, 0)	0.7282	0.02112	0.72851	1.66111	18.77781	0.05325	3.60555	123.69007	0	-0.34721	true
(-2, -10, 0)	0.7282	0.02112	0.72851	1.66111	18.77781	0.05325	3.60555	146.30993	0	-0.34721	true
(-10, 2, 0)	0.7282	0.02112	0.72851	1.66111	18.77781	0.05325	3.60555	123.69007	0	-0.34721	true
(-8, 8, 0)	0.55661	0.01614	0.55685	1.66111	20.83211	0.048	4.000	90.000	0	-0.42737	true
(8, 8, 0)	0.55661	0.01614	0.55685	1.66111	20.83211	0.048	4.000	0.000000	0	-0.42737	true
(8, -8, 0)	0.55661	0.01614	0.55685	1.66111	20.83211	0.048	4.000	90.000	0	-0.42737	true
(-8, -8, 0)	0.55661	0.01614	0.55685	1.66111	20.83211	0.048	4.000	180.000	0	-0.42737	true
(-6, 10, 0)	0.5126	0.01487	0.51282	1.66111	21.47324	0.04657	4.12311	75.96376	0	-0.45409	true
(6, 10, 0)	0.5126	0.01487	0.51282	1.66111	21.47324	0.04657	4.12311	14.03624	0	-0.45409	true
(-10, -6, 0)	0.5126	0.01487	0.51282	1.66111	21.47324	0.04657	4.12311	165.96376	0	-0.45409	true
(10, -6, 0)	0.5126	0.01487	0.51282	1.66111	21.47324	0.04657	4.12311	75.96376	0	-0.45409	true
(6, -10, 0)	0.5126	0.01487	0.51282	1.66111	21.47324	0.04657	4.12311	104.03624	0	-0.45409	true
(-6, -10, 0)	0.5126	0.01487	0.51282	1.66111	21.47324	0.04657	4.12311	165.96376	0	-0.45409	true
(-10, 6, 0)	0.5126	0.01487	0.51282	1.66111	21.47324	0.04657	4.12311	104.03624	0	-0.45409	true
(10, 6, 0)	0.5126	0.01487	0.51282	1.66111	21.47324	0.04657	4.12311	14.03624	0	-0.45409	true
(12, 0, 0)	0.47341	0.01373	0.47361	1.66111	22.09579	0.04526	4.24264	45.000	0	-0.48081	true
(0, 12, 0)	0.47341	0.01373	0.47361	1.66111	22.09579	0.04526	4.24264	45.000	0	-0.48081	true
(-12, 0, 0)	0.47341	0.01373	0.47361	1.66111	22.09579	0.04526	4.24264	135.000	0	-0.48081	true
(0, -12, 0)	0.47341	0.01373	0.47361	1.66111	22.09579	0.04526	4.24264	135.000	0	-0.48081	true

Figure 7: Tabulated Si [001] ZAP reflections. The table contains the (hkl) indices of reflection $\mathbf{i}$, its structure factor (real, imaginary, amplitude [V] & phase [degree], its length $[nm^{-1}]$, its corresponding lattice planes spacing [nm], the ratio of reflection $\mathbf{i}$ to reflection $\mathbf{i} = \mathbf{0}$ and their relative angle [degree], its Laue zone index, the length of its deviation vector $[nm^{-1}]$ and a flag indicating whether or not that the reflection has been selected for the calculation (always *true* when performing kinematical calculations).

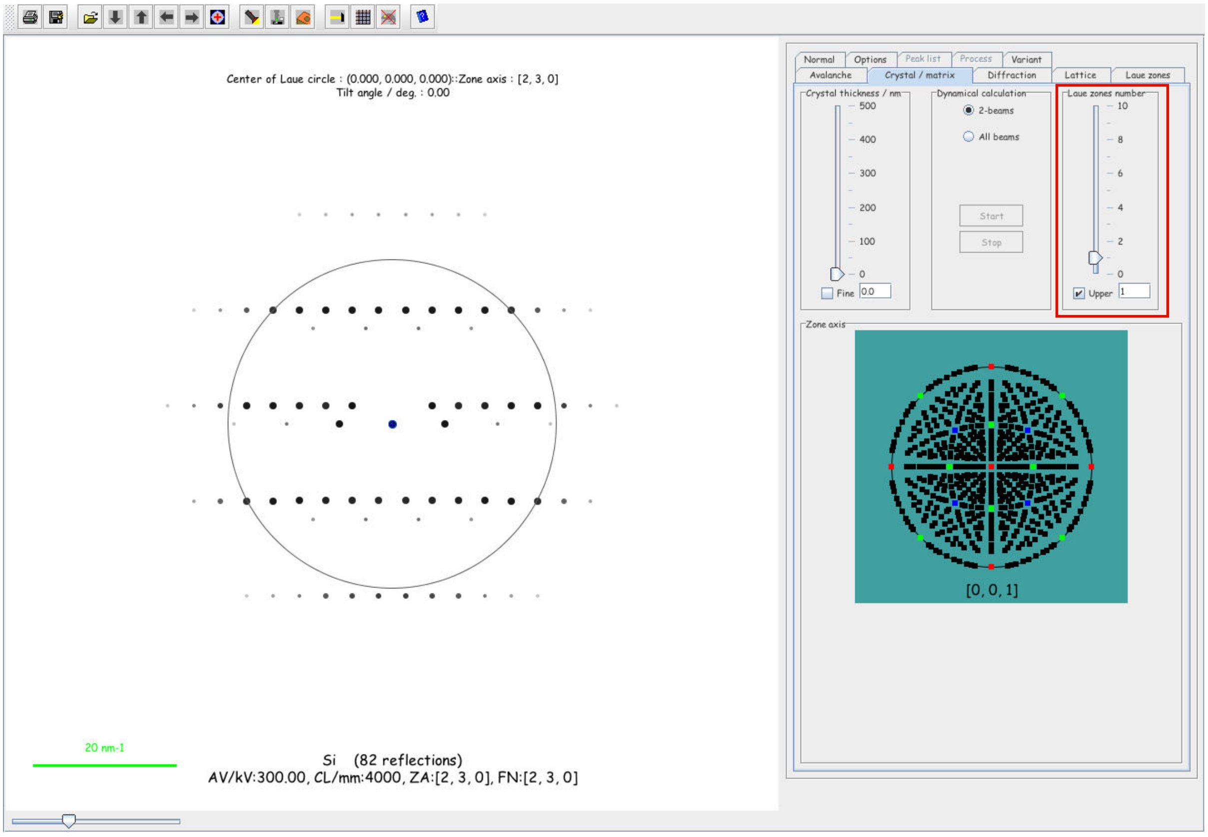


Figure 8: Kinematical Si [230] ZAP with ZOLZ and FOLZ reflections.

loaded. It is possible to keep some of them constant from calculation to calculation using the check boxes group 7 shon in Fig. 11.

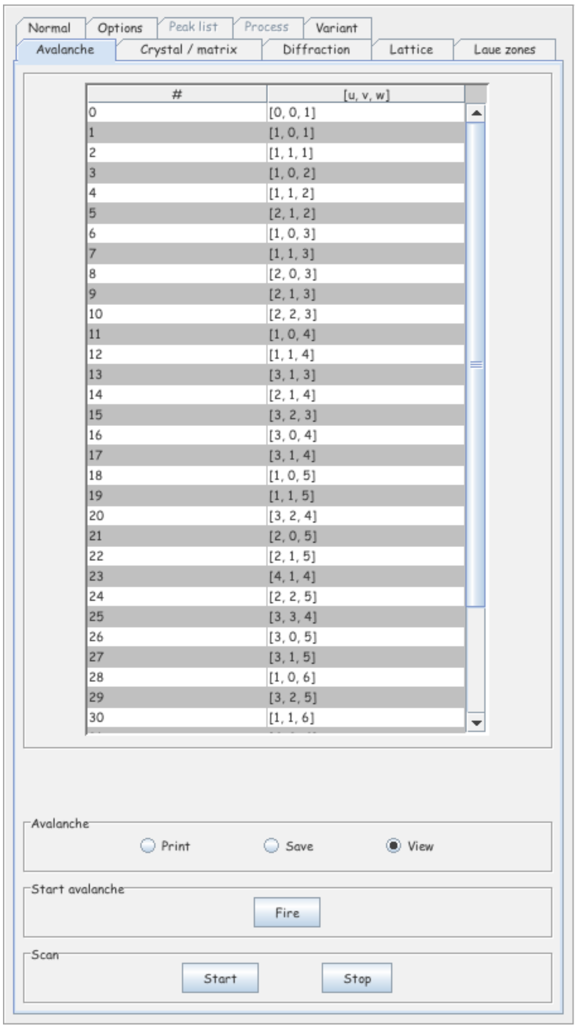


Figure 9: The *Avalanche* tab controls the crystal orientation and allows to print, save or display the selected ZAP.

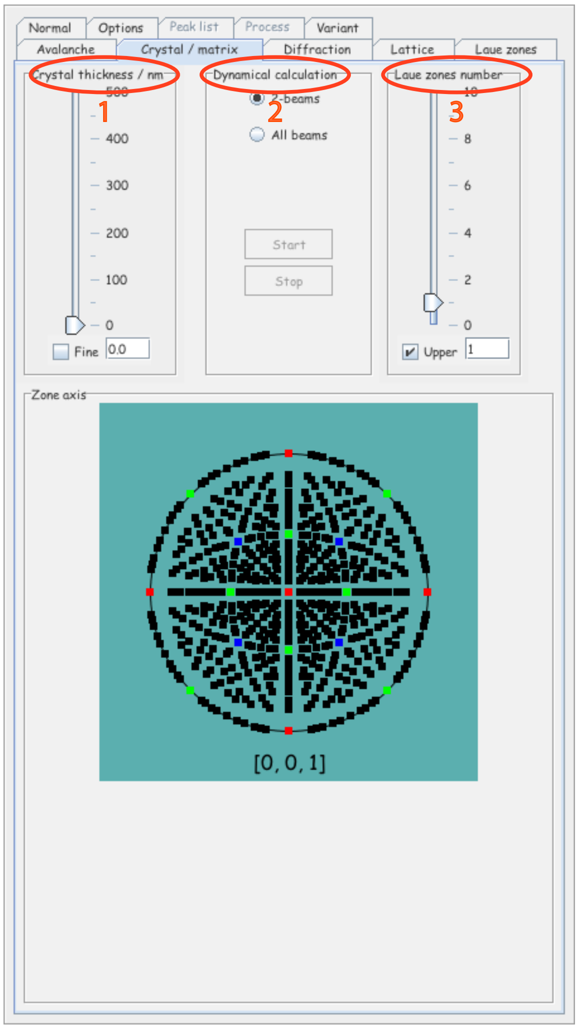


Figure 10: The *Crystal / matrix* tab controls the number of Laue zones to plot (3). Controls 1 & 2 allow to do dynamical ZAP calculations.

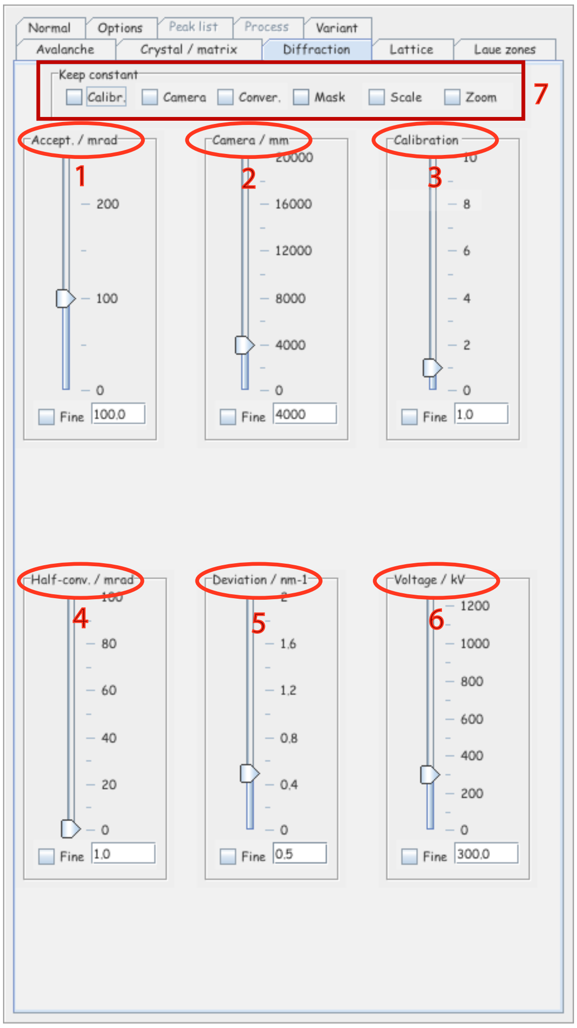


Figure 11: The *Diffraction* tab allows reflections with a deviation smaller than (5) $[nm^{-1}]$ and within a cone of (1) [mrad]. The check boxes group (7) allows to fix some of the ZAP plot parameters.

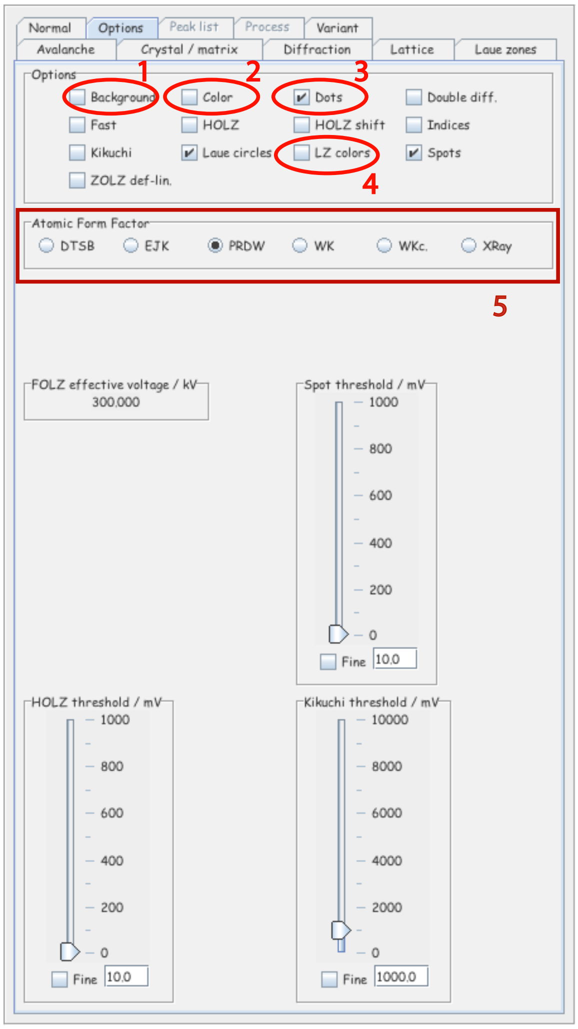


Figure 12: The *Options* tab allows to change the background (1), to color the Laue zone (2), to display spots (3) and to adjust the color scale of the different Laue zones (4). The radio buttons group (5) selects the source of the atomic scattering factors.

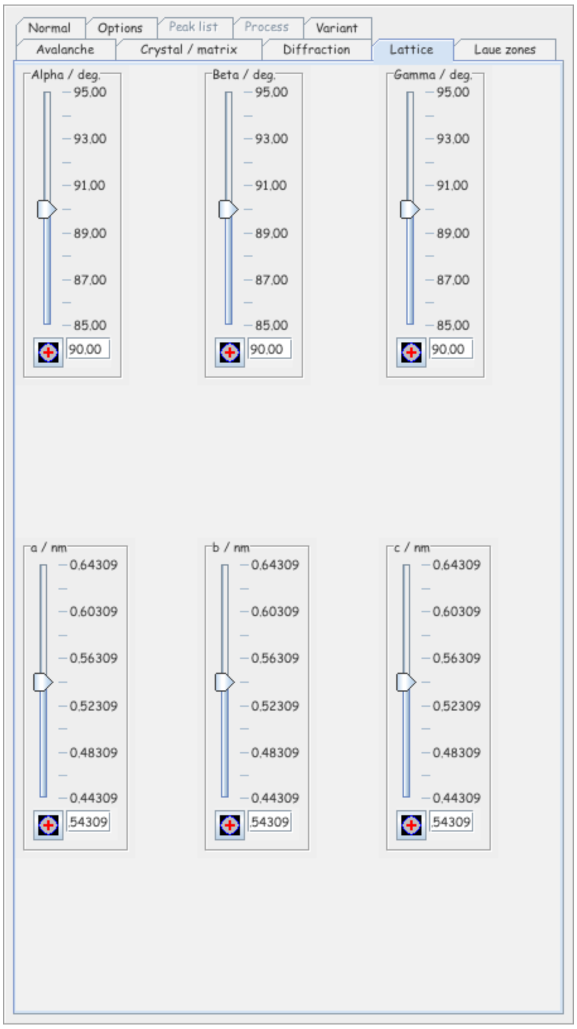


Figure 13: The *Lattice* tab allows to vary the lattice parameters.

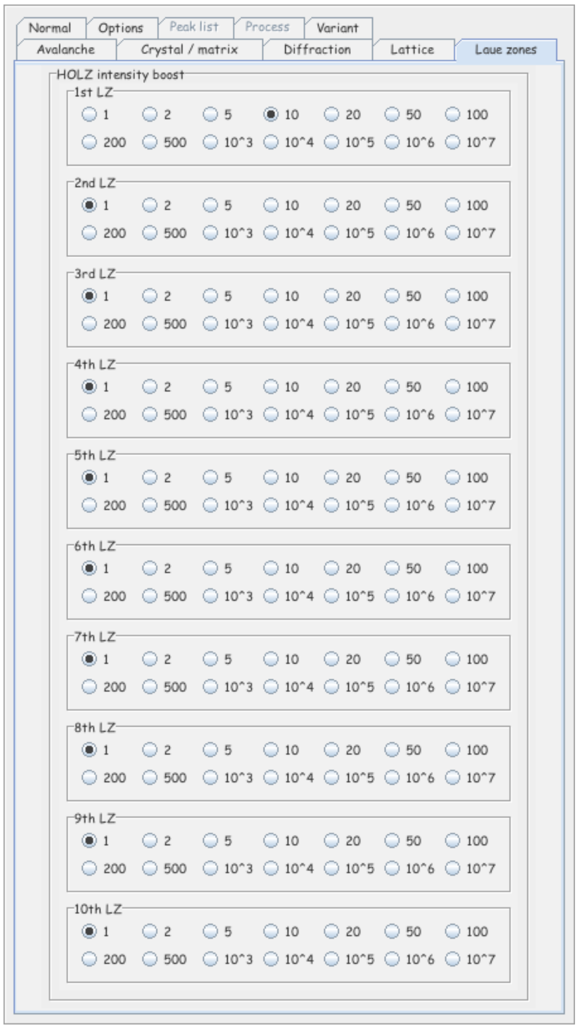


Figure 14: The *Laue zones* tab allows to boost the intensity of the high order Laue zone reflections.

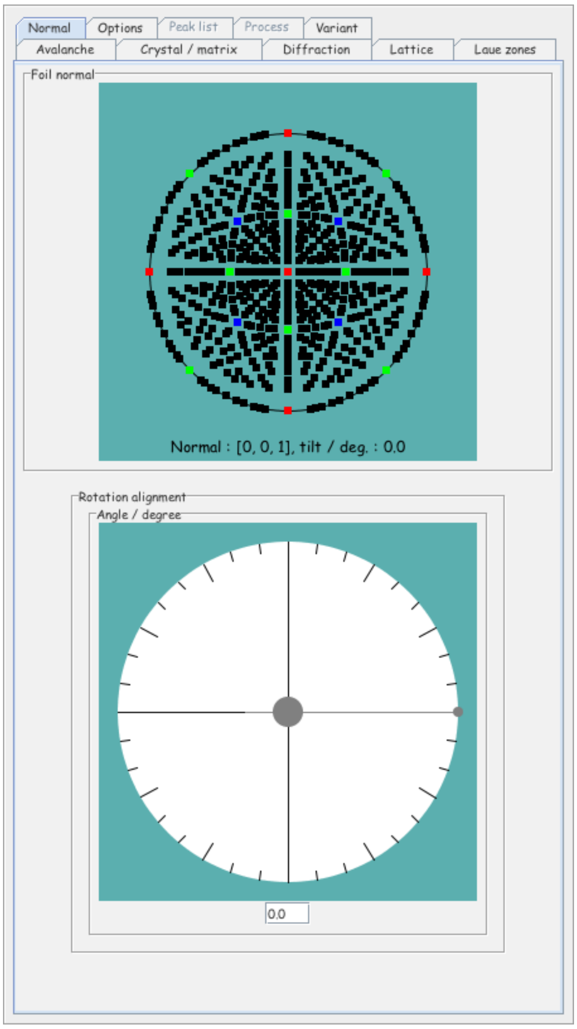


Figure 15: The *Normal* tab allows to change the orientation of the foil normal (by default it is set parallel to the ZAP direction).

Figure 16: Popup menu associated with the ZAP plot.

Finally to calculate a kinematical PED, the crystal is tilted away from the ZAP orientation by selecting the green cross and moving it away from the blue cross (Fig. 17). The tilt angle [degree] is shown as well as the indices of the center of the Laue circle (CLC)[2]. The popup menu associated with the ZAP drawing allows to reset the CLC or to cancel the ZAP translation (Fig. 16).

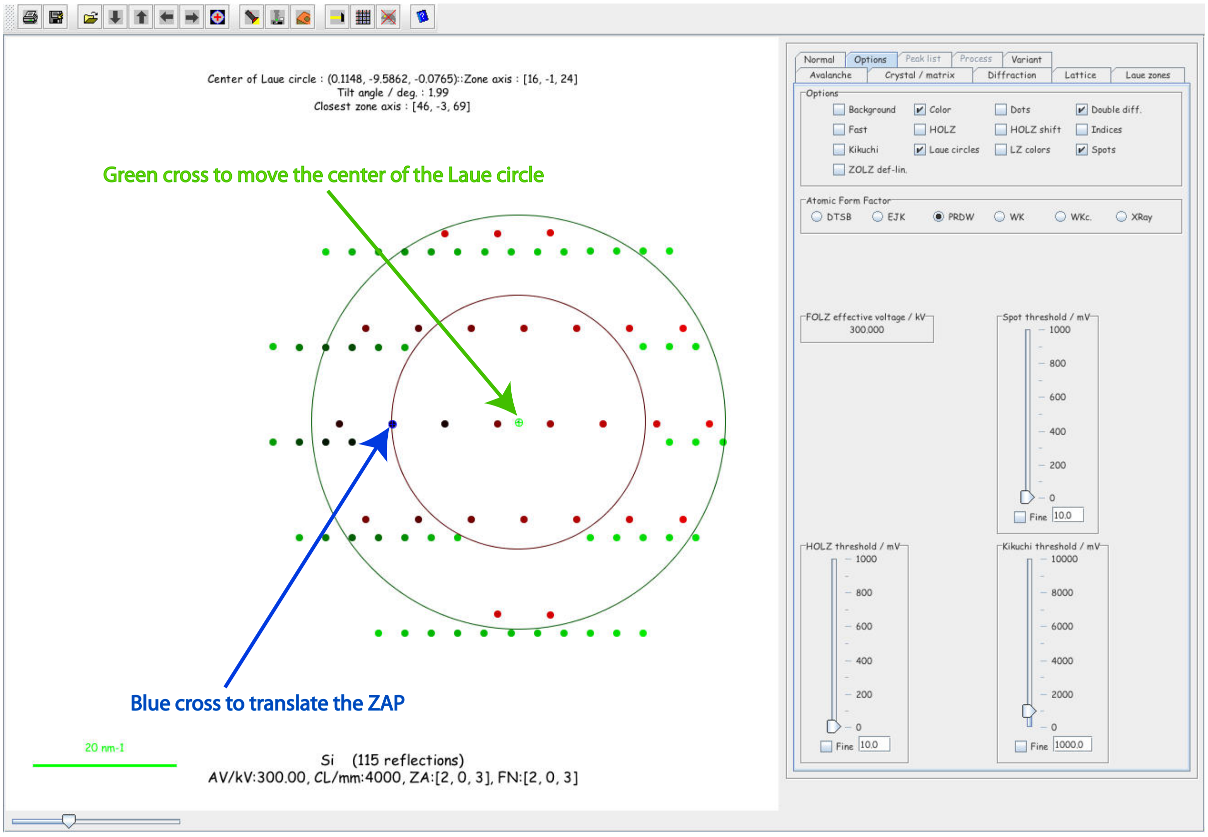


Figure 17: The ZAP is tilted by dragging the green cross.

The precession calculation is finally started using icon 1 of Fig. 18.

After completion, the kinematical PED pattern is displayed in a new frame (Fig. 19). The attached popup menu allows to display the PED using a logarithm scale. One can further improve the contrast of the high order Laue zone reflections using the radio buttons of the *Laue zones* tab[3] (Fig. 14).

[2]The CLC is the projection of the Ewald sphere center on a plane perpendicular to the incident electron beam direction. The intersection of the Ewald sphere and this plane is the Laue circle.

[3]The PED must be recalculated to include the HOLZ reflections intensity boost.

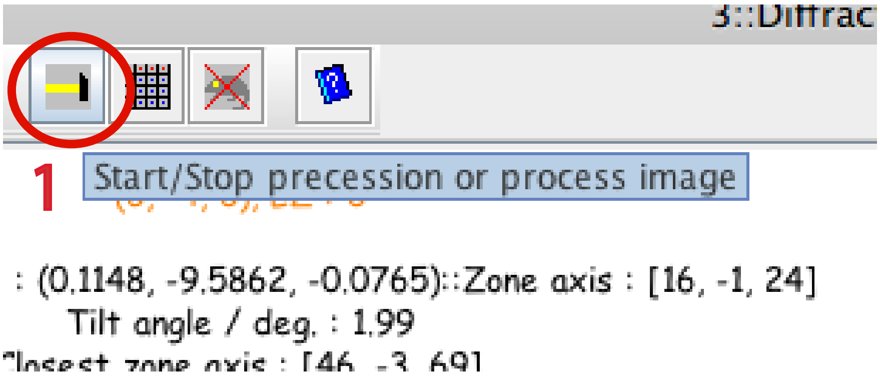


Figure 18: Icon 1 starts a kinematical PED calculation.

2.1 Remarks

- It is always better to start a PED calculation with a small number of reflections (100). It is always possible to increase the maximum deviation to include more reflections.
- The kinematical PED calculation is distributed on the available cores or processor of the computer. A good setting consists in specifying twice the number of cores / cpu[4] (Fig. 21).

[4]The number of cores / cpu is defining in menu *Parameters* → item *Preferences* tab *Debug*.

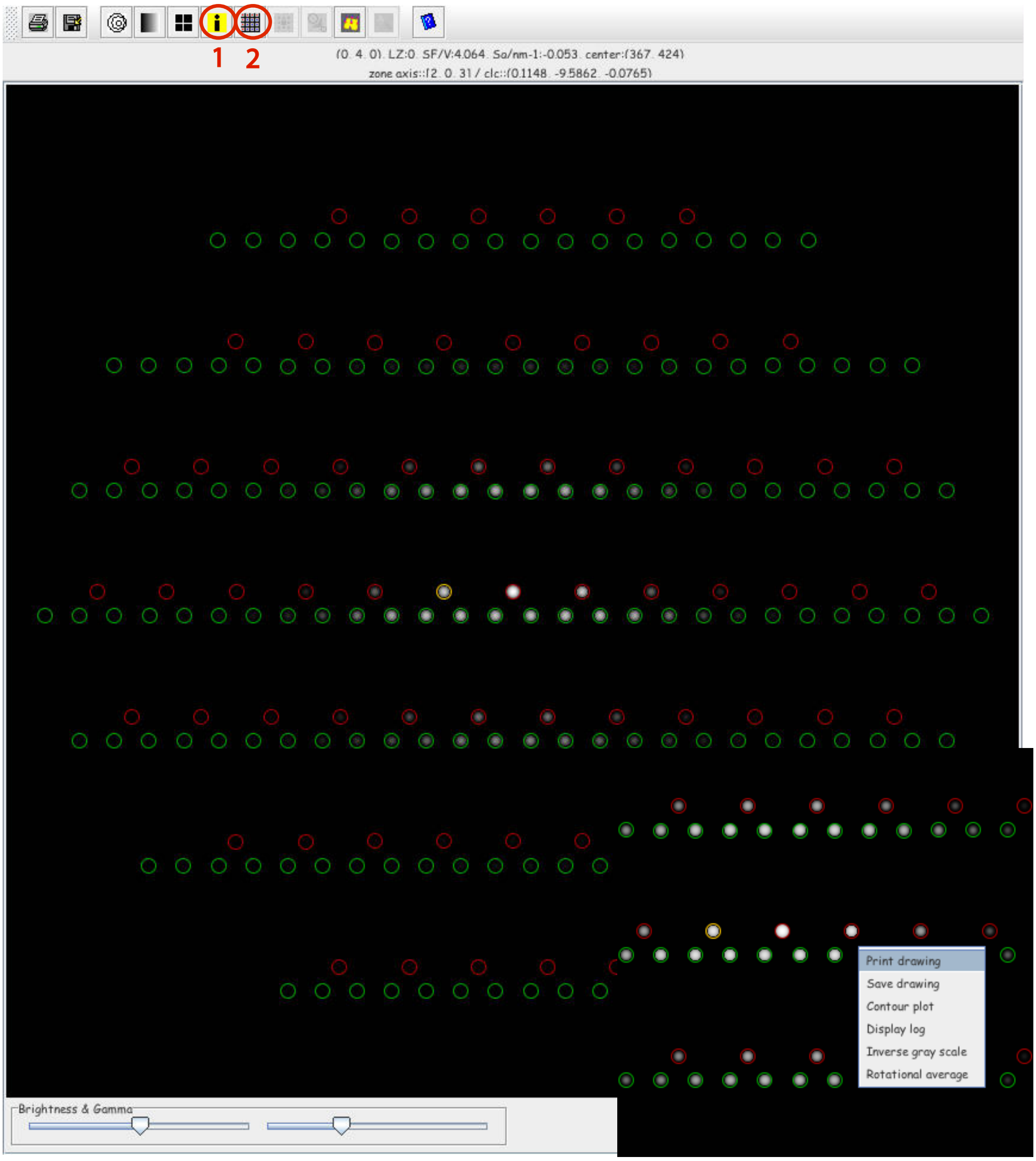


Figure 19: A kinematical PED with superimposed information (tool button 1) and its attached popup menu. Tool button 2 tabulates the intensities (Fig. 19).

Tabular list of reflections::Si::[2, 0, 3]

h	k	l	center.x	center.y	Intensity / a.u	Distance / n...	Amplitude / V...	Matrix
0	0	0	425	424	1.0	0.0	22.089294	true
-1	-1	1	440	404	0.8782879	3.189252	8.620229	true
-1	1	1	410	404	0.87846637	3.189252	8.620229	true
-1	-3	1	469	404	0.8399851	6.1069527	3.8569107	true
-1	3	1	381	404	0.84026927	6.1069527	3.8569107	true
0	4	0	367	424	0.5347928	7.365262	4.064029	true
0	-4	0	483	424	0.53484005	7.365262	4.064029	true
-1	5	1	352	404	0.8111967	9.567756	1.8879842	true
-1	-5	1	498	404	0.81080407	9.567756	1.8879842	true
5	-1	-3	440	508	0.8766506	10.89337	1.5367619	true
5	1	-3	410	508	0.8767216	10.89337	1.5367619	true
5	3	-3	381	508	0.84356546	12.074313	1.2969388	true
5	-3	-3	469	508	0.8432767	12.074313	1.2969388	true
-1	-7	1	527	404	0.7215453	13.149623	1.11563	true
-1	7	1	323	404	0.7218068	13.149623	1.11563	true
6	2	-4	396	529	0.23054779	13.779143	1.4452714	true
-6	-2	4	454	319	0.2306693	13.779143	1.4452714	true
6	-2	-4	454	529	0.23064841	13.779143	1.4452714	true
-6	2	4	396	319	0.23055157	13.779143	1.4452714	true
5	-5	-3	498	508	0.74737954	14.143413	0.971441	true
5	5	-3	352	508	0.747811	14.143413	0.971441	true
0	8	0	309	424	0.18847474	14.730524	1.2661119	true
0	-8	0	541	424	0.18857186	14.730524	1.2661119	true
-7	-1	5	440	299	0.6261879	15.9462595	0.7564591	true
-7	1	5	410	299	0.62633187	15.9462595	0.7564591	true

Figure 20: Tabulated kinematical PED. The intensity scale is arbitrary and within numerical errors the symmetry of the ZAP must be conserved, i.e. equivalent reflections must have approximately the same value.

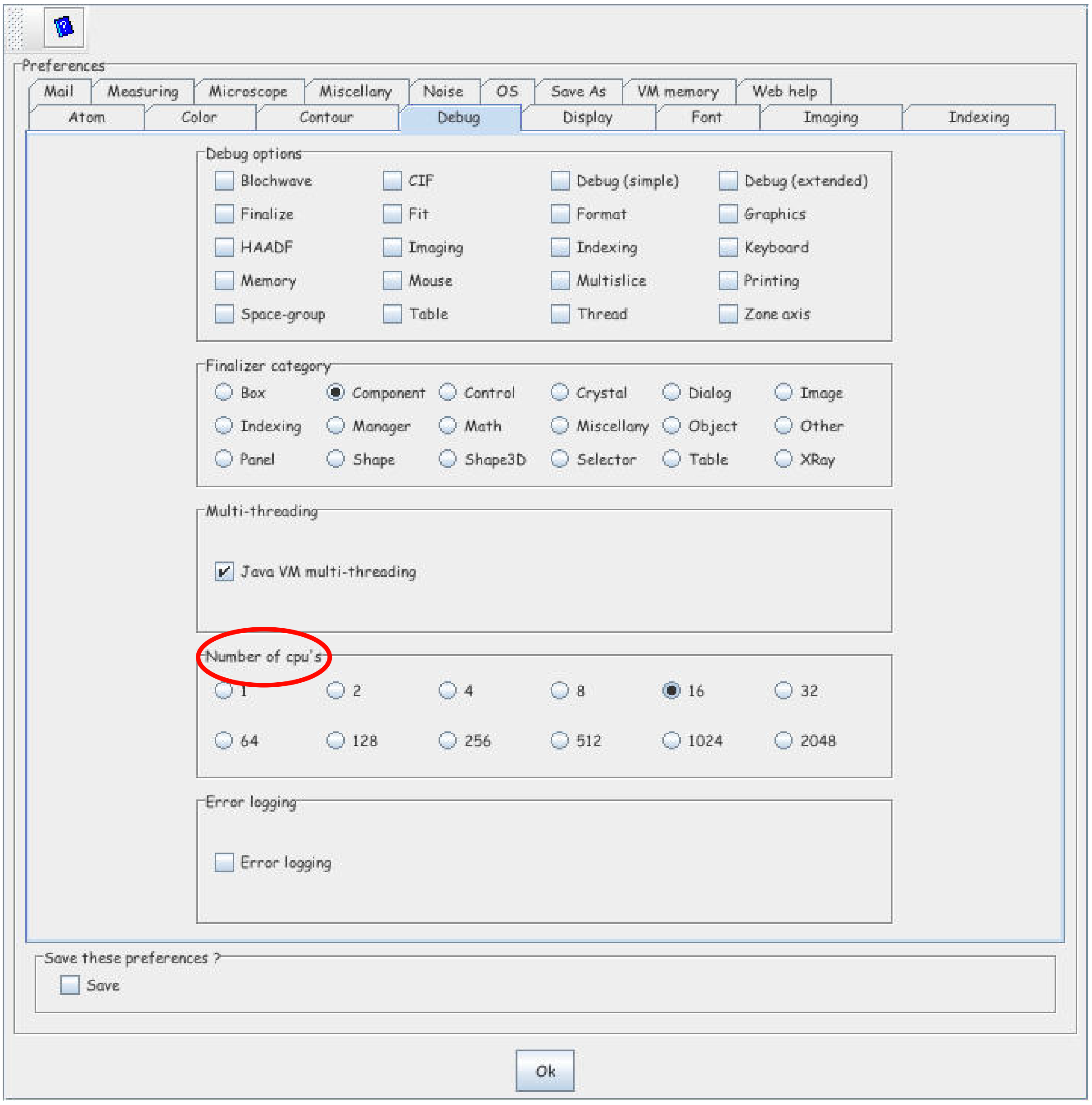


Figure 21: Setting the parameter *Number of cpu's* for a dual quad-core Mac Pro.

3 Dynamical PED: details

Calculations of PED patterns taking into account dynamical (or multiple) scattering are obtained using the Bloch wave method, selecting menu item *Blochwave* of menu *Imaging* (Fig. 22).

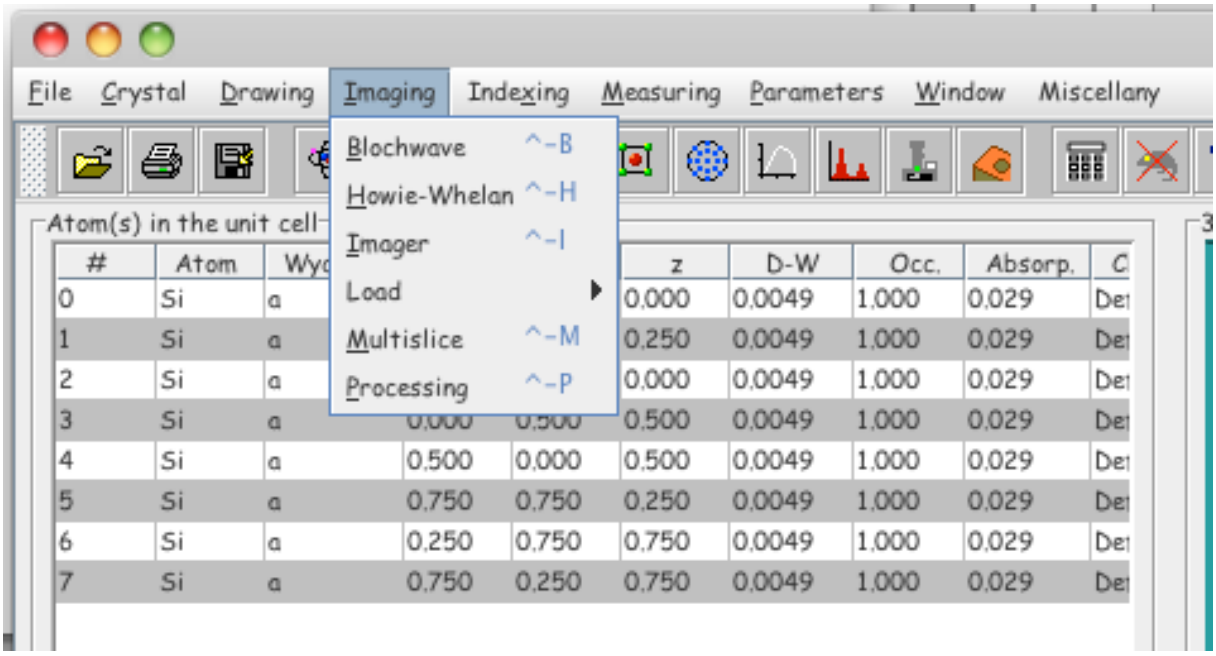


Figure 22: PED patterns are calculated using the Bloch wave method.

Select the *CBED* tab and sets the ZAP [uvw] indices, Laue zones number and maximum deviation using icon 5 of Fig. 23 (specimen dialogue)[5].

The following tabs group the PED calculation controls:

1. **Illumination** tab (Fig. 24).
2. **Iteration** tab (Fig. 25).
3. **Laue zones** tab (Fig. 26).
4. **Scan control** tab (Fig. 27).

Typical settings are:

[5]Always start a new calculation with not more than 30 to 40 reflections since jems automatically selects the reflections that have the largest contribution to diffraction for any illumination orientation.

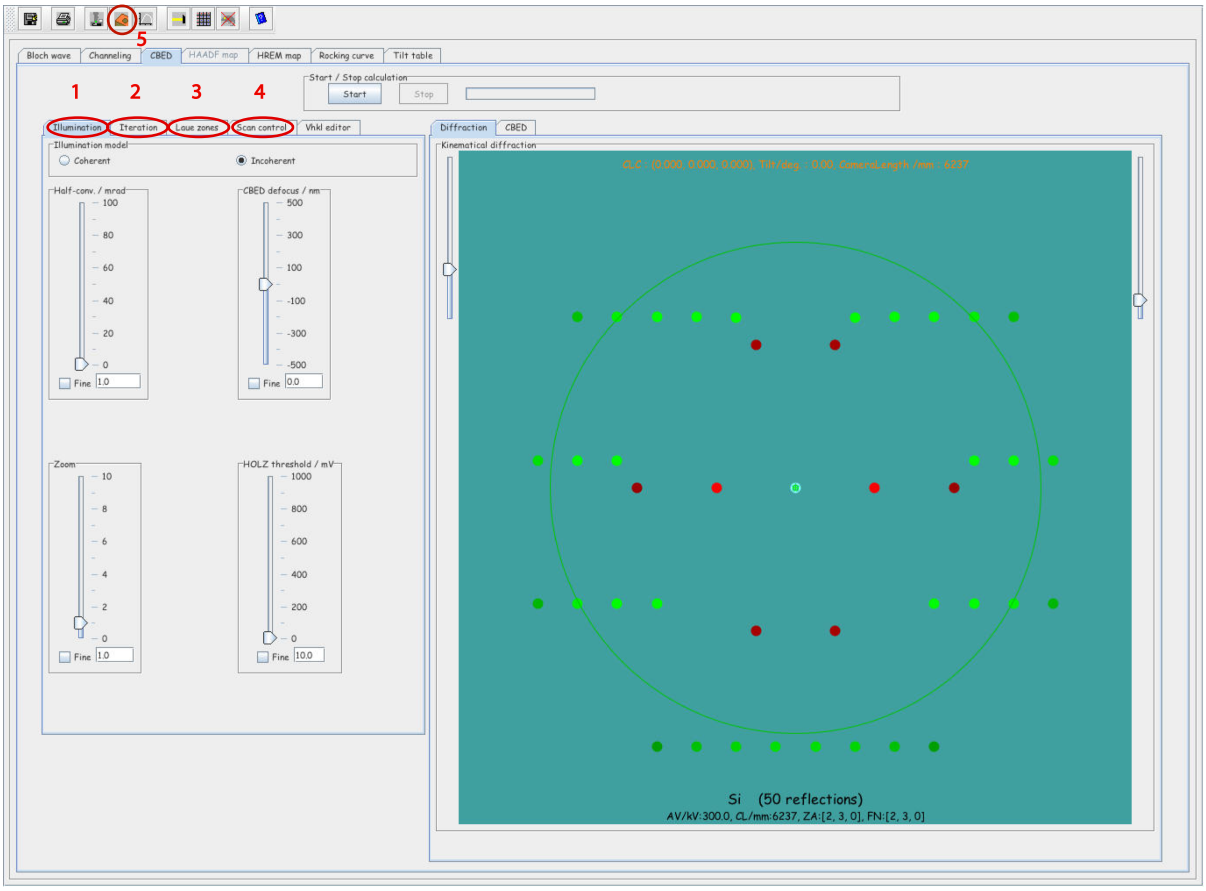


Figure 23: Dynamical PED patterns are calculated using the controls of the *CBED* tab. Icon (5) activates the *Specimen* dialogue that defines the [uvw] indices of the ZAP, the number of Laue zones to take into account and the number of reflections (maximum deviation).

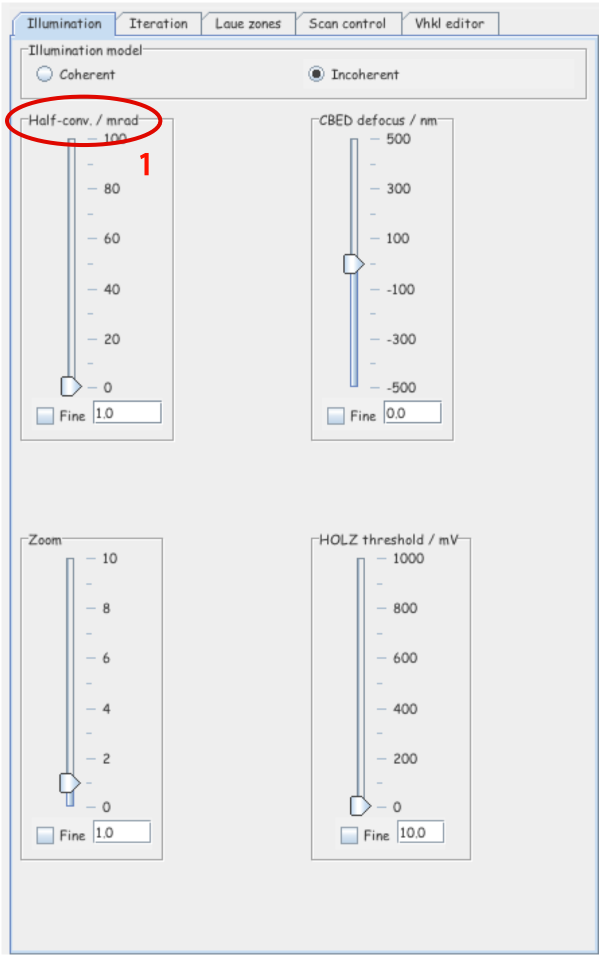


Figure 24: The ***Illumination*** tab allows setting the convergence of incident electron beam to the minimum value (0.1 [mrad]).

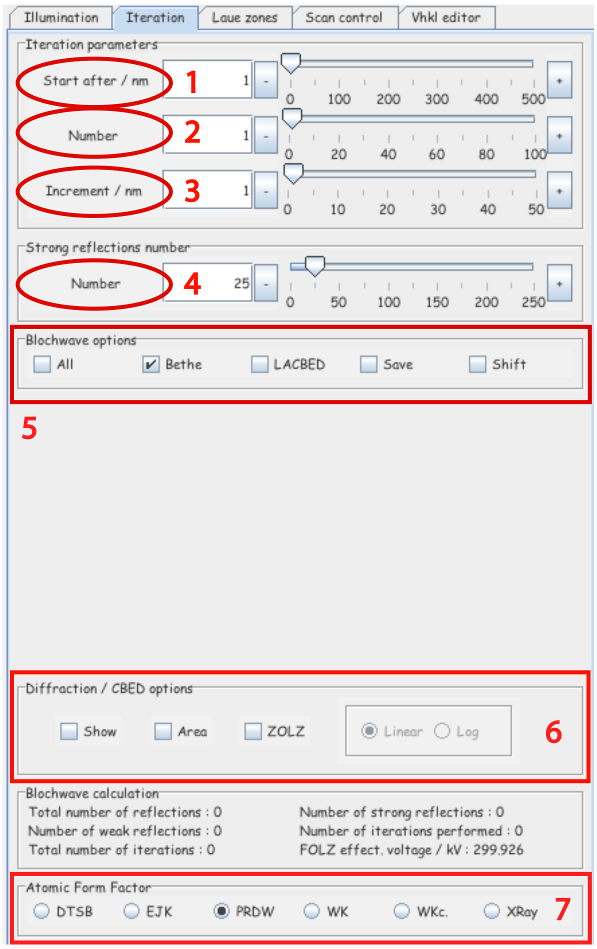
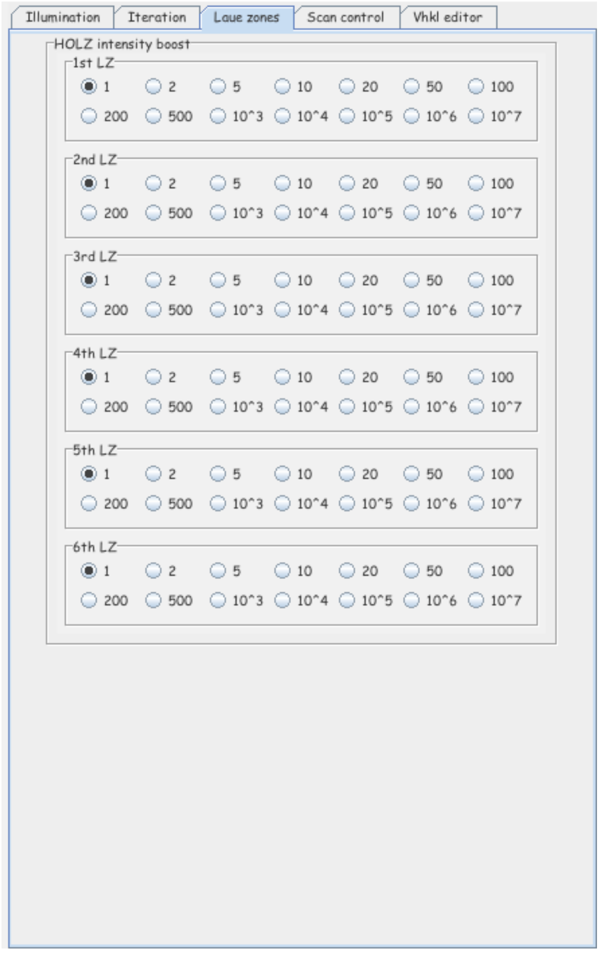


Figure 25: The ***Iteration*** tab groups controls to define the starting specimen thickness (1), the number of PED to calculate (2), the specimen thickness increment between 2 PEDs (3), the number of *reflections* (4), parameters controlling the Bloch wave calculations (5) some options used to display the PEDs (6) and the source atomic scattering factors (7).



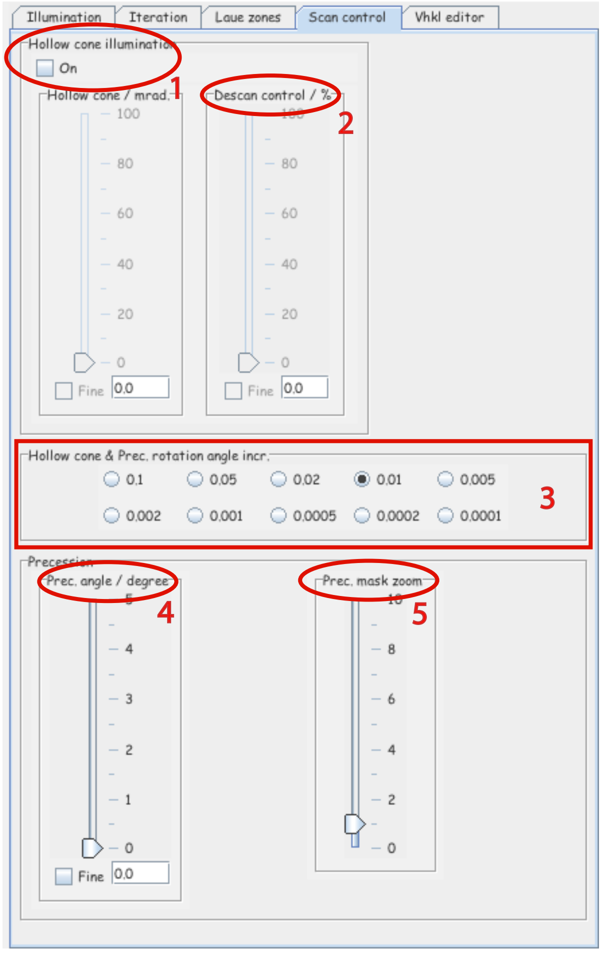


Figure 26: The ***Laue zones*** tab allows to multiply the intensity of the HOLZ reflections by a integer factor.

Figure 27: The ***Scan control*** tab groups the PED scan controls. When Hollow cone illumination (1), the precession **de-scan** is turned off ; a partial or full **de-scan** is selected using (2). The increment of the Hollow cone & Precession rotation angle is selected using (3). Slider (4) sets a particular precession angle and slider (5) controls the diameter of the **circular mask** put at the reflections' position in order to measure the diffracted intensity.

- **Microscope:**
  1. Accelerating voltage: 100 kV
  2. Camera length: 2500 mm
- **Illumination tab**:
  1. **Half-conv. / mrad**: 0.1[6]
- **Iteration tab**:
  1. **Start after /nm**: 5
  2. **Start after /nm**: 40 (to calculate PED from 5 nm to 205 nm thick crystal)
  3. **Increment /nm**: 5
  4. **Number**: 25
  5. **Show**: *selected*, **ZOLZ**: *selected*
- **Scan control tab**:
  1. **Hollow cone & Prec. rotation incr.**: 0.02[7]

The **Blochwave options** control the number of reflections that are taken into account (Fig. 25, controls group 5). For each illumination orientation the reflections with a deviation smaller than the maximum deviation are selected. The reflections are then categorized as **strong** or **weak**. Weak reflections can be taken into account using the **Bethe potential** approximation:

- **All** when selected takes into account all the reflections both strong or weak.
- **Bethe** when selected introduces the weak reflections as a perturbation of the strong ones.
- **Bethe** when **not** selected, only strong reflections are considered[8].

With these settings (except the *Illumination Half-conv.* in order to make the spots visible), and Si [230], 100 kV, camera length 2500 mm and 38 reflections, Fig. 28

[6]A larger convergence increases largely the calculation time. A conical illumination requires the calculation of the CBED disks' intensity, i.e. many iterations for a given illumination orientation.)

[7]A larger increment makes the PED calculation faster, but may break the PED pattern symmetry.

[8]Fastest iterations since the calculation time of the Blochwave method with n reflections scales as n^3.

is obtained. The illumination tilt is selected by moving the green cross at the pattern center (Fig. 29). Fig. 31 shows the diffraction pattern at a particular orientation.

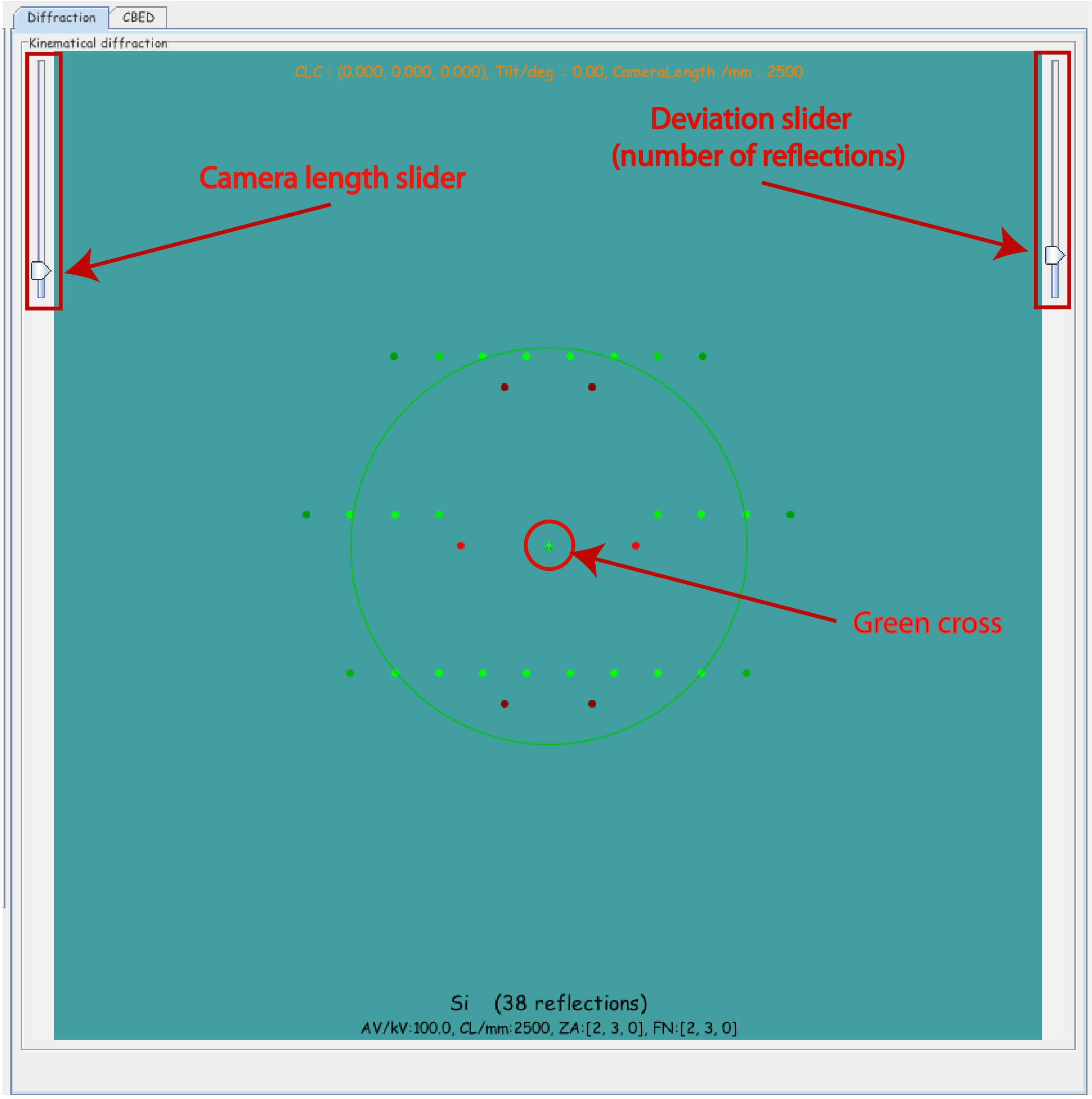


Figure 28: Typical PED starting conditions. The green cross at the pattern center can be moved using the mouse to tilt the illumination.

The tab **CBED** shows the PED under calculation (Fig. 31) or after completion of

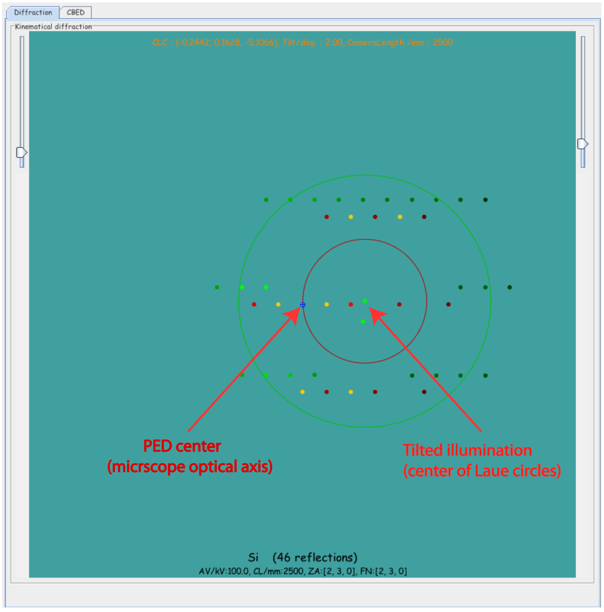


Figure 29: Tilted CBED pattern. The center of the Laue circle is moved using the mouse to impose an illumination of 2^o.

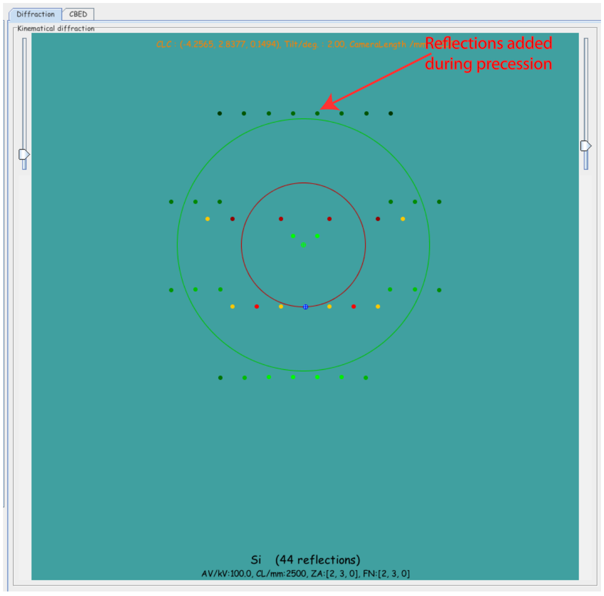


Figure 30: During the PED calculation, some reflections too distant to the Ewald sphere are removed from the Bloch wave calculation and new reflections close enough to the Ewald sphere added.

the PED calculation (Fig. 32)[9]. Note that the sliders **Thickness** and **Contrast** allow to display the PED for the different crystal thicknesses (stored in the arrays) and to improve the contrast. When the PED calculation is finished a mask can be superimposed on the PED (**Integration mask**) or the displayed PED array tabulated (**Array tabulation**).

The **Save** checkbox of the Blochwave options (Fig. 25, controls group 5) when selected before starting the PED calculation will save the stack of PED arrays as *.jems* images[10].

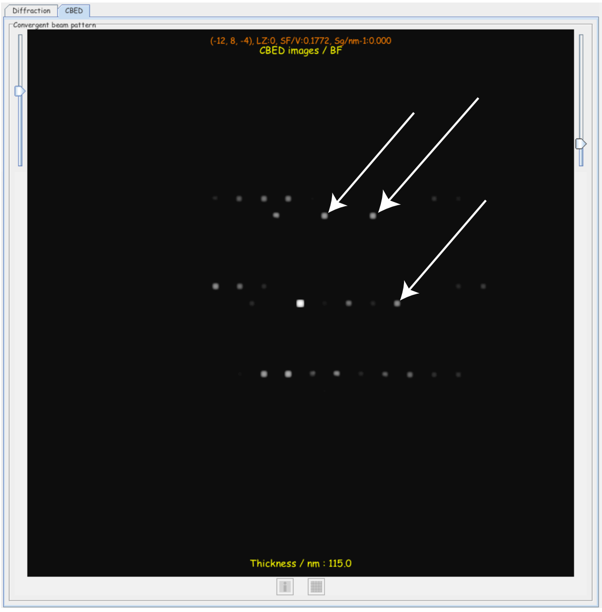


Figure 31: The reflections' intensity are accumulated in the stack of PED images. The arrows points to some PED *spots* added to 115 nm image at a particular illumination orinetation.

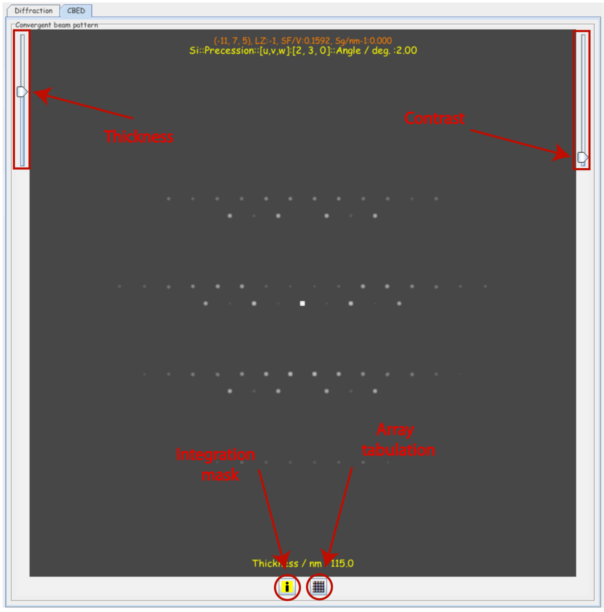


Figure 32: After completion of one revolution the PED is complete and the reflections intensity accumulated in the arrays stack. The *Thickness* slider allows to step through the thickness stack. The *Contrast* slider modifies the contrast of the PED. The left toolbutton at the bottom of the PED display the integration mask (and the indices of the reflections) while the right one tabulates the array).

The intensity integrated by the mask are tabulated using icon 2 of Fig. 35. The tabulated PED spots intensity is shown in Fig. 36 for the specimen thickness selected

[9]For any illumination orientation the diffracted intensities are accumulated in 2-D arrays.
[10]The stack can be loaded using menu *Imaging* → item *Load stack*.

(using the thickness slider of Fig. 32). The integration mask size is adjustable (Fig.27, Fig.34).

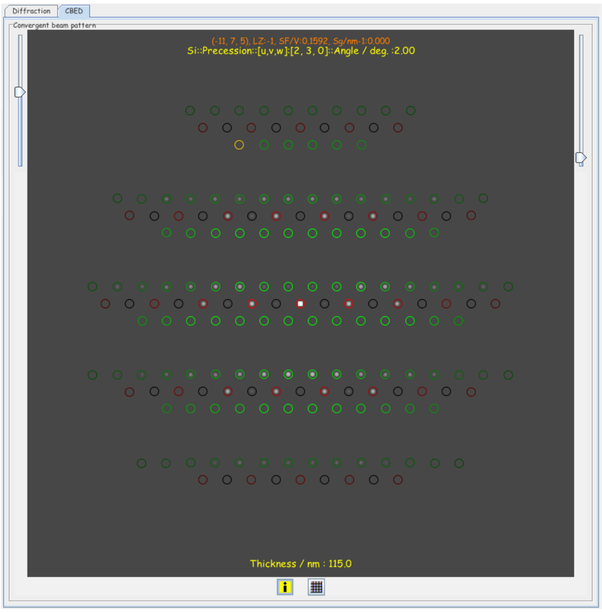


Figure 33: A mask is placed around the reflections to integrate their accumulated intensity (here default the mask).

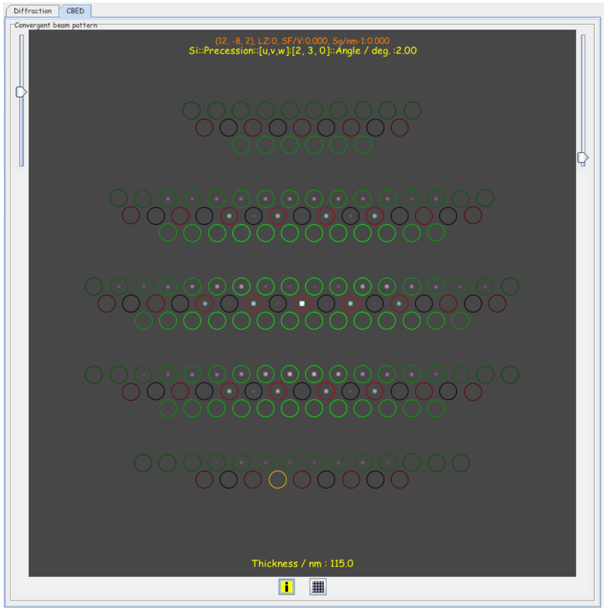


Figure 34: The size of the circular mask holes can be increased using slider 5 of the **Scan control** tab.

Each reflection of Fig. 36 can be selected and the integrated intensity saved for further processing, for example using Mathematica (Fig. 37) or plotted as a function of specimen thickness (Fig. 38). Icon 1 of Fig. 36 starts the **Charge flipping** analysis of the PED (see section 4.3).

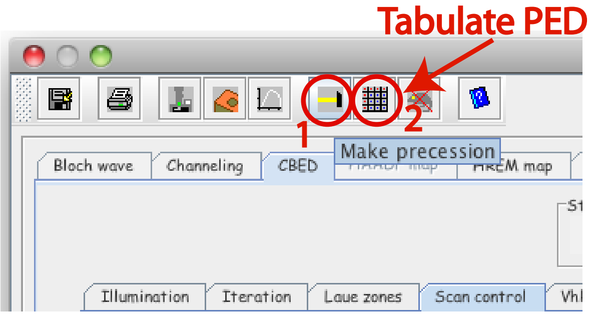


Figure 35: The reflections' intensity are tabulated using the *Tabulate PED* button.

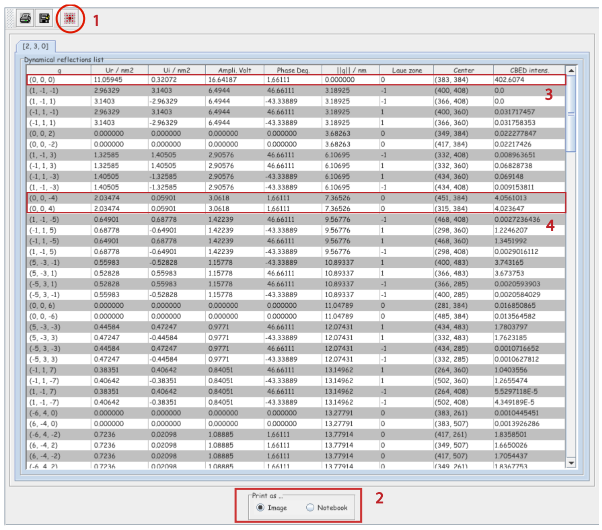


Figure 36: At the selected crystal thickness (here 115 nm) the reflections properties are show as a table. Button 1 activates the *Charge flipping* processing of the PED, controls 2 allow to save the table as a Mathematica notebook, lines 3 and 4 emphasize reflections (000), (004) and (00-4). Note the slight difference in the intensity of the (004) and (00-4) reflections (a smaller PED rotation increment reduces their difference).

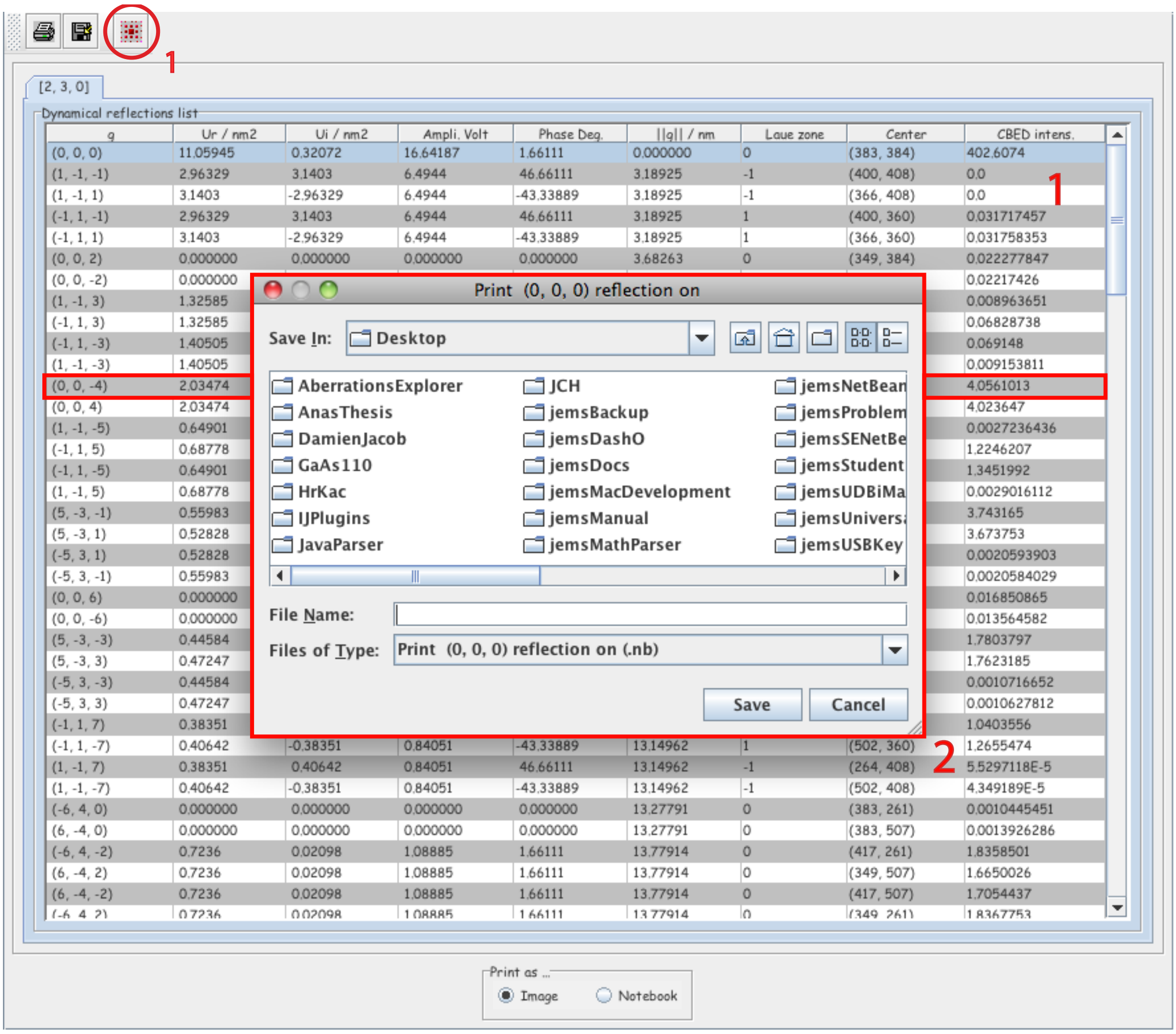


Figure 37: When a reflection is selected, a dialogue is displayed that allows to save the table. It is followed by a plot of the selected reflection as a function of crystal thickness (Fig. 38).

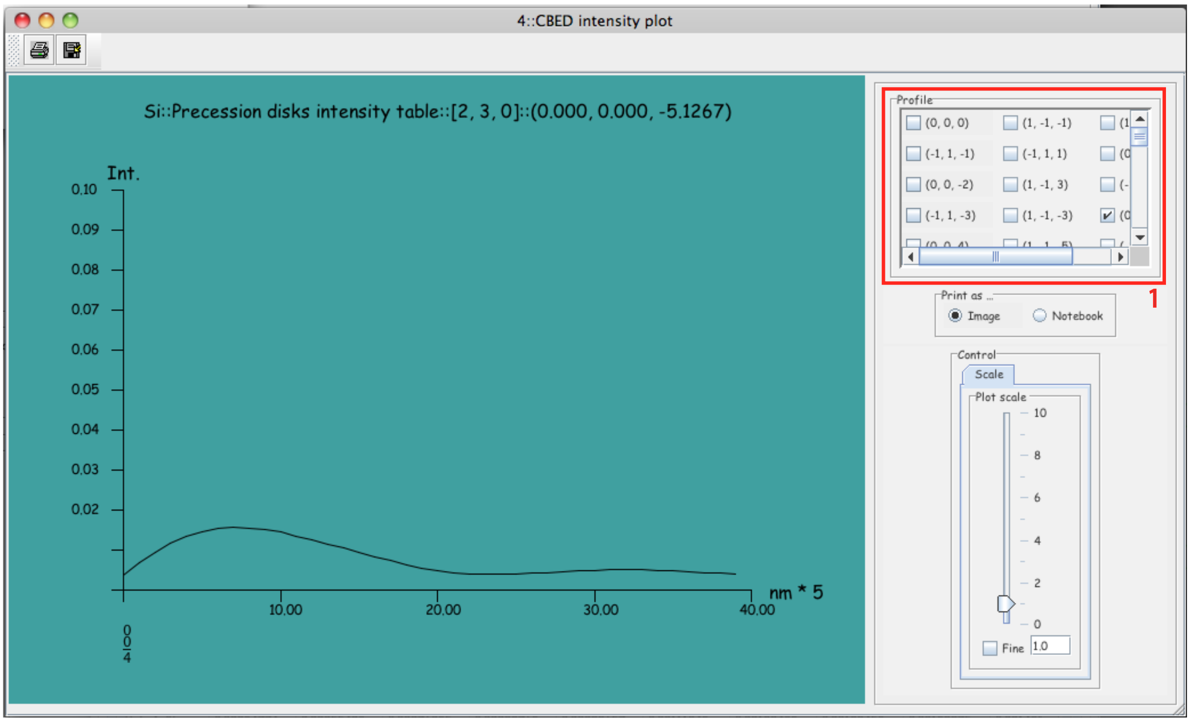


Figure 38: The plot controls and popup menu allow to change the plot intensity scale or to display several reflections. The plot can be printed as a Mathematica notebook.

4 Final remarks

4.1 Symmetry of the PED

1. The PED pattern must display the symmetry of the SAED diffraction pattern. When the increment of the illumination rotation angle is too large (Fig. 27), some reflections may never be at exact Bragg condition during the PED formation. In such a case it is necessary to set a smaller increment.

2. It is never obvious to set the most appropriate number of reflections for calculating a particular PED pattern. Always start with a small number of reflections then add some more and compare the tabulated intensities.

4.2 Example: andalusite

A kinematical and a dynamical SAED patterns of andalusite [001] are shown in Fig. 40 and Fig: 41. When electrons are propagating precisely down the [001] andalusite direction, dynamical extinctions can be observed (screw axis $\perp$ to [001]). A slight crystal tilt put some intensity at the position of these dynamical extinctions. One can consequently infer that precession at low precession angle should also significantly put intensity there.

The next figures (Figs.43, 44, 45 and 46) show PED pattern of Andaluzite [001], 100 nm thick, for different precession angles (1, 2, 3 and 4^o). Note that dynamical diffraction effects are more pronounced at low precession angles. They tend to disappear with increasing precession angle and the pattern consequently gets closer to a kinematical SAED.

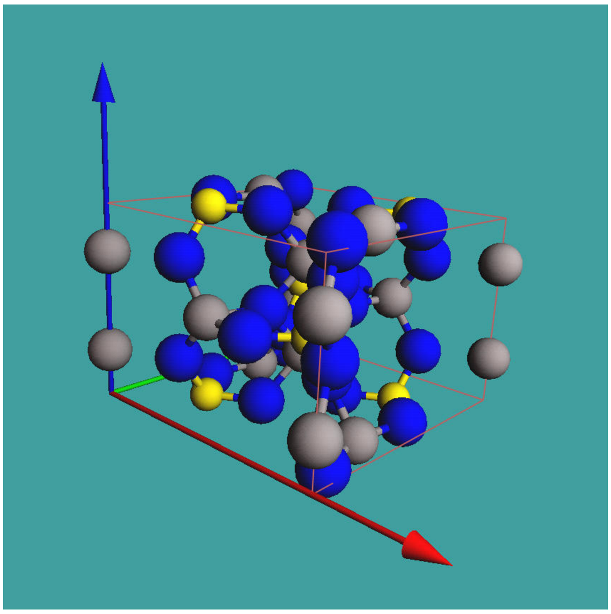


Figure 39: Andalusite (Si: yellow, Al: gray, O: blue).

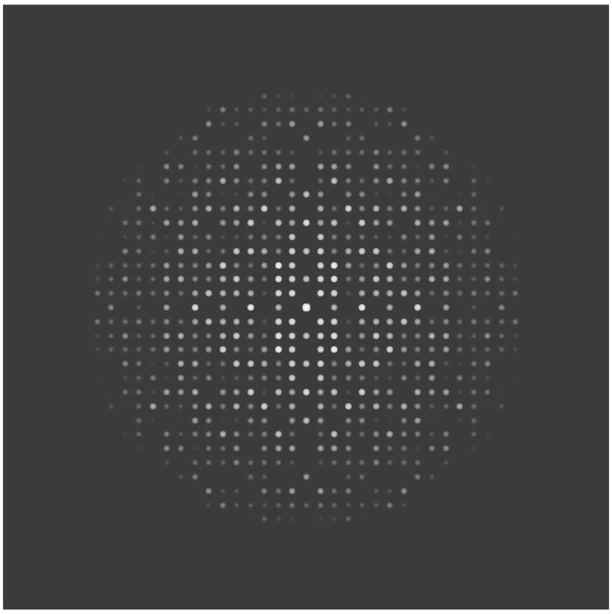


Figure 40: Andalusite [001] kinematical SAED pattern.

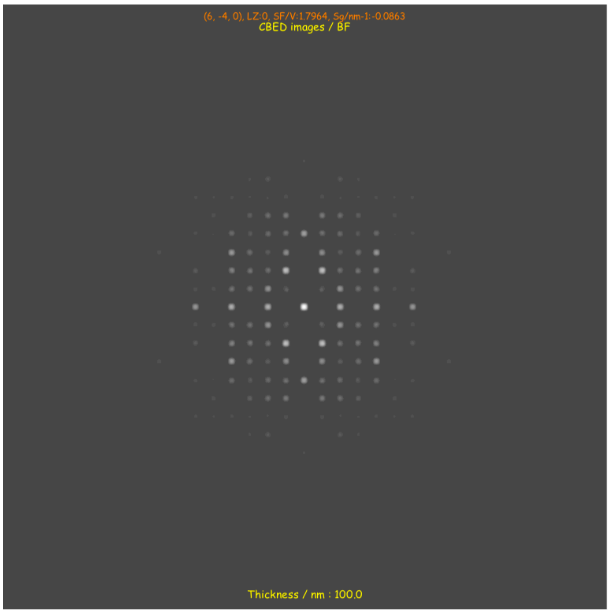


Figure 41: Andalusite [001] dynamical SAED pattern (exact [001] orientation).

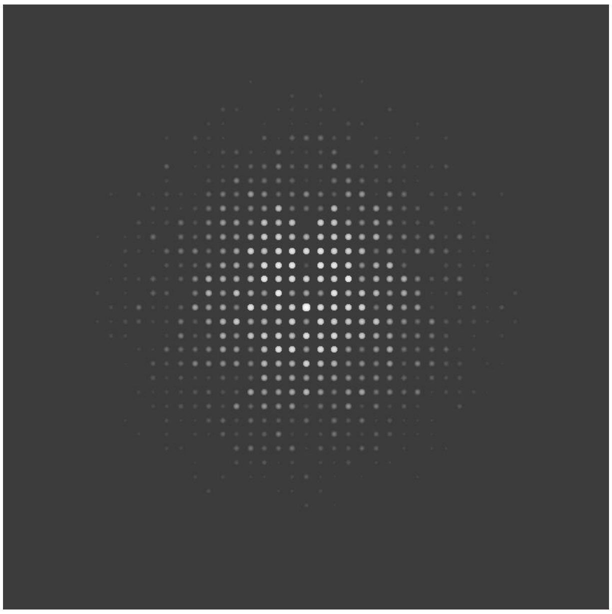


Figure 42: Andalusite [001] dynamical SAED pattern (0.15^o tilt of [001]).

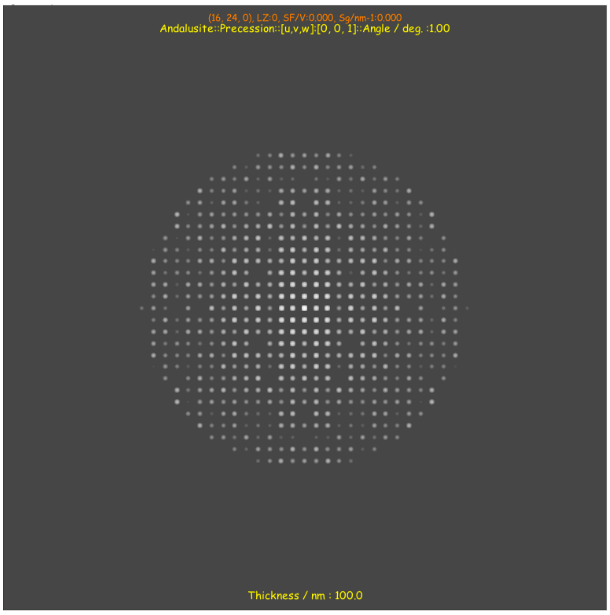


Figure 43: .

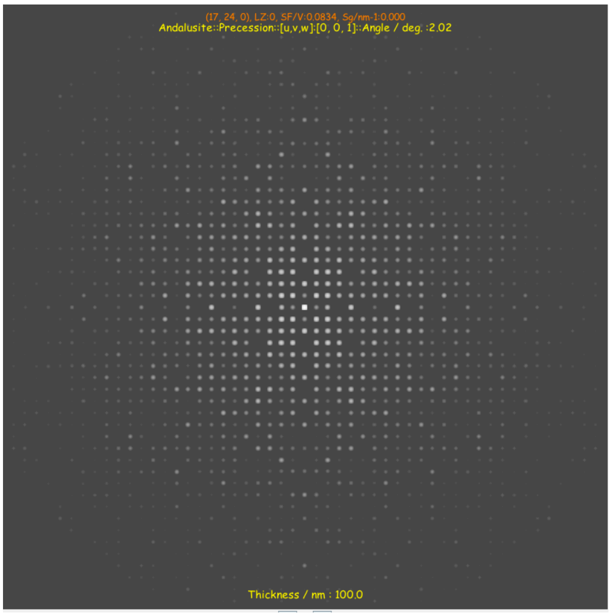


Figure 44: .

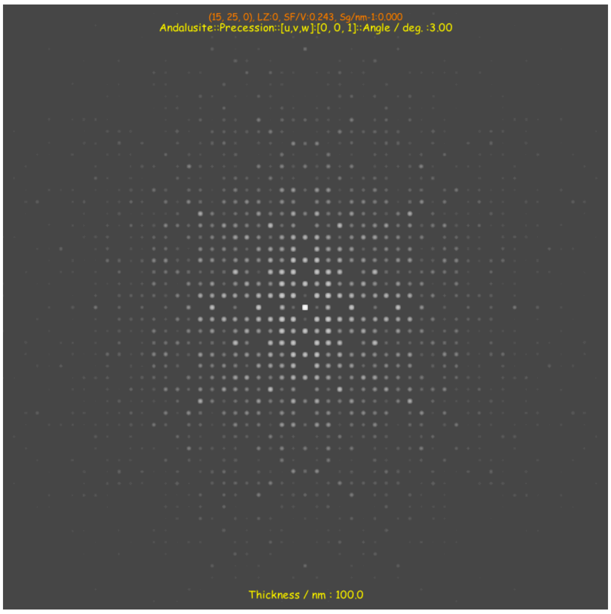


Figure 45: .

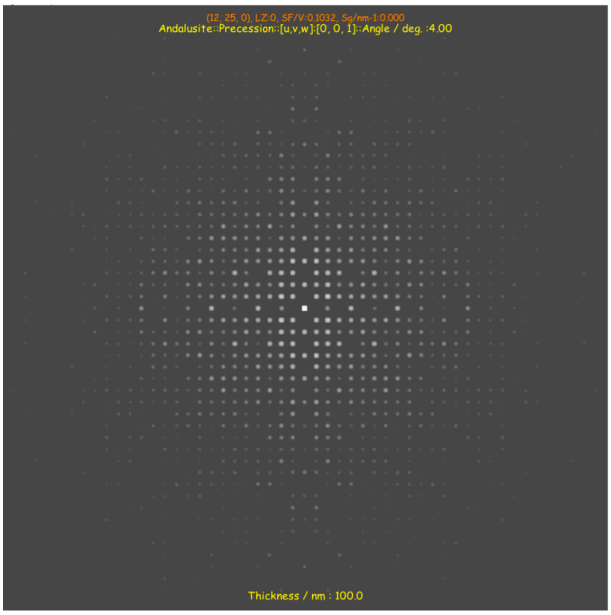


Figure 46: .

4.3 Charge flipping

Charge flipping reconstruction of the projected potential is possible (Fig. 47). The procedure does not always perform well with 2-D PED's[11].

With simple structure, charge flipping in 2-D seems to provide the proper projected potential. For BeO (Fig. 48 and Fig. 49), the [001] projected potential and the charge flipping potential map, reconstructed from a simulated PED pattern of a 30 nm thick crystal, are in good agreement (Fig. 50 and Fig. 51)[12].

[11] Pretty often a potential map similar to the Patterson map is reconstructed as a result of the initial choice of the random phases assigned to the reflections.

[12] Dynamical diffraction effects should be checked before attempting to reconstruct the projected potential map.

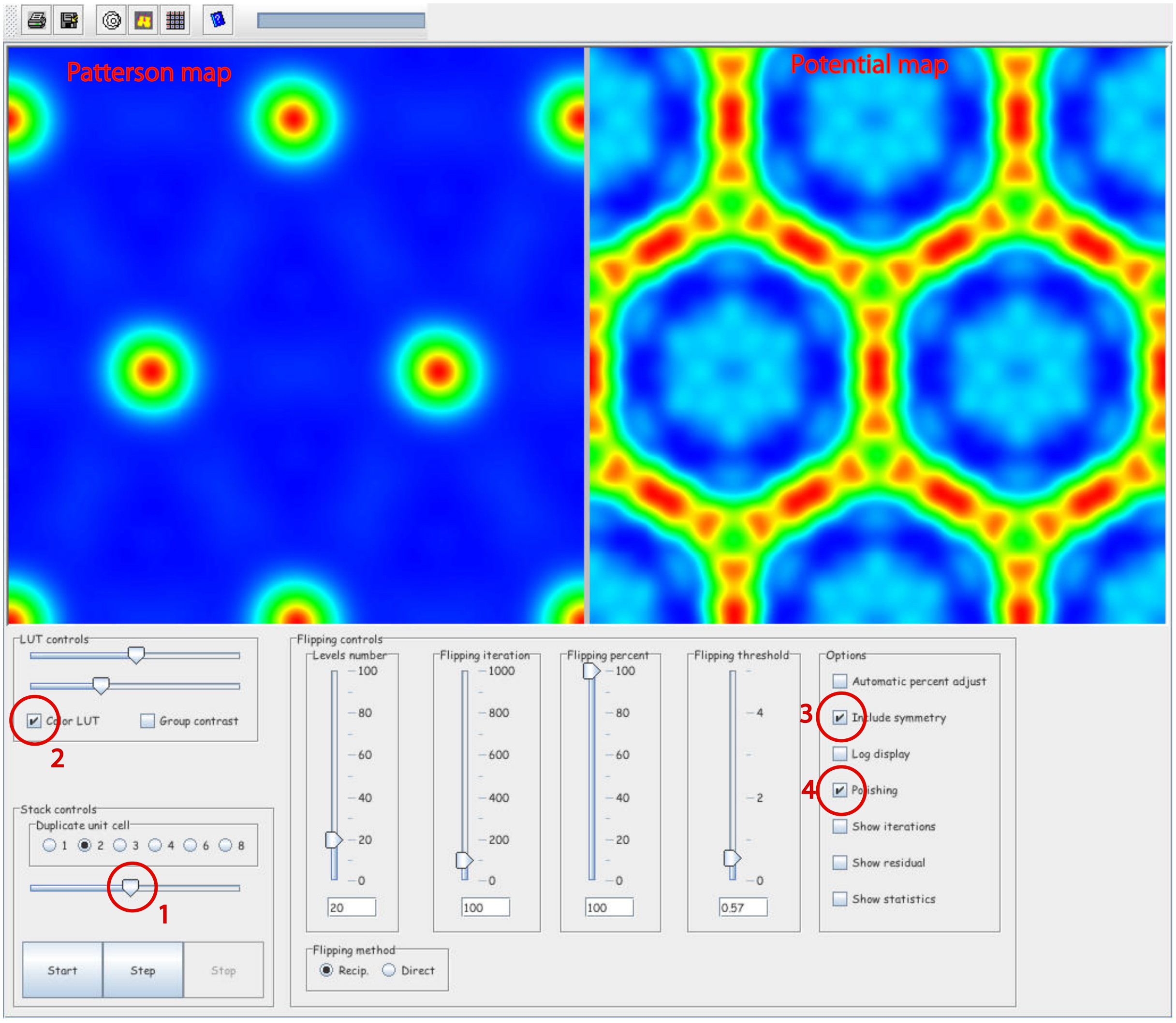


Figure 47: Charge flipping dialogue. Slider 1 selects the crystal thickness, checkbox 2 selects a color lookup table, 3 introduces symmetry in the reconstruction, 4 adds a polishing step at the end of the charge flipping procedure. The Patterson map of BeO [001] is shown besides the reconstructed potential map. For thick crystals the potential map can differ significantly from the projected potential as shown here.

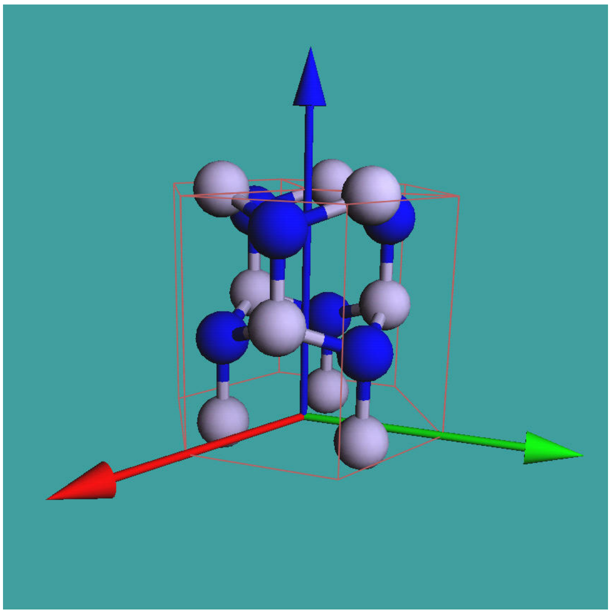


Figure 48: 3-D model of BeO (Be:gray, O: blue).

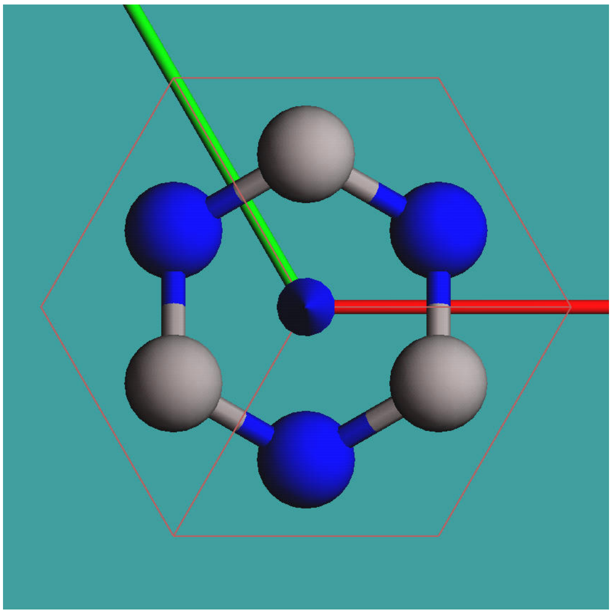


Figure 49: [001] BeO projection.

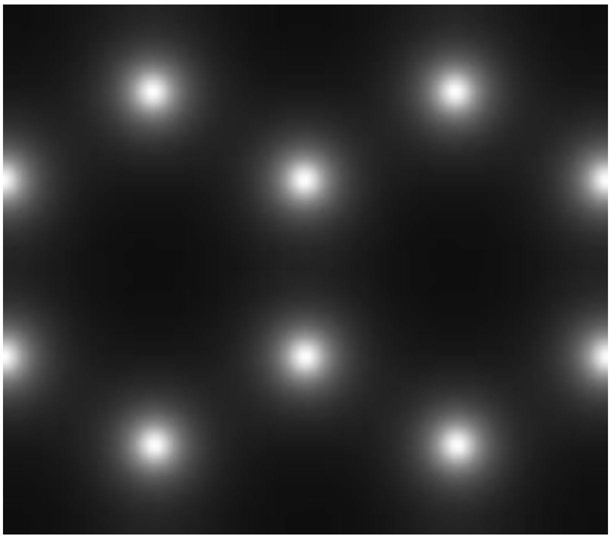


Figure 50: [001] BeO projected potential.

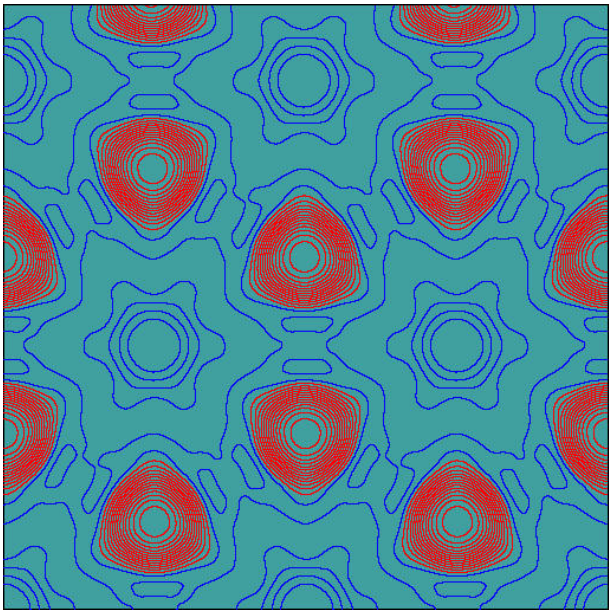


Figure 51: BeO projected potential reconstructed by charge flipping algorithm (30 nm thick crystal).