jems GUI

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The **Goniometer** menu item of jems menu **Measuring** opens a frame that allows to figure out what angles to apply to a double-tilt or tilt-rotation specimen holder in order to align a crystal in a particular $[uvw]$ crystallographic zone axis. Aligning a crystal with reference to the TEM optical axis requires to figure out the value of 3 angles of rotations defined as follow:

1. **D**ouble-**T**ilt : α rotation of axis defined by the specimen holder axis (perpendicular to the microscope optical axis), β for a rotation perpendicular to the specimen holder axis and θ of $[uvw]$ crystallographic direction.

2. **T**ilt-**R**otation : α rotation along the specimen holder axis, θ perpendicular to α along the microscope optical axis when $\alpha = 0$ and ϕ also of $[uvw]$ crystallographic direction.

With the help of the procedure described in this document the alignment of the crystal in any accessible $[uvw]$ crystallographic direction is made simpler and faster. One procedure defines the orientation of the crystal with respect to the microscope reference frame using 2 $[uvw]$ identified zone axes while the other is using one zone axis and the angle of its attached SAED with the specimen holder axial direction (O_x). It should be noted that the proposed alignment procedure using 2 crystallographic zone axes offers a way to improve the crystal orientation settings recursively, since identifying $[uvw]$ two crystallographic directions separated by a larger angle renders the crystal orientation more accurate.

Since the alignment procedure using a **DT** or **TR** specimen holder are almost identical (see section 1.2, only the procedure for orienting a crystal on a **D**ouble-**T**ilt specimen holder will be detailed in section 1.1.

1.1 Double tilt specimen holder

The goniometer programme allows to compute the (α, β) angles necessary to align anti - parallelly to the electron beam a particular zone axis either using a **Double-Tilt**. The alignment requires to specify 2 angles (α, β) and a third angle θ to fully orientate the crystal with reference to the microscope optical axis (O_z) and the specimen holder O_x and O_y axes (with O_x the specimen holder axial direction).

With $(\alpha, \beta) = (0, 0)$ the O_z axis is marked by a red circle at the stereogram centre. The red arrows labeled α and β define the O_x axis, α tilt axis, and the perpendicular O_y axis, β tilt axis (Fig. 1). The crystal orientation can be specified using either 2 identified zone axes or a single one and the rotation of its associated SAED pattern with respect to O_x. Here zone axis 1, $[1, 2, 3]$, aligned with O_z when $(\alpha, \beta) = (20, 12)$ and zone axis 2, $[0, 1, 1]$ aligned when $(\alpha, \beta, \theta) = (4.8, 0, -126)$. The $[uvw]$ zone axis indices $[-7, 189, 162]$ of the oriented crystal are show below the stereogram. Note that they are pretty close to $[0, 1, 1]$ as it should be.
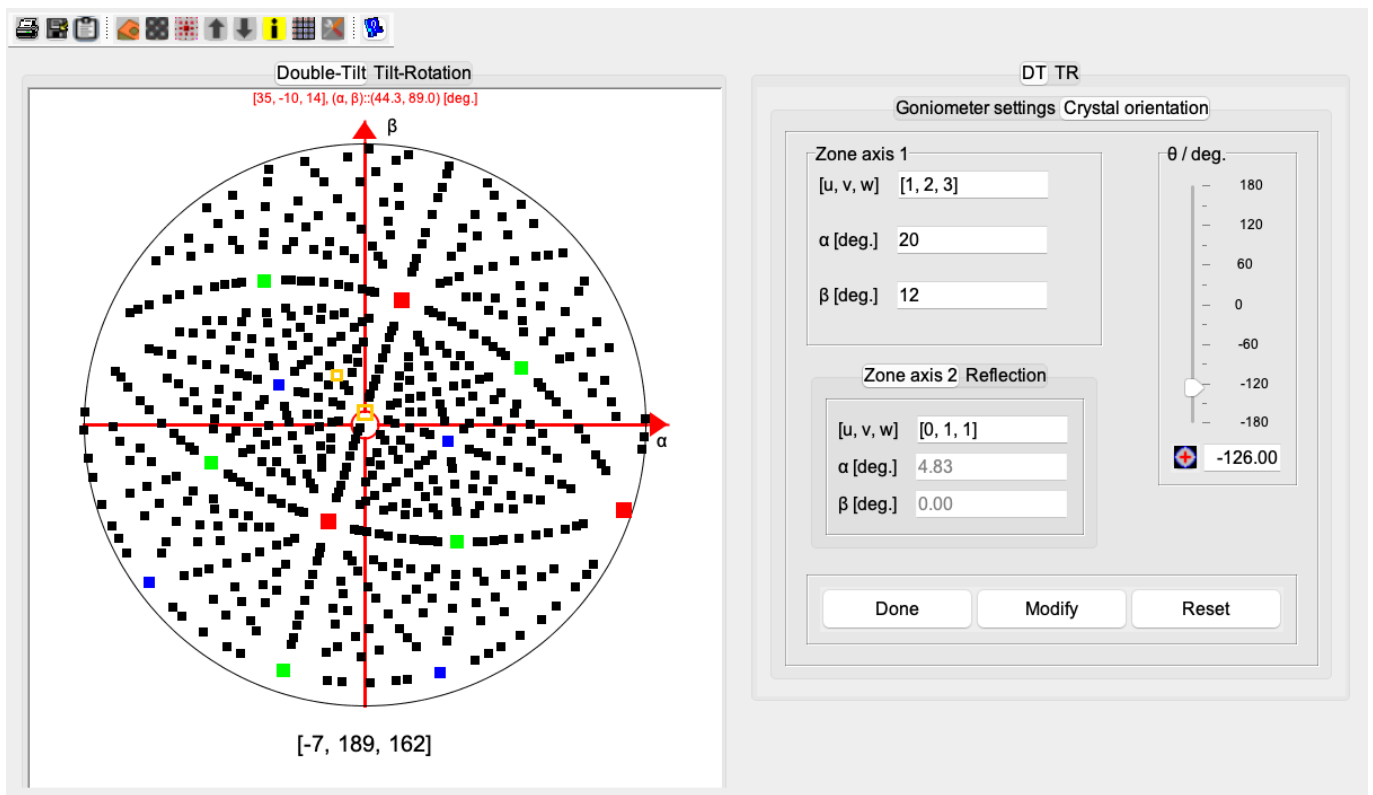

Figure 1: Double-tilt settings using 2 $[uvw]$ crystallographic zone axes ($[1, 2, 3]$, $[0, 1, 1]$). With $(\alpha, \beta) = (0, 0)$ the crystal $[uvw]$ orientation is $[-7, 189, 162]$.

1.1.1 Crystal orientation using 2 crystallographic zone axes

Orienting the crystal using 2 identified crystallographic zone axes proceed as follow when mounted on a double-tilt specimen holder.

1. Rotate the specimen holder in order to align (anti-parallel to the electron beam) a particular crystal zone axis (here $[1, 2, 3]$). Put the zone axis $[uvw]_1$ indices and the (α, β) angles provided by the specimen holder into the controls of panel **Zone axis 1**, tab **Crystal orientation** (Fig. 1).

2. Rotate again the specimen holder until a second zone axis is identified (here $[0, 1, 1]$). Put its $[uvw]$ indices into $[u, v, w]_2$ text field of tab **Zone axis 2**. Then use the θ rotation to match the calculated (α, β) of this zone axis with the measured angles (TEM goniomter). Assuming the measured (α, β) are (5, 0), a θ rotation of -125.4 degrees must be introduced to match the calculated and measured angles.

   The 2 zone axes are marked on the stereogram by yellow squares. Their $[uvw]$ indices are provided either by showing the indices (**i**) or using the popup menu (see **??**). Pointing them using the mouse will show their indices as well as the (α, β) rotation angles required to put them at the stereogram centre.

   Using the (α, β) controls of the **Goniometer settings** panel one can verify the crystal alignment (Figs. 2, 3).
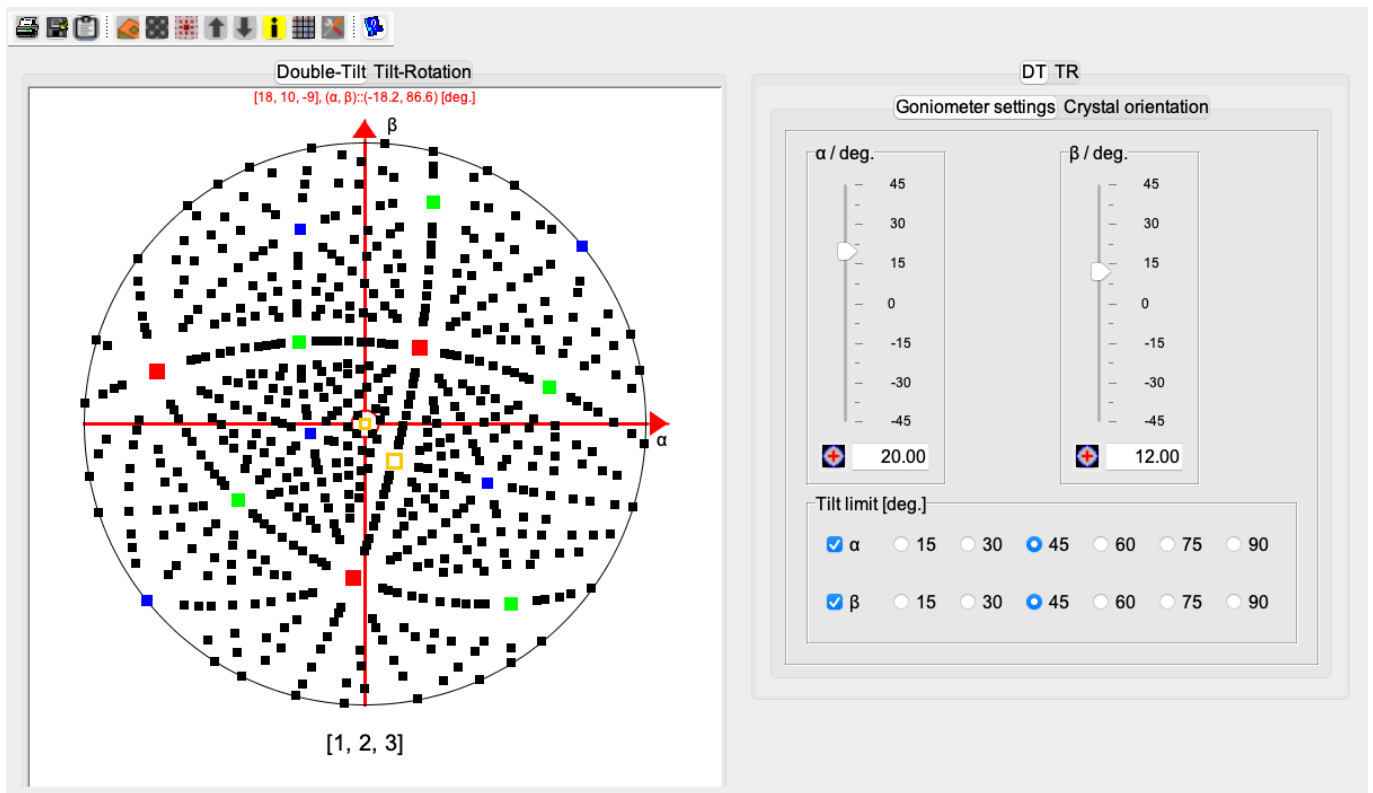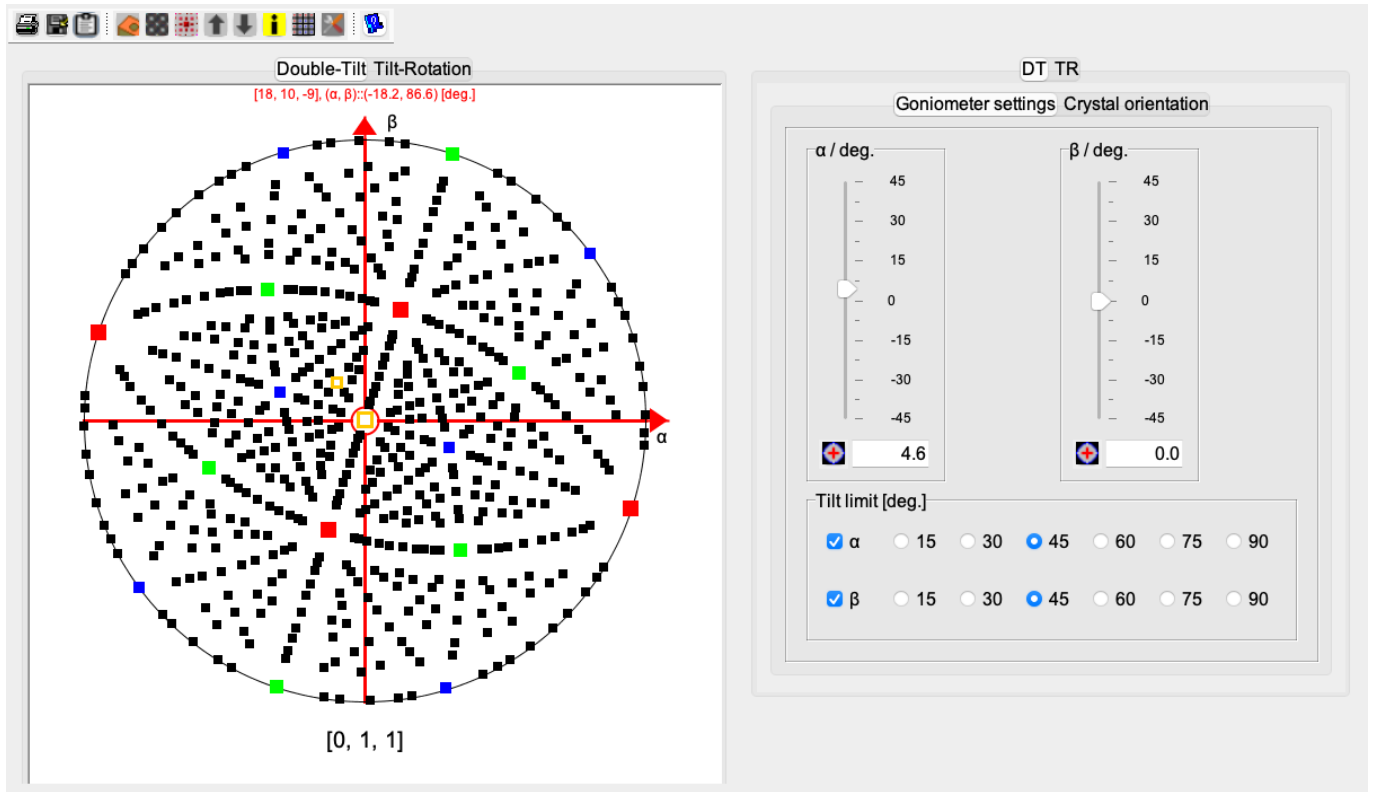

Figure 2: Goniometer settings of oriented crystal using 2 zone axes. With $(\alpha, \beta) = (20, 12)$ zone axis $[uvw]_1$ is aligned with O_z.

The keyboard arrows $\uparrow$, $\downarrow$, $\leftarrow$ and $\rightarrow$ can be used to tilt the crystal or to change the angle values displayed by the controls. Also after selecting a slider, the displayed value can be modified using the $\uparrow$, $\downarrow$ arrows [1].

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[1]this jems feature is available for slider controls.

Figure 3: Goniometer settings of oriented crystal using 2 zone axes. With $(\alpha, \beta) = (4.6, 0)$ zone axis $[uvw]_2$ is aligned with O_z.

1.1.2 Crystal orientation using 1 zone axis

Orienting the crystal using a single identified crystallographic zone axes proceed as follow when mounted on a double-tilt specimen holder. Getting the first zone axis is similar to the two zone axes orientation procedure.

1. Rotate the specimen holder in order to align (anti-parallel to the electron beam) a particular crystal zone axis (here $[1, 2, 3]$). Put the zone axis $[uvw]_1$ indices and the (α, β) angles provided by the specimen holder into the controls of panel **Zone axis 1**, tab **Crystal orientation** (Fig. 1).

2. Measure the angle between a single or a line of identified reflections and the specimen holder O_x axis. Select tab **Reflection** and put the **(hkl)** indices of the identified reflection into text field (h, k, l) [2]. The $[uvw]_1$ SAED pattern is now plotted over the stereogram (Fig. **??**). The θ rotation control rotates the stereogram (rotation axis $[uvw]_1$). θ should be set to the measured angle[3].

Using the (α, β) controls (α, β) of the tab **Goniometer settings**, the stereogram can be rotated in order to align the a particular $[uvw]$ zone axis with the microscope optical axis (Oz-axis) (Fig. 11a).

When the orientation of the crystal is completed use the buttons:

- **Done** : to freeze the crystal orientation settings.

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[2]The reflection must belong to the **Z**ero-**O**rder **L**aue **Z**one.

[3]The diffraction parameters, i.e. camera length, beam half-convergence, etc, as well as thresholds used to filter out Kikuchi, HOLZ lines or diffraction spots are modified using the popup menu item *Show diffraction parameters*.

- **Modify** : to modify the crystal orientation.

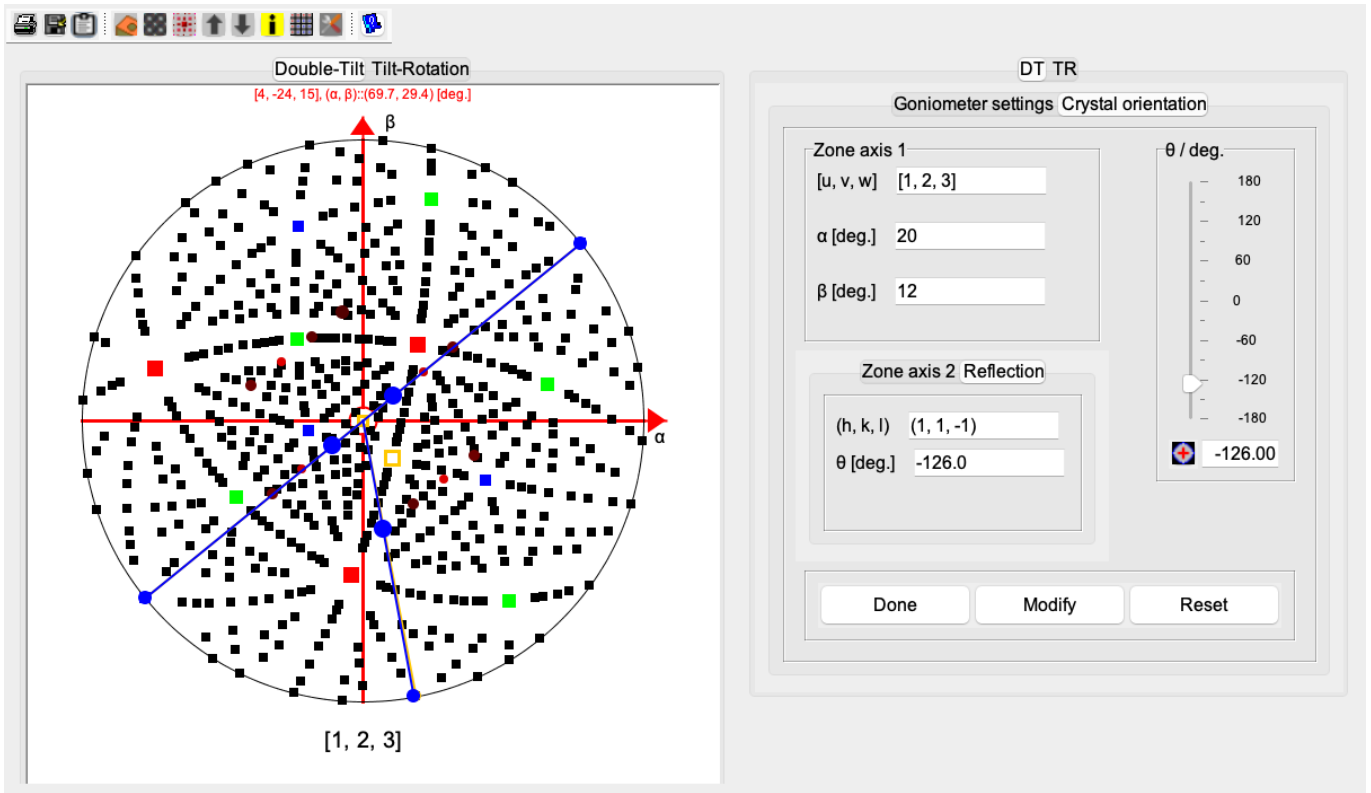- **Reset** : to reset the orientation settings.

Figure 4: Crystal orientation using a single identified $[uvw]_1$ zone axis and the θ angle of the O_x specimen holder and the $[uvw]_1$ SAED pattern (blue reflections).

To improve the SAED pattern's visibility, decrease the number of $[uvw]$ zone axes ($\downarrow$, Fig. 5) and modify the SAED parameters using the popup menu attached to the stereogram (Fig. 6a) to open the **Diffraction parameters** dialogue (Fig. 6b).

Modifying the *Half-conv.* (beam half-convergence), *Camera* (camera length) and *Accept.* (objective aperture acceptance angle) has improved the SAED visibility overlayed on the stereogram. Puting $[uvw]$ and (hkl) indices to the zone axes (Fig 8a) and SAED spots could also help as well as magnifying the stereogram (Fig. 8b).

Selecting again the **Goniometer settings** tab the (α, β) tilt angles set to $(0, 0)$ and the crystal zone axis $[-7, 189, 162]$) is align with O_z (Fig. 9).
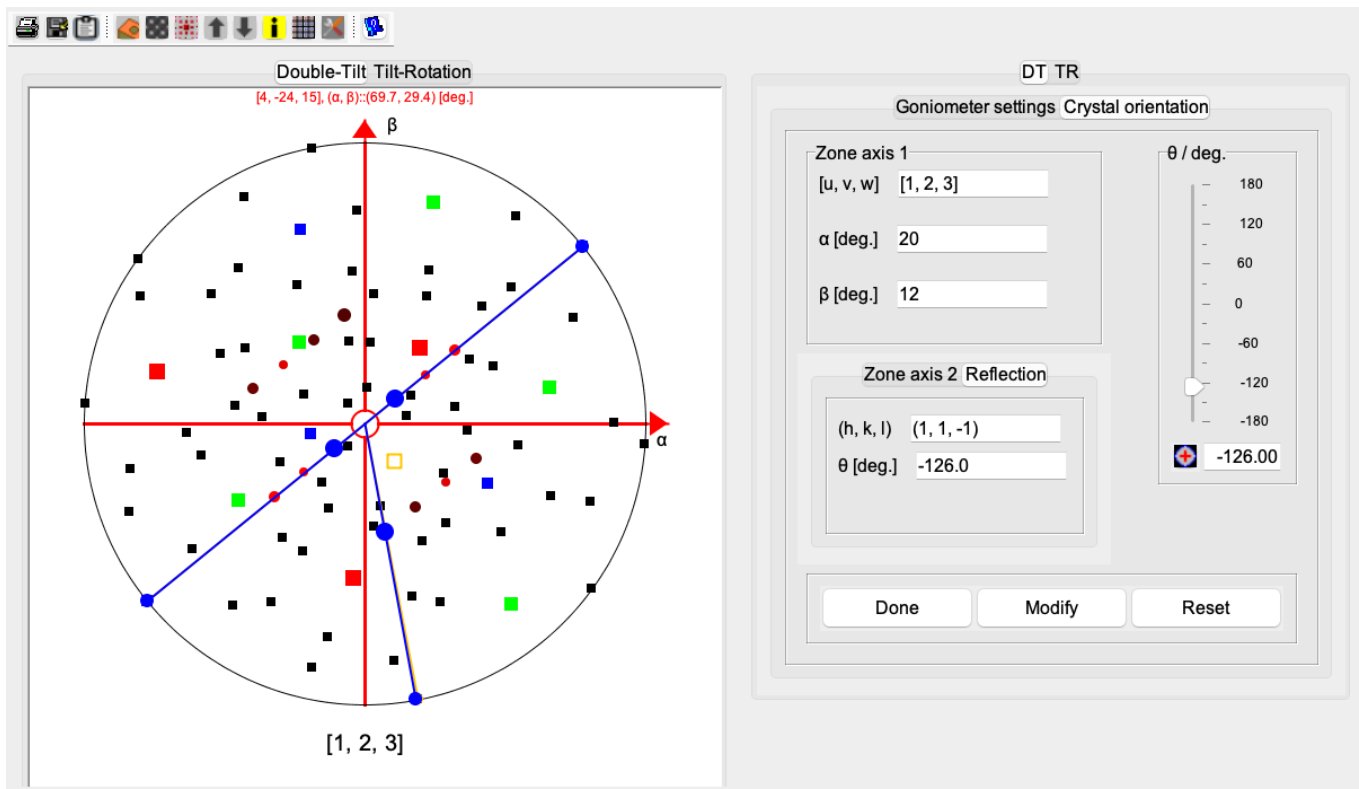
Figure 5: Reduced number of [*uvw*] crystallographic zone axes to improve SAED visibility.
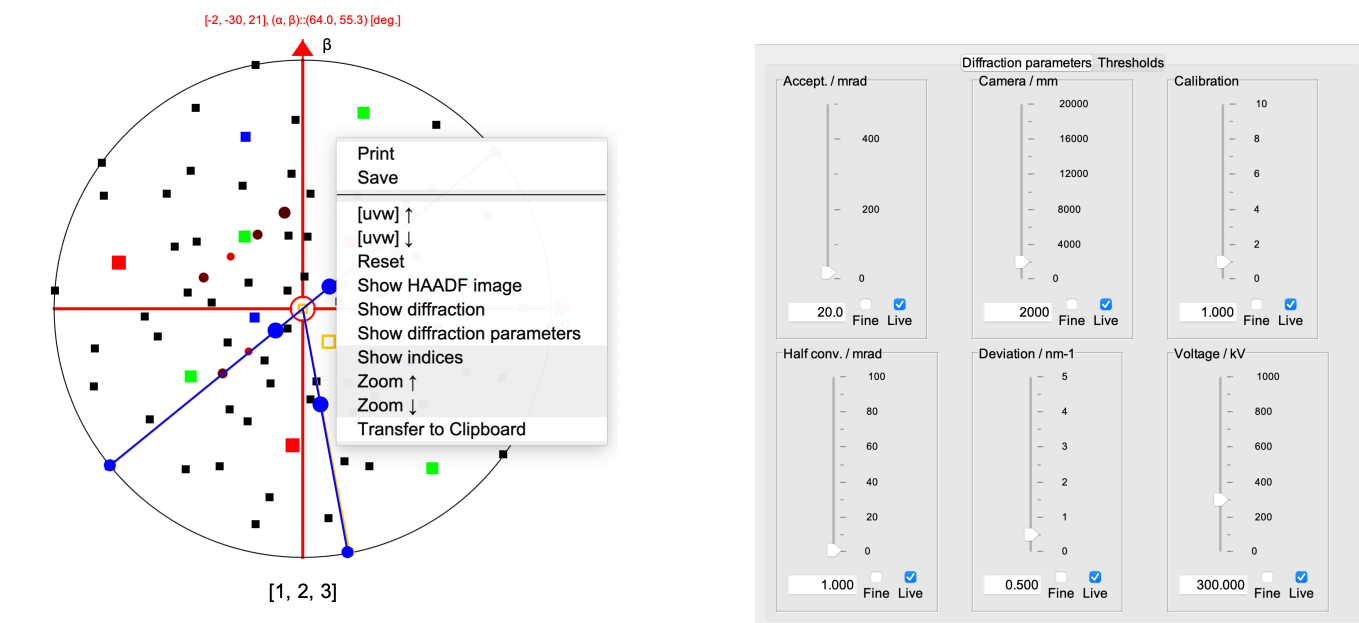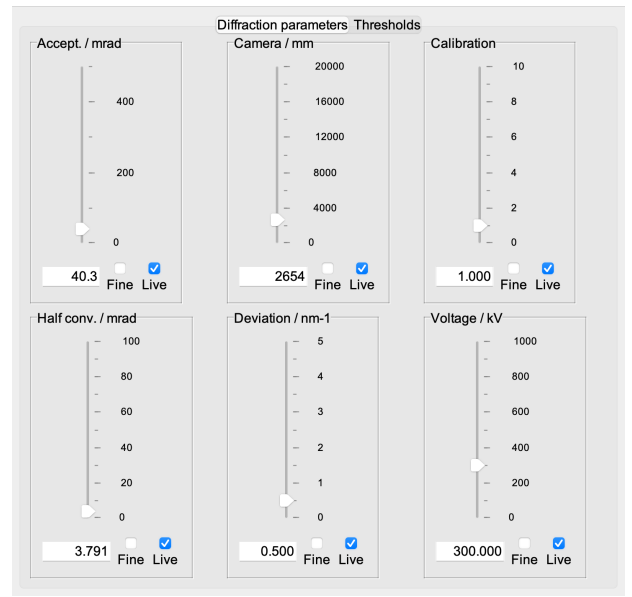

(a) Popup menu attached to the goniometer stereogram.

(b) Dialogue to modify the SAED parameters (camera length, half-beam convergence, etc).

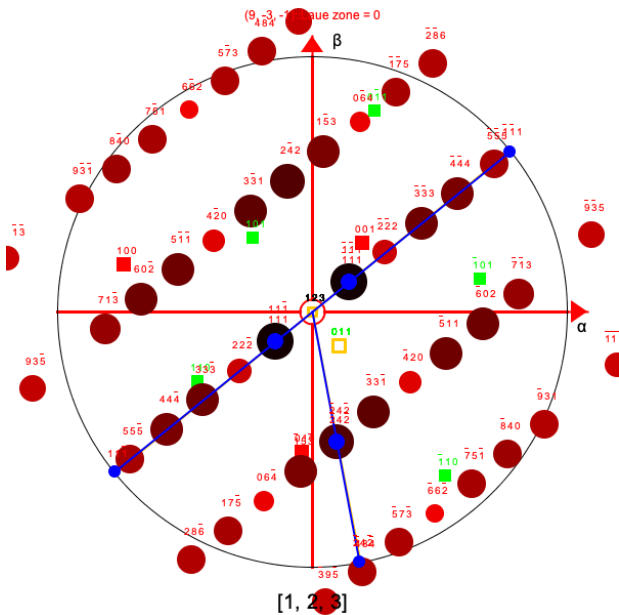Figure 6: Popup menu and dialogue to modify the SAED parameters.
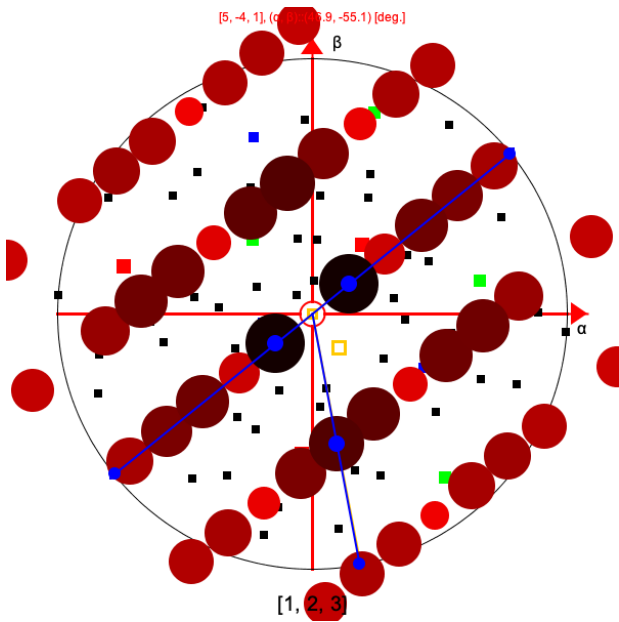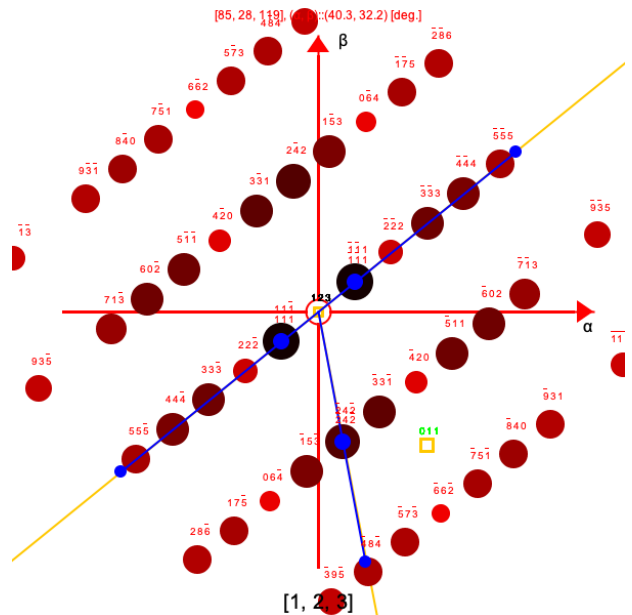
(a) Modified SAED parameters.

(b) New *Half-conv.*, the *Camera* and *Accept.* parameters.

Figure 7: Modifying the SAED parameters.

(a) Indexed [*uvw*] crystallographic axes and SAED (*hkl*) reflections.

(b) Magnified goniometer stereogram.

Figure 8: Indexing and magnifying the goniometer stereogram.
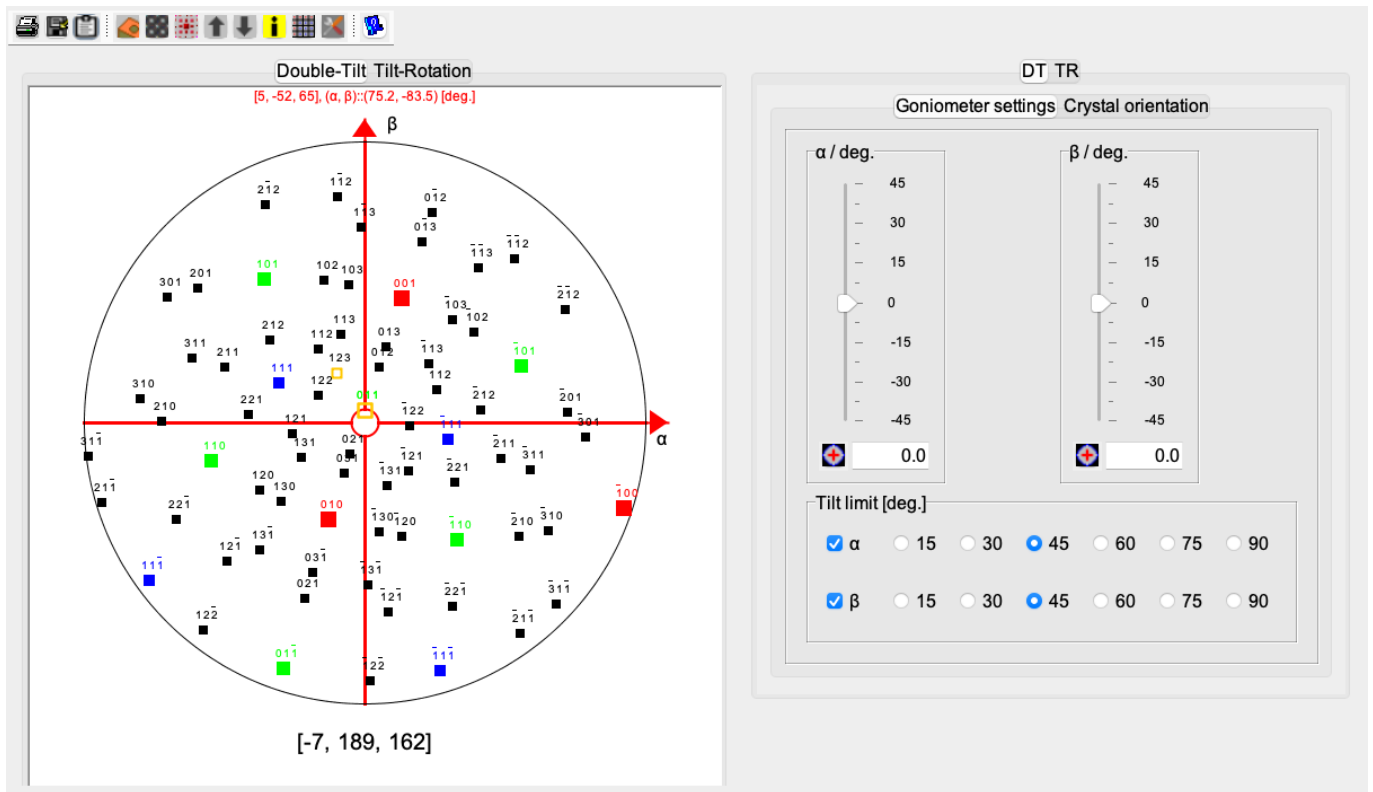
Figure 9: $\alpha = 0$, $\beta = 0$.

1.1.3 Tool buttons

The tool buttons allow to:

- ![] : print the whole goniometer frame.

- ![] : save the whole goniometer frame .

- ![] : transfer the whole frame to the clipboard.

- ![] : open the specimen dialogue (Fig. 10a).

- ![] : show HAADF images within the projection approximation (Fig. 10b).

- ![] : show SAED patterns.

- ![] : increase the number of displayed $[uvw]$ zone axes (Fig. 10c).

- ![] : decrease the number of displayed $[uvw]$ zone axes (Fig. 10d).

- ![] : add $[uvw]$ or $[uvtw]$ (hexagonal) indices to each zone axis.

- ![] : create a table of zone axes accessible using the goniometer (Fig. 17a).

- ![] : superpose a *Wulff net* on the oriented stereogram (Fig. 15).
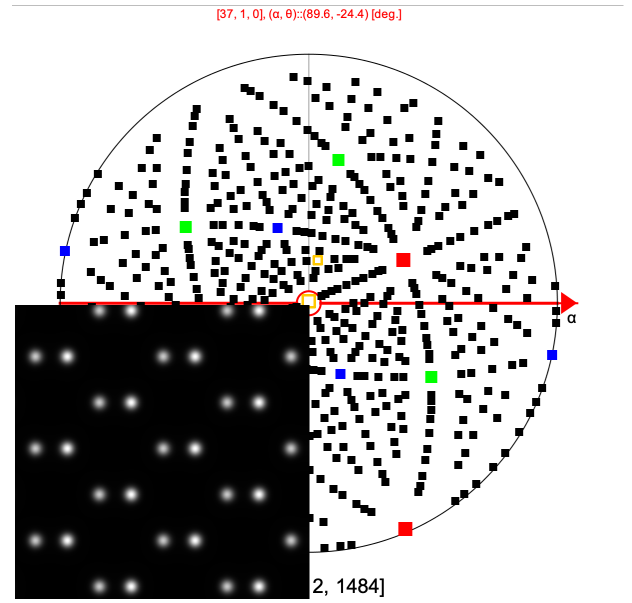
- ![] : display a help file.

1.1.4 Control tabs

The controls tabs allow to rotate the stereogram and to specify the range of the (α, β) tilts (**Tilt limit**). The rotation directions follow the right handed rules of geometry. This can be change using the (α, β) check boxes.
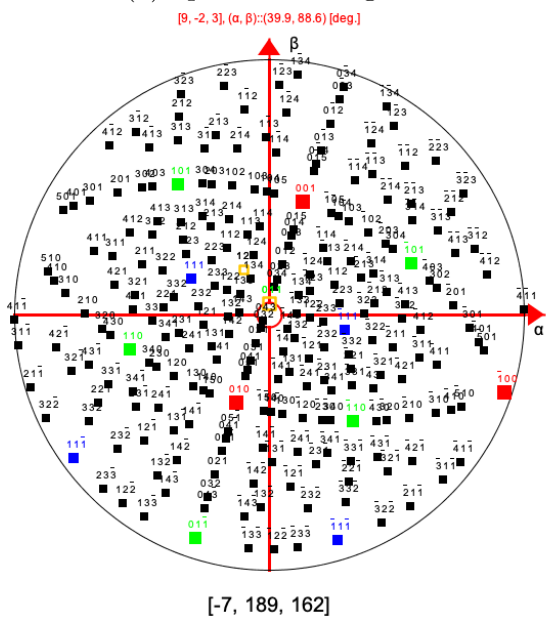
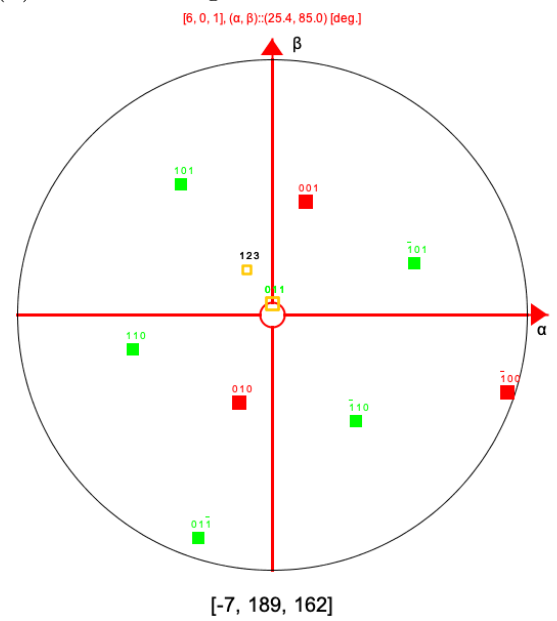Figs 11a and 11b shows the sliders controlling the α and β rotations.

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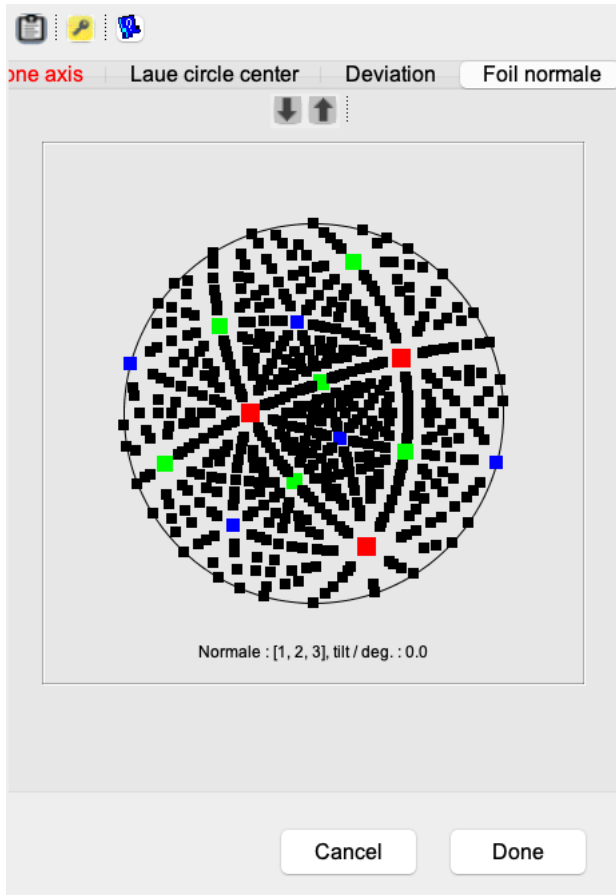
(a) Specimen dialogue.
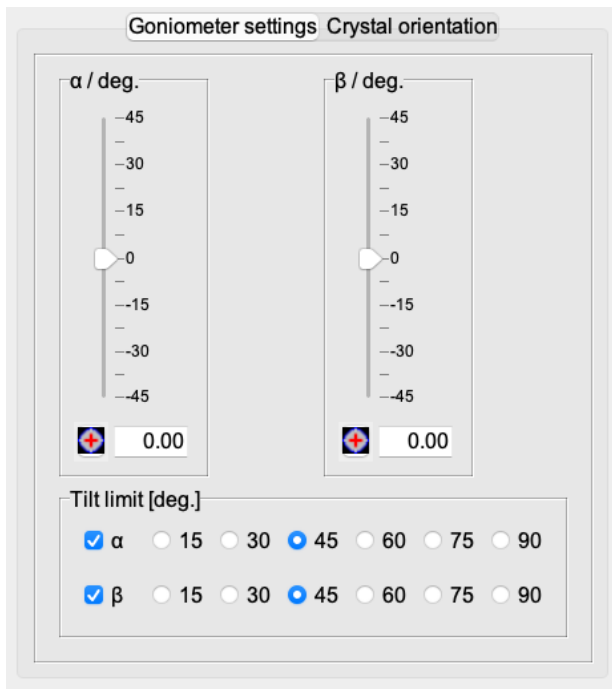
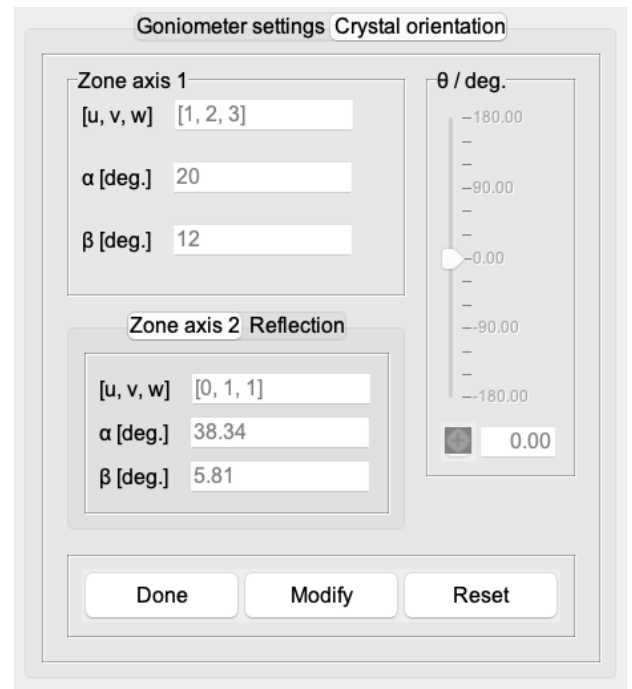(b) HAADF image of last clicked zone axis.

(c) Increasing the [uvw].

(d) Decreasing the [uvw].

Figure 10: Increasing and decreasing the [uvw].

- α : the rotation is defined by the specimen holder axis (Ox - axis).

- β : the rotation is perpendicular to the specimen holder (Oy - axis).

(a) Goniometer ($\alpha = 0$, $\beta = 0$) controls.

(b) Goniometer settings of oriented crystal.

Figure 11: Goniometer and orientation tabs.

1.1.5   Stereogram popup menu

The popup menu items attached to the stereographic projection allow to:

- **Print** : print the drawing.

- **Save** : save the drawing.

- **More zones** : increase the number of plotted zones axis.

- **Less zones** : decrease the number of plotted zones axis.

- **Reset**: set (α, β) to (0, 0) degrees.

- **Show HAADF image** : show the HAADF image of the last selected zone axis (Fig. 12).

- **Show diffraction** : display the SAED pattern of the last selected zone axis (Fig.13).

- **Show diffraction parameters** : open a dialogue to modify the diffraction parameters and HOLZ, Kikuchi or spot thresholds.

- **Show indices** : attach indices to the plotted zone axis (Fig. 16a).

- **Show range** : show the accessible zone axes (Fig. 14).

- **Zoom** ↑ : magnify the stereogram drawing(Fig. 16b).

- **Zoom** ↓ : demagnify the stereogram drawing.

- **Transfer to Clipboard** : transfer the drawing to the clipboard.

The diffraction pattern is hidden when leaving the **Reflection** tab. Going back to the **Goniometer settings** tab will center the stereogram (here along the zone axis $[-7, 189, 162]$).
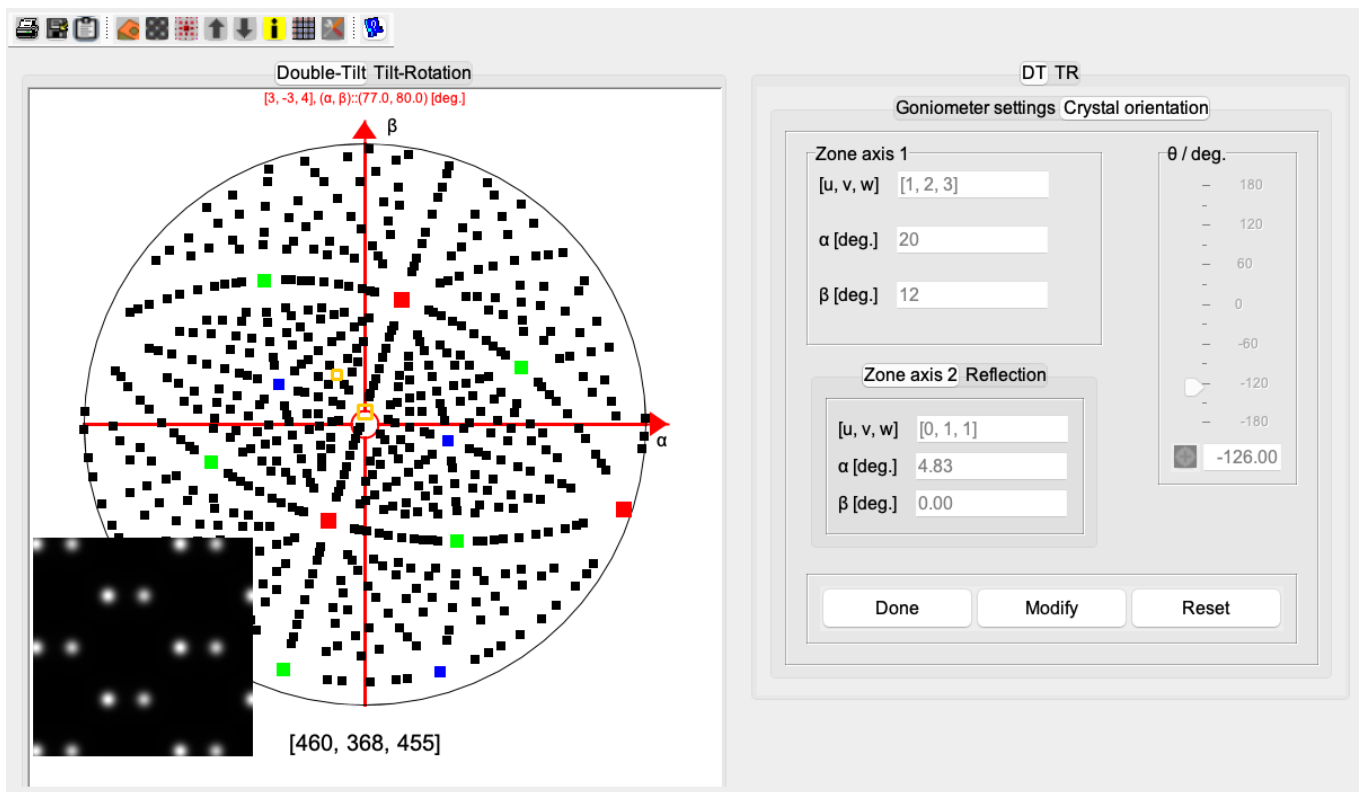
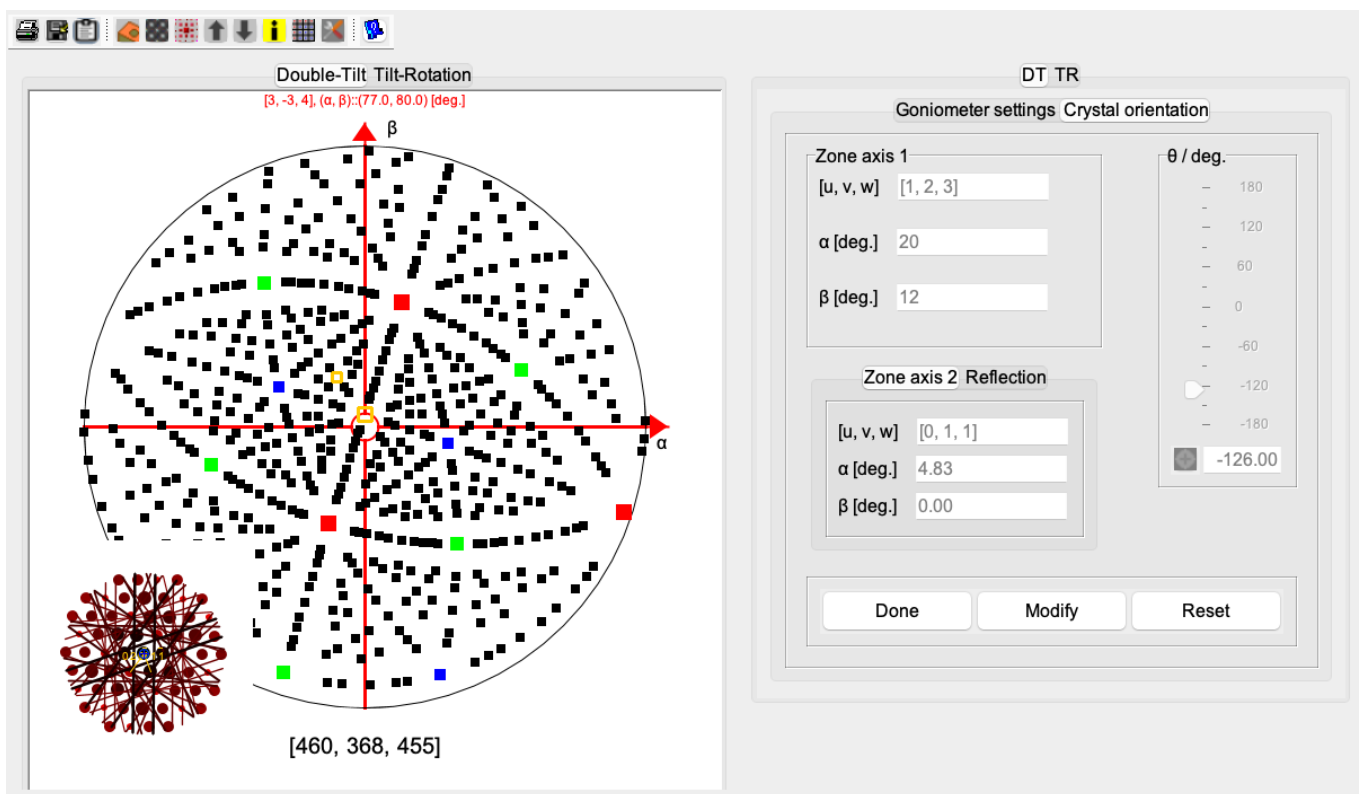Figure 12: HAADF image displayed at stereogram's bottom left corner.

Figure 13: SAED pattern displayed at stereogram's bottom left corner.
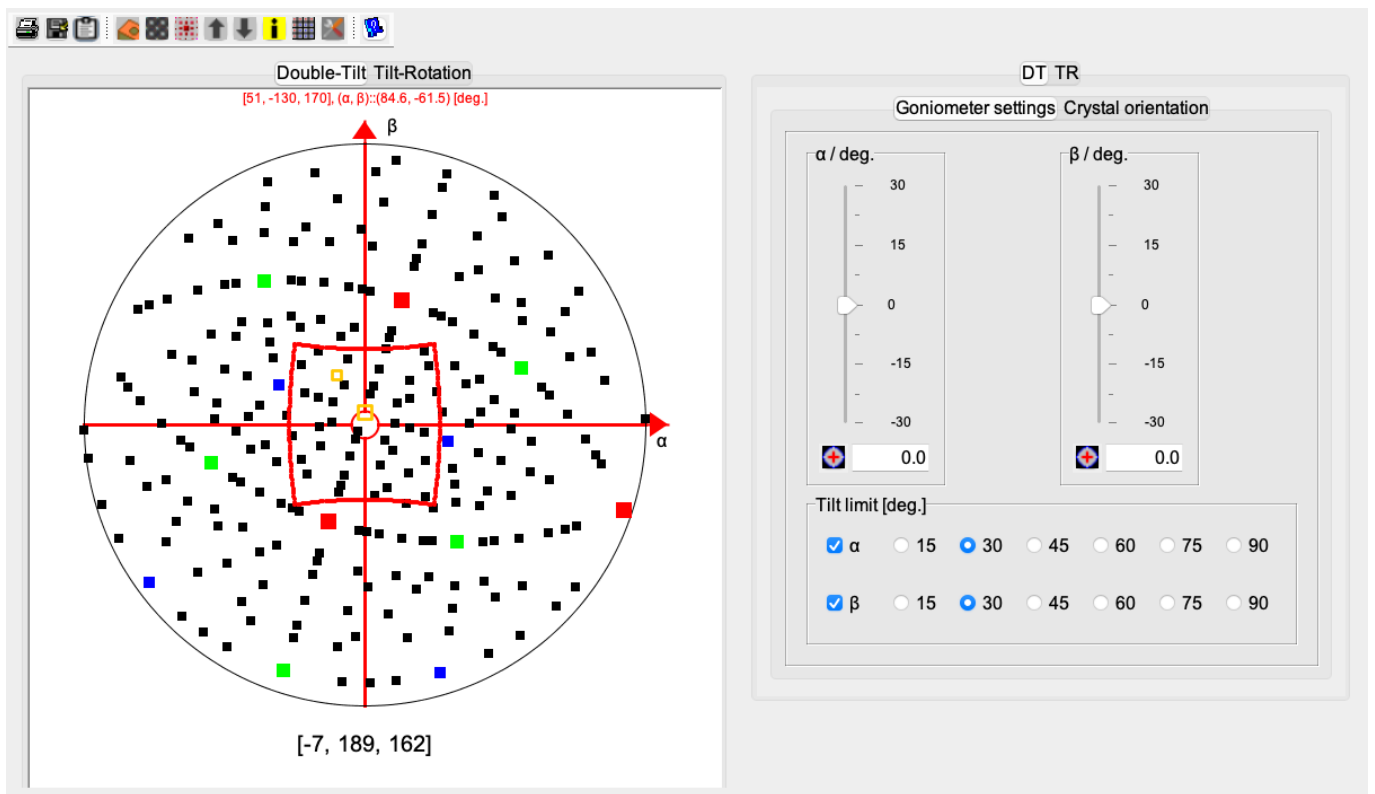
Figure 14: The accessible zone axes for a specimen holder allowing maximum α and β tilts of $\pm$ 30 degrees .
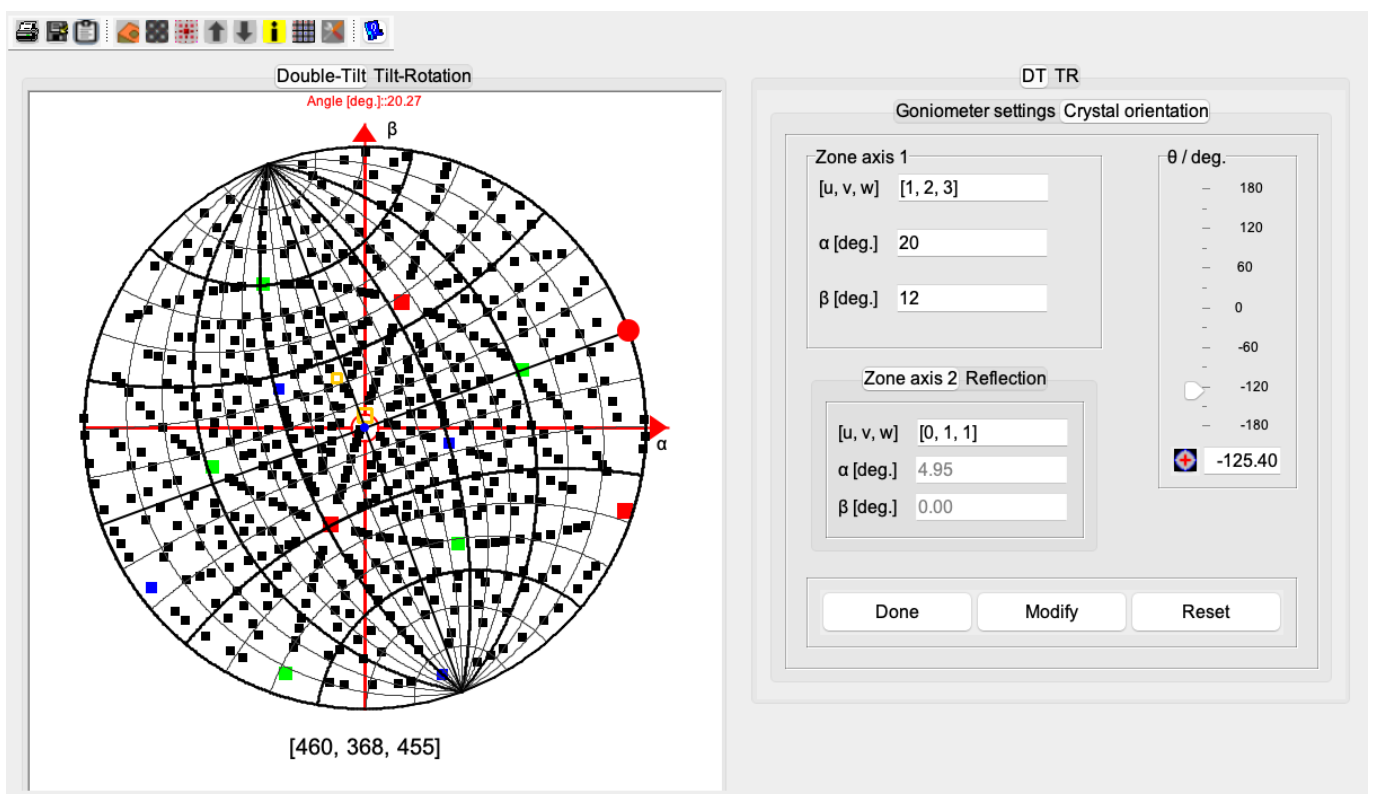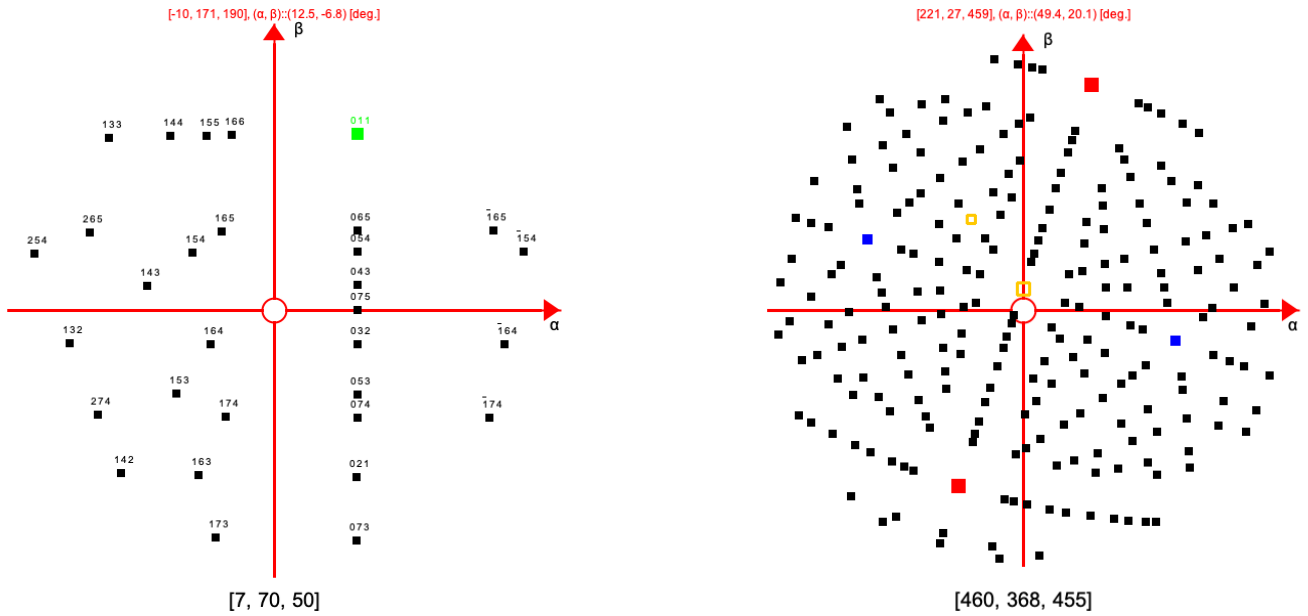

Figure 15: Wulff-net superposed on the stereogram. It is rotated using the Red dot and can be used to measure angles.

(a) Attached indices to the plotted zone axes.

(b) Stereogram magnified by 2.

Figure 16: Magnifying the stereogram drawing and adding zone-axis indices.

1.1.6 Goniometer details

A table of accessible zone axis (Fig. 17a) provides the (α, β) angles that align a tabulated zone axis. Up to 4 zone axes can be selected and their SAED put at the corners of the stereogram (Fig. 17b).

1.1.7 Stereogram with SAED pattern or HAADF images

Moving the mouse on the stereogram provides the (α, β) angles of the mouse position. A mouse click on any square (zone axis) will display its indices and angles as well as the associated diffraction pattern and HAADF image at the bottom corners of the stereogram (Fig. 18). As soon as the mouse leaves the square theses drawings are suppressed.

[u,v,w]	$g_1::(h,k,l)$	$g_2::(h,k,l)$	α [deg.]	β [deg.]
[0, 5, 4]	(2, 0, 0)	(0, 8, -10)	-1.19	2.05
[0, 4, 3]	(2, 0, 0)	(0, 6, -8)	-2.89	2.61
[0, 3, 2]	(2, 0, 0)	(0, 4, -6)	-5.91	3.61
[-1, 5, 4]	(1, 1, -1)	(-6, 2, -4)	-3.94	-6.40
[-1, 4, 4]	(0, -2, 2)	(8, 0, 2)	1.63	-9.46
[0, 5, 3]	(2, 0, 0)	(1, 3, -5)	-8.49	4.48
[-1, 4, 3]	(1, 1, -1)	(-4, 2, -4)	-6.36	-8.19
[1, 5, 4]	(-1, 1, -1)	(-6, -2, 4)	1.59	10.48
[0, 4, 5]	(2, 0, 0)	(0, 10, -8)	10.85	-1.96
[1, 4, 4]	(0, -2, 2)	(8, -2, 0)	7.90	9.66
[-1, 3, 3]	(0, -2, 2)	(6, 0, 2)	0.59	-12.52
[-1, 5, 3]	(-2, 2, -4)	(-6, 0, -2)	-11.45	-4.94
[0, 3, 4]	(2, 0, 0)	(0, 8, -6)	12.55	-2.55
[-1, 4, 5]	(-1, 1, -1)	(-6, -4, 2)	7.91	-10.46
[1, 4, 3]	(-1, 1, -1)	(-6, 0, 2)	0.68	13.34
[0, 2, 1]	(2, 0, 0)	(0, 2, -4)	-12.66	5.90

(a) Table of accessible crystallographic zone axes.
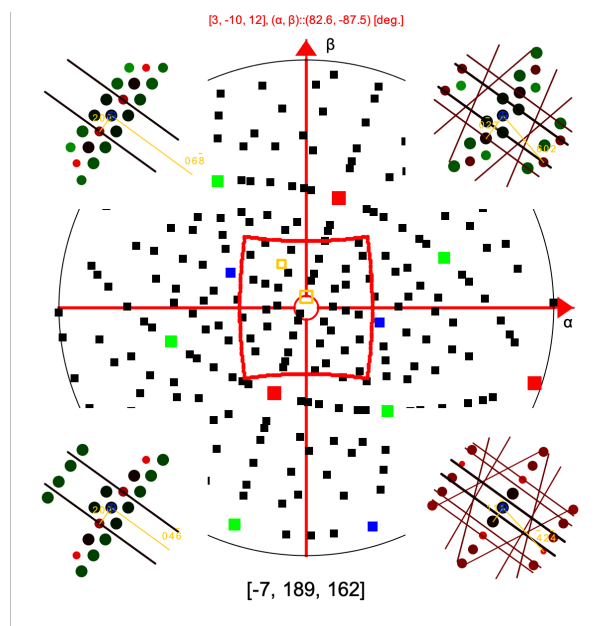
(b) SAED put at the stereogram corners.

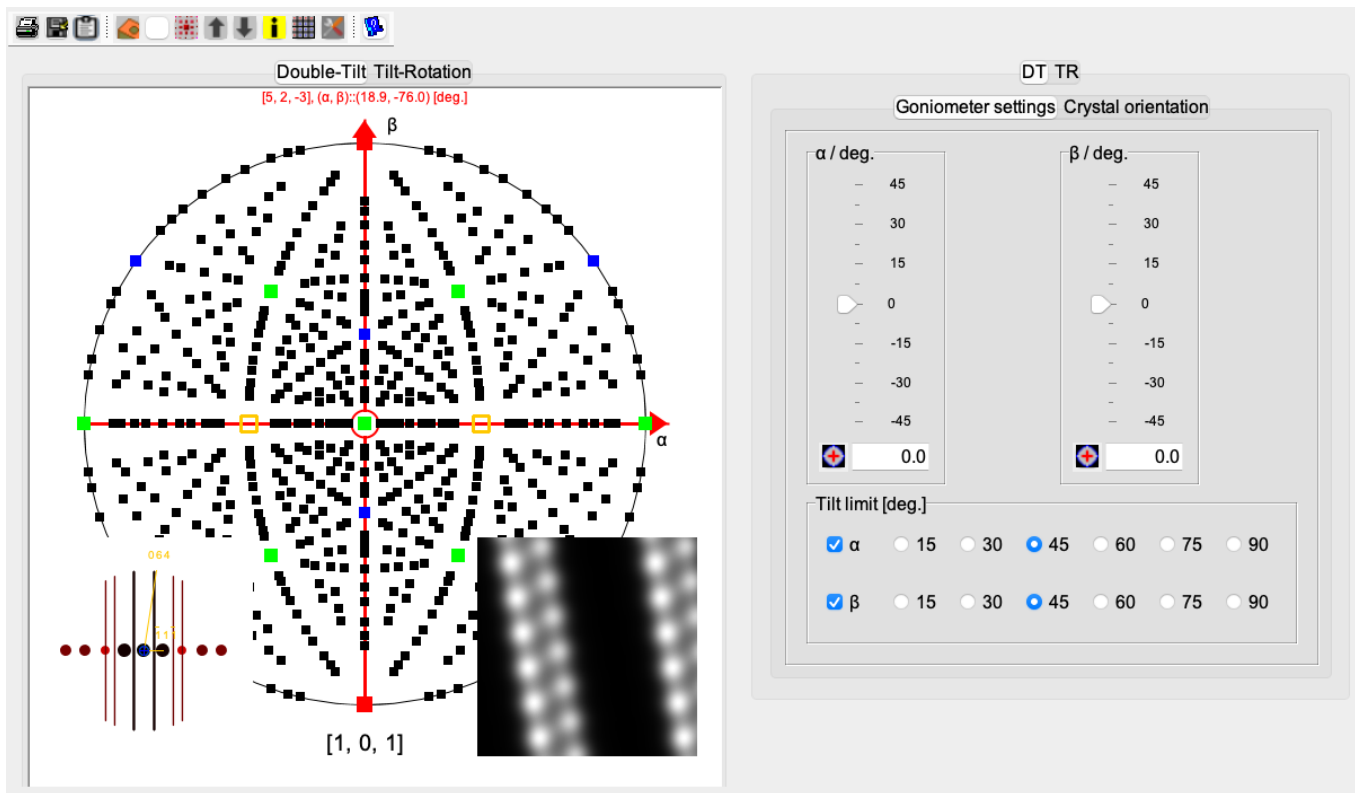Figure 17: SAEDs of 4 selected zone axes.

Figure 18: SAED and HAADF images displayed at the bottom corners of the stereogram.

1.2 Tilt-rotation specimen holder

The controls to calculate the crystal orientation using a **TR** specimen holder are identical to those used by a **DT** holder. The differences concern the labelling of the rotation axes [4].

Graphically the red line and arrow labelled β are missing on the **TR** stereogram plot (Fig. 19).
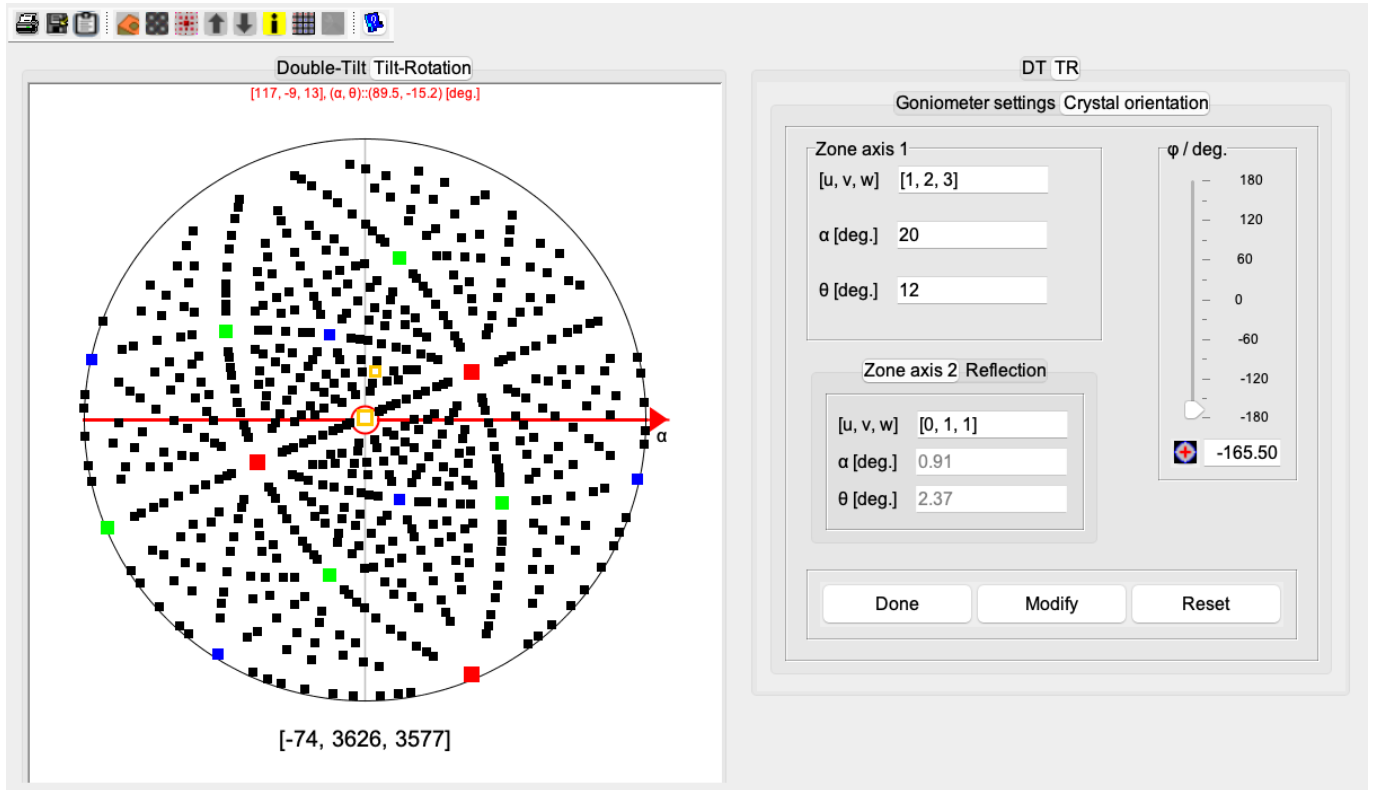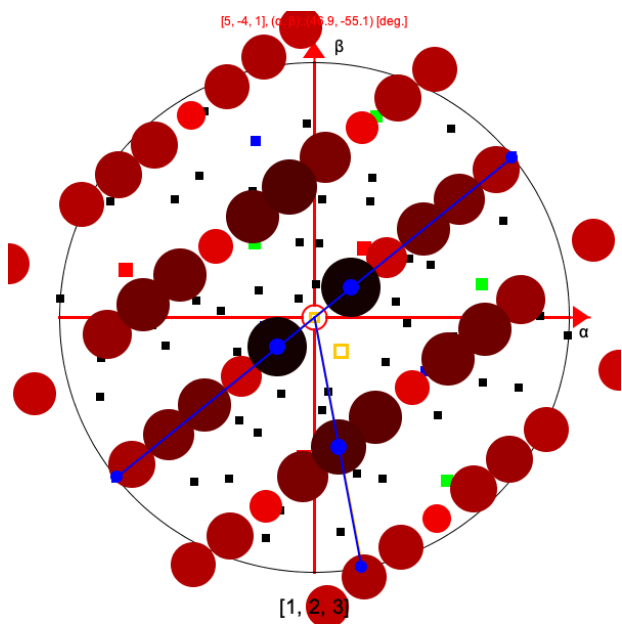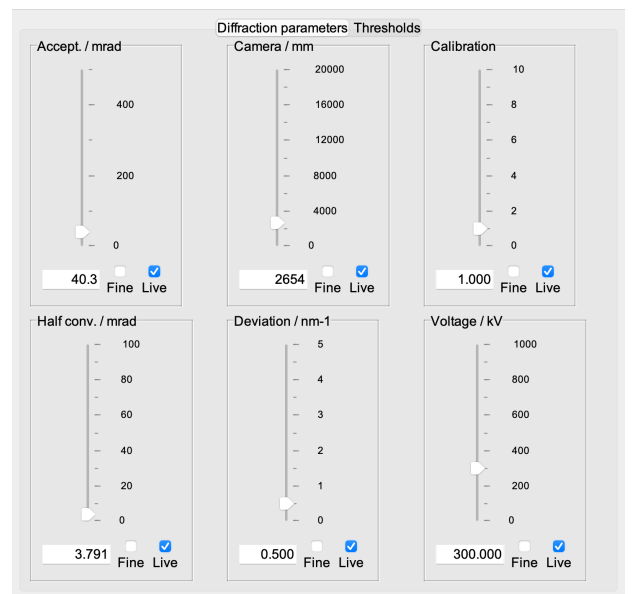

Figure 19: Tilt-rotation settings using 2 $[uvw]$ crystallographic zone axes ($[1, 2, 3]$, $[0, 1, 1]$). With $(\alpha, \theta) = (0, 0)$ the crystal $[uvw]$ orientation is $[-7, 189, 162]$.

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[4]Indeed for the very same 2 $[uvw]$ crystallographic zone axes and sets of angles (α, β) and (α, θ) the crystal orientations are different.

(a) Modified SAED parameters.

(b) New *Half-conv.*, the *Camera* and *Accept.* parameters.

Figure 20: Modifying the SAED parameters.