User Manual of τompas

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What is τompas?

τompas (TEM On-line Multi-purpose Analyzing System) is a software tool to interactively demonstrate pole figures, Kikuchi patterns, defect projections and quantified crystallographic data based on sample holder tilt angles.

The aim of τompas is to help researchers with frequently used conventional TEM techniques, and enhance the experiment efficiency by reducing human effort. τompas is a one-stop solution of TEM on-line crystallographic analysis. With τompas, one can easily design the route of sample tilting, instantly interpret Kikuchi patterns, and directly get the indices of features in images.

How to use τompas?

The interface of τompas

The interface of τompas consists of a menu on the top, a display area with pages, a status bar at the bottom and a control panel on the right, as shown in Figure 1. With the menu and the control panel, one can modify the parameters used in simulation. The status bar can display the indices of mouse position when the mouse is on a pole figure or a Kikuchi pattern, as well as the scale of the Kikuchi pattern.

The first page of display area, as shown by Figure 1, presents zone axis orientations, positions where two or more lattice planes intersect with each other, weighted by the number of contained lattice planes. The big circles of lattice planes are shown in the second page (Figure 2). The third page (Figure 3) shows simulated Kikuchi patterns and the fourth (Figure 4) shows the projection of line and planar features of known indices.

The display area is designed to react to users' mouse inputs. The frequent operations in TEM, such as tilting the sample and change the camera lens, are simulated by mouse dragging and wheel rotating. The graphs shown in display area are digitized: the indices of each point on the graph is displayed on the status bar; the indices of zone axes, big circles and Kikuchi bands are visible on mouse hovering; the zone axes can also be directly reached by right clicking.

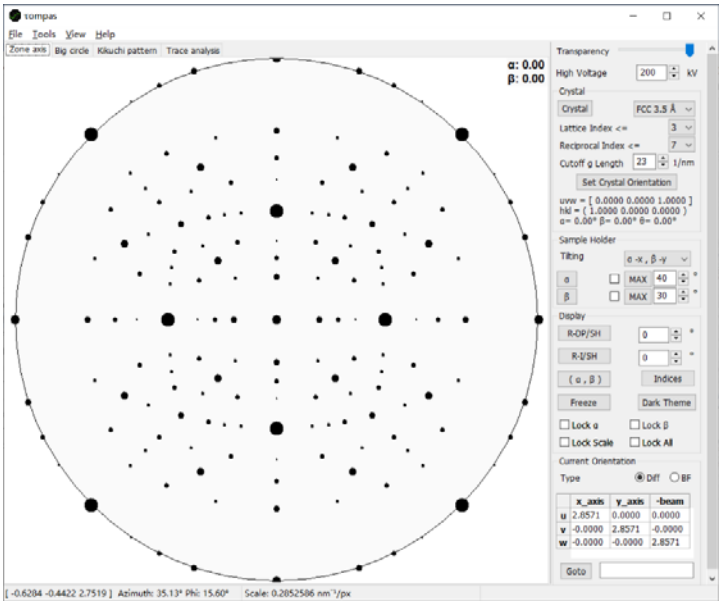

Figure 1 The first page of τompas, showing zone axes in a pole figure

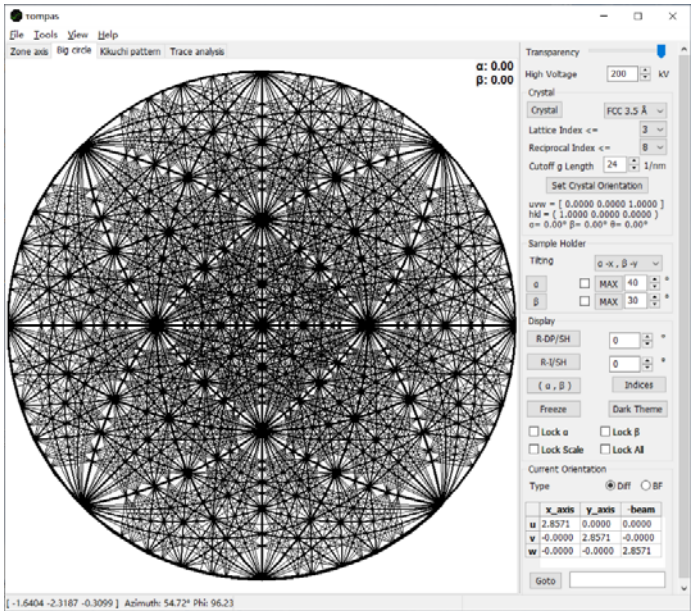

Figure 2 The second page of τompas, showing big circles in a pole figure

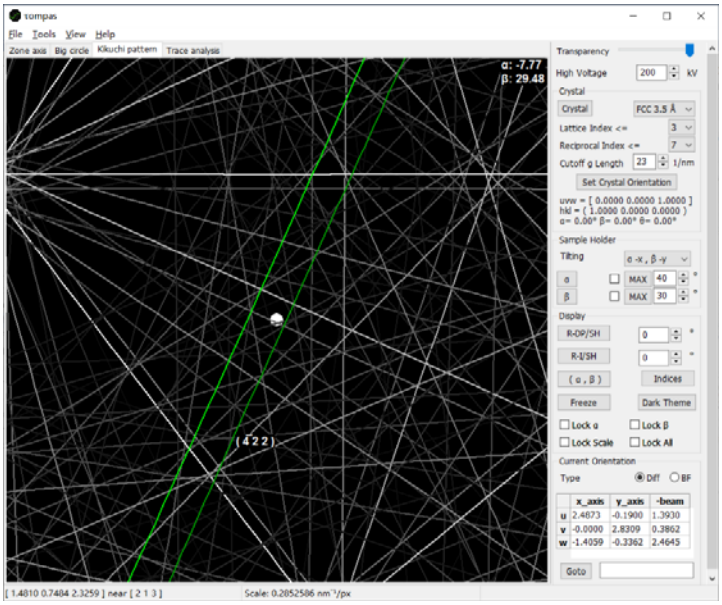

Figure 3 The third page of τompas, showing a Kikuchi pattern

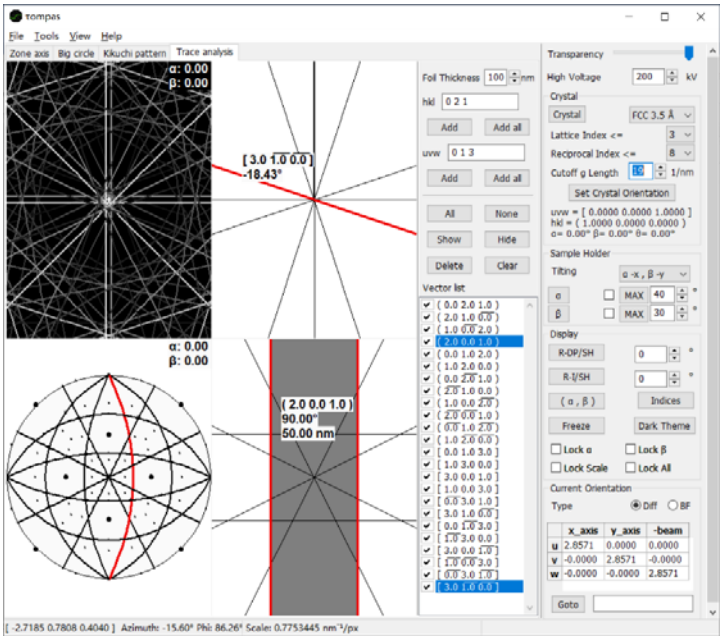

Figure 4 The fourth page of τompas, showing a pole figure, a Kikuchi pattern and features' projection altogether

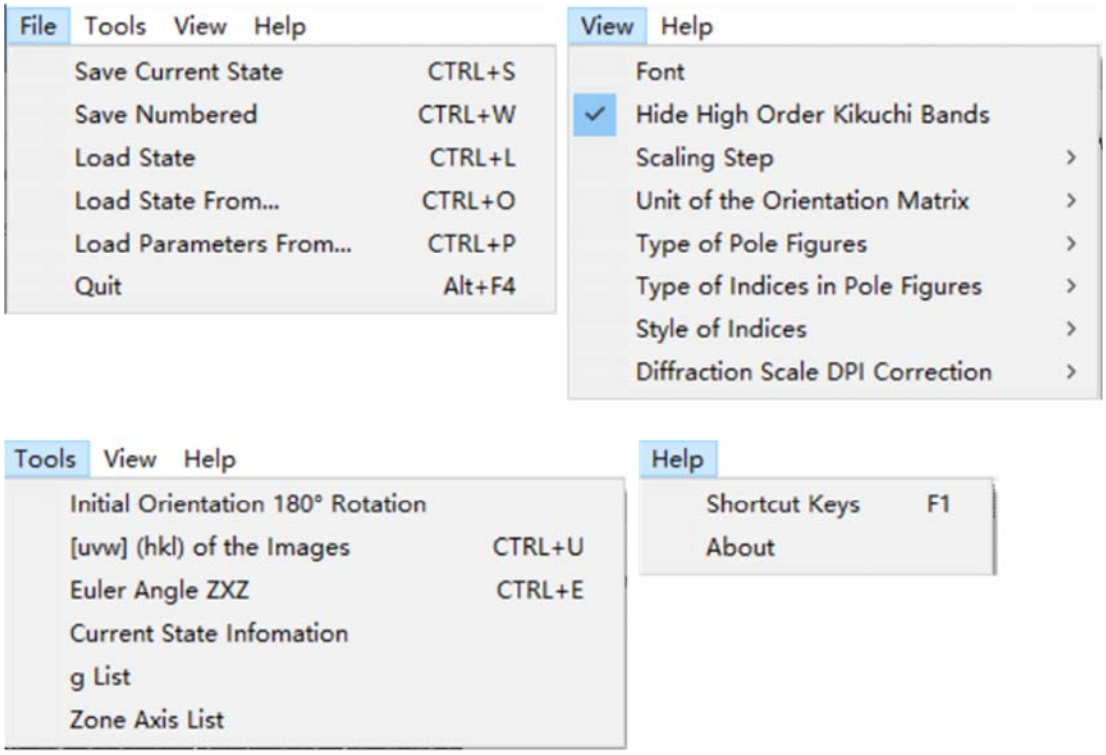

Figure 5 The menu of τompas

The menu of τompas offers some functions to export information and adjust the look of τompas, as shown in Figure 5 and Table 1.

Table 1 Menu items and their functions

Item	Function
Save Current State	Save current state to state.ini
Save Numbered	Save current state to state%Time%.ini
Load State	Load state from state.ini
Load State From	Load state from a selected file
Load Parameters From	Only load TEM parameters from a selected file
Quit	Exit the program
Initial Orientation 180° Rotation	Rotate the crystal by 180° to eliminate the 180° ambiguity on initial orientation
[uvw] (hkl) of the Images	Send [uvw] (hkl) to clipboard
Euler Angle ZXZ	Extract & Set the orientation by ZXZ Euler Angles. (0,0,0) means c//z and a*//x on the screen
Current State Information	Show the parameters needed to reproduce the current view
g list	Copy the list of reciprocal vectors drawn in the pole figure
Zone Axis list	Copy the list of real vectors drawn in the pole figure
Font	Set the font used in the display area
Hide High-order Kikuchi bands	Hide high-order Kikuchi bands
Scaling Step	Adjust the step of mouse wheel zooming

Item	Function
Unit of the Orientation Matrix	Choose from hkl or uvw style of orientation matrix and the length of column vectors
Type of Pole Figures	Choose between lower sphere and upper sphere pole figures*
Type of Indices in Pole Figures	Choose the direction of orientation indices in pole figures*
Style of Indices	Choose between Latex type minus sign or the usual type minus sign
Diffraction Scale DPI Correction	Correct the scale of Kikuchi patterns when the screen has DPI scaling
Status information	Show the parameters needed to reproduce the current view
DPI	Change DPI set to make the scale of Kikuchi patterns correct
Shortcut Keys	Display the keyboard inputs that the display area can receive
About	The information about τompas

*Usually, the zone axes are described by the index of the reversed electron beam direction (from the screen to the electron gun), which means they are vectors on the upper sphere of pole figures. However, a Kikuchi pattern is a gnomonically projected lower sphere, and it moves in the same direction with the lower sphere pole figure when being tilted. Therefore, to work better with Kikuchi patterns and to respect the habit of zone axis indices, the default pole figure is a lower sphere one with upper sphere indices, which is quite different from other pole figures.

The control panel offers full control of the crystal lattice, sample holder, and the display area, while providing direct information of crystal orientation, as listed in Table 2.

Table 2 Control panel items and their functions

Item	Function
Transparency	Change transparency of τompas, to compare with experimental Kikuchi patterns and images
High voltage	Change high voltage of TEM
Crystal	Change crystal lattice
Lattice index <=	Max index of zone axes to be displayed
Reciprocal index <=	Max index of reciprocal vectors to be displayed
Cutoff g length	Max length of reciprocal vectors to be displayed
Set crystal orientation	Set crystal orientation by [uvw] (hkl)
Sample holder: Tilting	Tilting axes of the sample holder, first 4 for double-tilt, the other 4 for tilt-rotation
Sample holder: α & β	Reset tilting angle α or β to zero
Sample holder: checkbox	Hide big circles out of the holder tilting range
Sample holder: max	Limit the tilting angles within the holder tilting range
Sample holder: numbers	Change the holder tilting range

Item	Function
R-DP/SH	The right-handed rotation from the holder to diffraction patterns. Click the button to reset
R-I/SH	The right-handed rotation from the holder to images. Click the button to reset
(α, β)	Display the tilt angles of mouse position in pole figures
Indices	Display indices of zone axes in pole figures
Freeze	Stop refreshing display area
Dark theme	Change the theme of display area to reduce eye strain in TEM room
"Lock" checkboxes	Lock the scale of the display area or tilting angles
Current orientation type	Choose from display the orientation matrix of Kikuchi patterns or that of images
Orientation matrix	The current crystal orientation matrix, could be copied by clicking
Goto	Receive α, β positions or uvw positions and directly change orientation

Preparation before the TEM session

Determine tilting axes of sample holder and magnetic rotation angles

The coordinate system of τompas is shown in Figure 6. The x axis is along the long axis of sample holder, and z axis is anti-parallel to the electron beam. For double-tilt sample holders, usually the sample is tilted along y axis firstly and then tilted along x axis, and for tilt-rotation sample holders, usually the sample is rotated along z axis firstly and then tilted along x axis. The sign of tilting angles depends on the convention used by TEM, which should be explained in the manual of the sample holder, or can be inferred by observing the holder rotation while increasing α. For example, the double-tilt sample holder used on FEI Tecnai G2 20 has a tilting axis of $-x$ for α and $-y$ for β. This convention can be easily checked by switching the tilting method after setting up rotation angles, lattice parameters and the crystal orientation, as the crystal orientation at a random (α, β) will change with the tilting method.

The image-diffraction pattern rotation angle should be determined following the standard procedure on textbooks. Here we explain how to determine the relative rotation between the sample holder and the image. Move the sample holder slightly along its long axis (the x+ direction of τompas coordinate system), either by hand or by electronic devices, and compare the images taken before and after moving. The angle from screen x axis to the displacement vector is the R-I/SH, as shown in Figure 7.

Once these parameters are determined using a sample holder at some magnification of images and diffraction patterns, there is no need to change the tilting method unless the holder is changed, nor to change the rotation angles unless the magnification is changed. The parameters can be saved. And they can be loaded for each session on the same TEM afterwards.

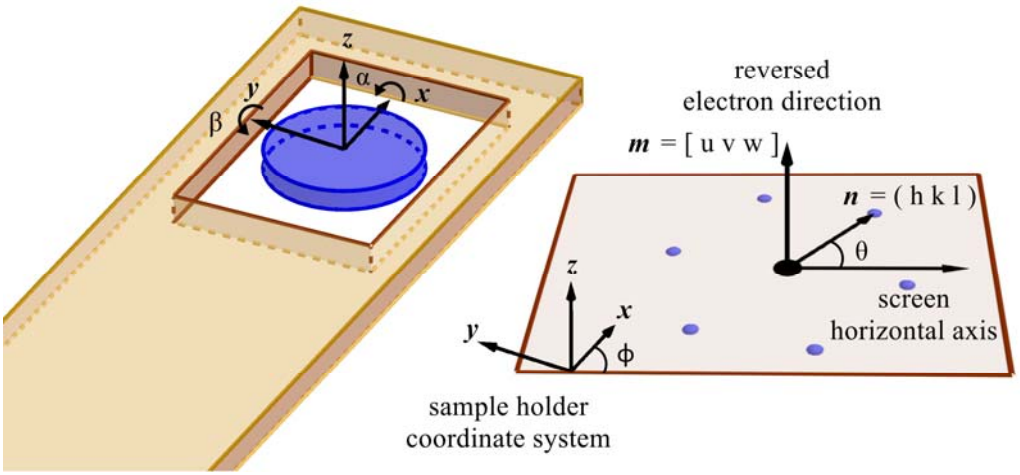

Figure 6 The coordinate system of τompas

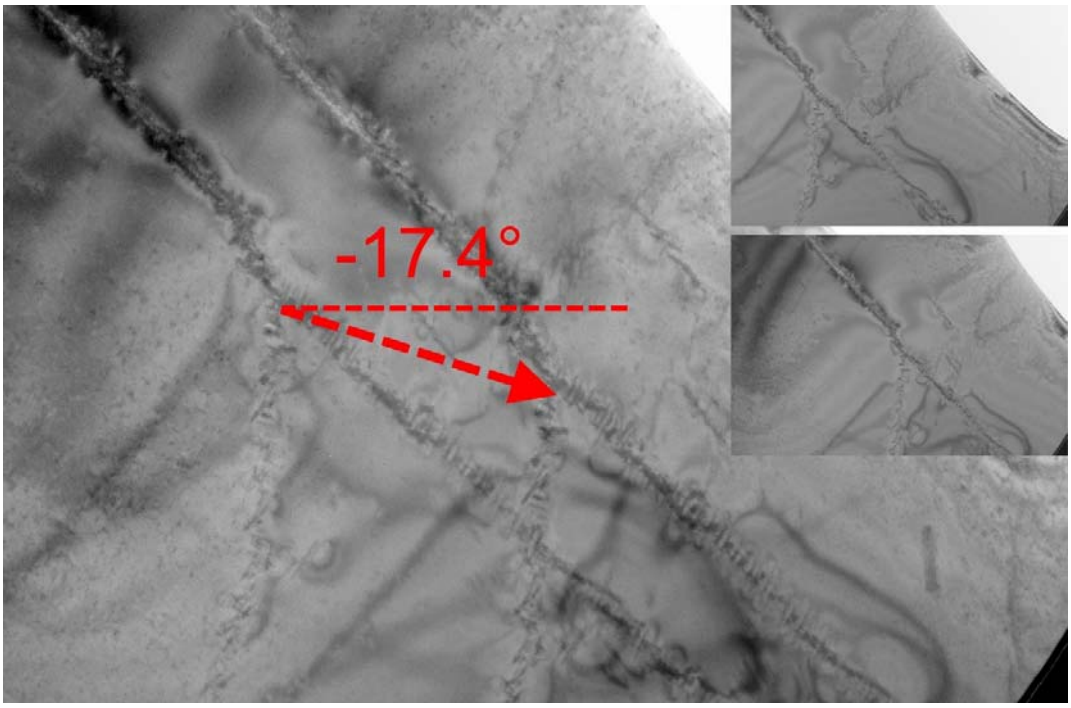

Figure 7 Demonstration of determining R-I/SH by image difference

Input crystal lattice parameters

τompas only requires a knowledge of basic lattice parameters and the space group, and **ONLY SYSTEMATIC EXTINCTION** is considered, which should give good enough simulation for crystals without coincidence extinction in most cases. The crystal structure can either be input by clicking the *Crystal* button and using the dialog shown in Figure 8, or be selected from the frequently used structures on the right side.

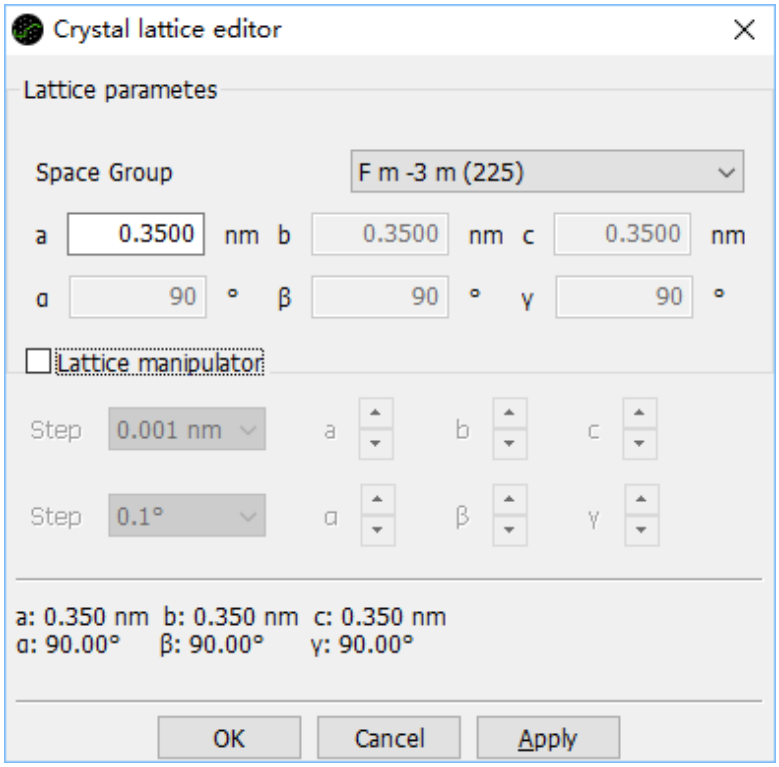

Figure 8 Dialog to input and manipulate lattice parameters

During a TEM session

Set crystal orientation

To use τompas on a grain, a linkage between the real crystal orientation and the simulated one must be established. This can be done by inputting the crystal orientation at an arbitrary (α, β) position. For simplicity, we recommend to use a diffraction pattern at a low-index zone axis, as shown in Figure 9. These settings of crystal orientation are adopted in the following parts of this manual. Of course, if the zone axis doesn't contain a 2-fold axis, simply using one diffraction spot will end in an 180° ambiguity of crystal orientation. This can be easily corrected by clicking the *Crystal orientation 180 rotation* item in *Tools* menu.

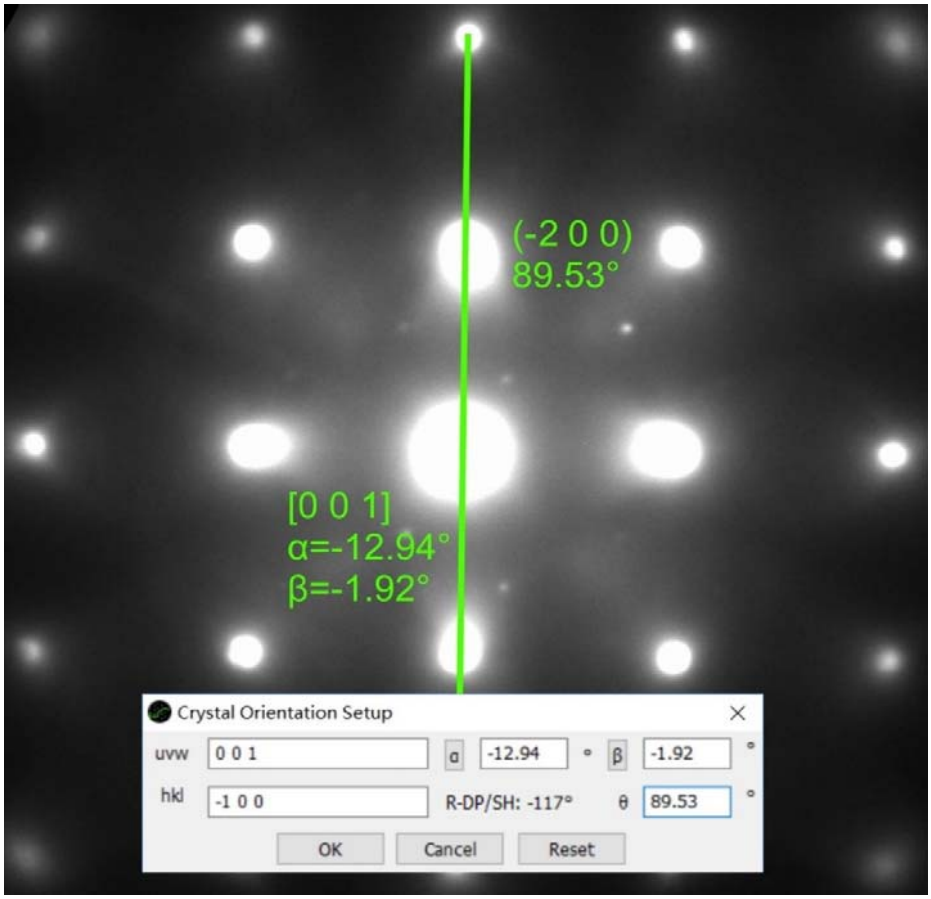

Figure 9 Crystal orientation setup: an example of FCC [0 0 1] zone axis

Navigate sample tilting

The zone axes point in pole figures can be activated by mouse hovering and show the (α, β) tilt angles of this zone axis. The big circles in pole figures can also be activated to show indices. When the (α, β) in the control panel is activated, the (α, β) of the mouse position is displayed, as shown in Figure 10. This feature can be used to navigate the sample tilting to any point needed by the operator.

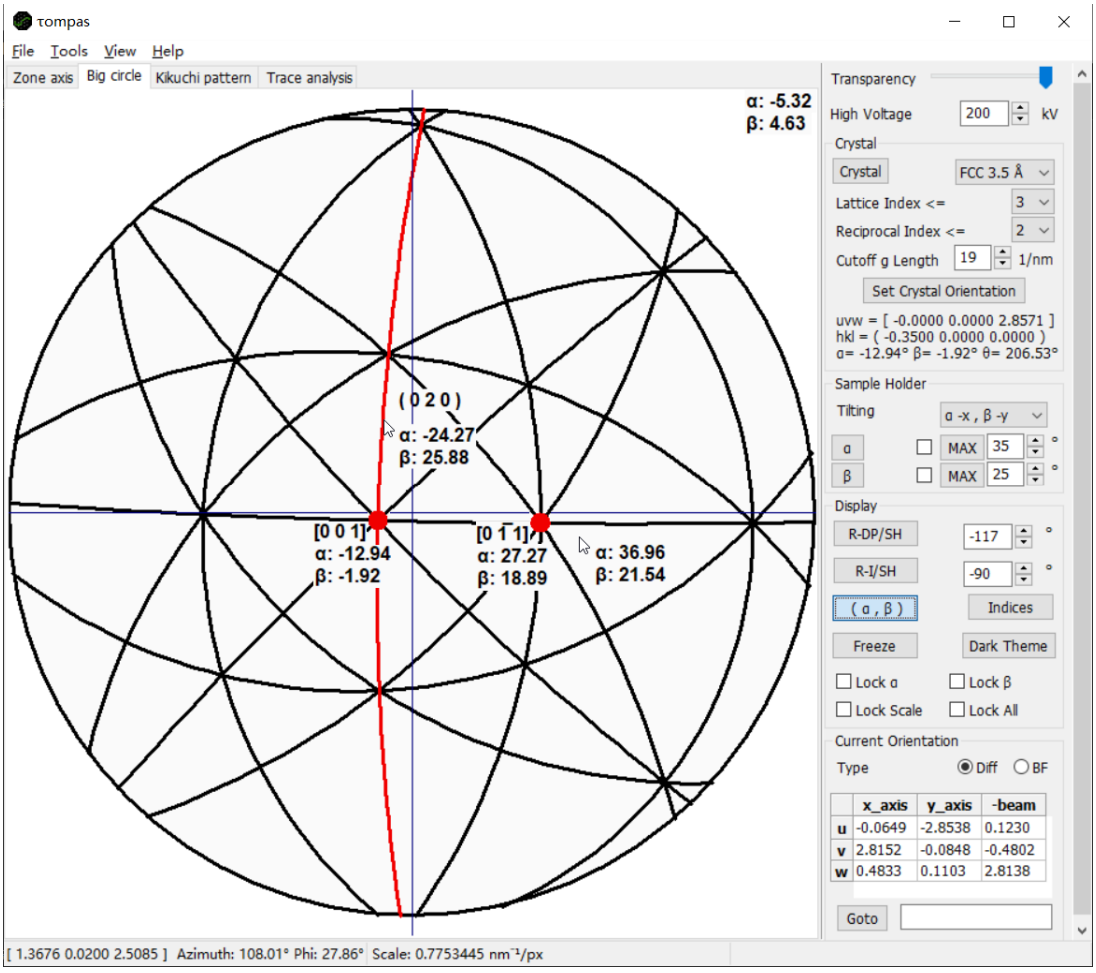

Figure 10 Sample tilting navigation

Design diffraction contrast analysis

τompas could be helpful in designing complicated optical conditions, such as diffraction contrast analysis. As is known to all, to determine the Burger's vector of a dislocation needs at least two **g**s with $\mathbf{g} \cdot \mathbf{b} = 0$. However, the needed **g**s may not be reachable due to the sample holder tilting range. For example, as shown by Figure 11, if **g**s with indices no greater than 2 are preferred, and the tilting range is set as $\alpha \leq 35°$, $\beta \leq 25°$, the **g**s within the tilting range cannot be used to determine if the **b** is [0 1 1] (missing on the right side), but can fulfill the need to determine other $<$ 0 1 1 $>$ family Burger's vectors. The useful positions of two-beam condition can be known by the method described in *Navigate sample tilting* part.

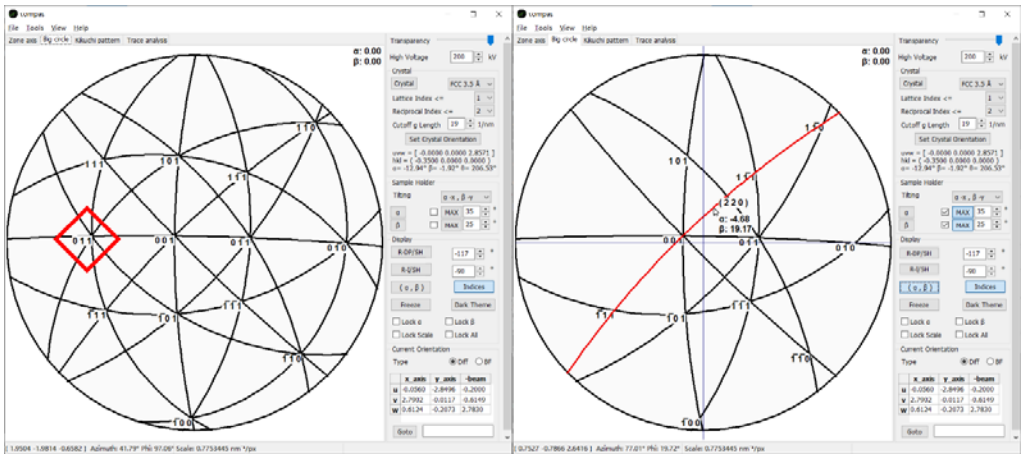

Figure 11 A demonstration of all low-index (≤ 2) **g**s (left) and reachable **g**s (right) for diffraction contrast analysis

Interpret Kikuchi patterns by matching

The interpretation of Kikuchi patterns usually requires lots of efforts, especially on indexing and measuring Kikuchi bands. With τompas, Kikuchi patterns can be interpreted by a simple simulating-matching process. As shown in Figure 12, after setting the crystal orientation with the same parameter as the example at *Set crystal orientation* part, a Kikuchi pattern is taken at $\alpha = -36.21°$, $\beta = 22.89°$. The first step is to use *Goto* function (Table 2 the last one) to input the same sample holder tilt angles shown by Figure 12 upper-right. Then the transparency of τompas should be adjusted to become an overlay of the experimental Kikuchi pattern, as shown by Figure 12 lower-left. From then on, the simulated pattern (Figure 12 lower-right) is identical to the experimental one. The indices of the bands in the pattern, also known as indices of plane normal drawn from the center spot, can be directly read in $\tau ompas$ in the way shown by Figure 3, and the orientation matrix is shown on the control panel for convenience. Besides, the lattice parameters can be tuned using the dialog shown in Figure 8, to get a better matching with the experimental pattern.

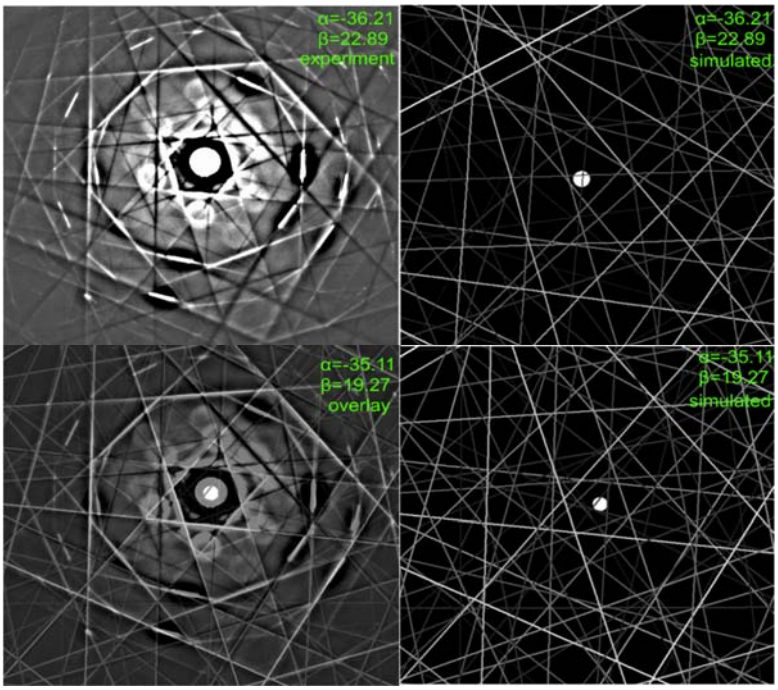

Figure 12 Interpret Kikuchi patterns by overlay-matching

Determine indices of line and planar features

τompas has a function to simulate the geometrical projection of line and planar defects in bright field images. This feature enables the user to roughly determine the indices of defects from a range of known results without the need of measurements. Since the projection of an interface already includes the projection of traces, i.e. line features, here we use an example of twin interface projection show how this function works.

In FCC crystals, the twin interface is usually one of {1 1 1} vectors. As shown by Figure 13, where the image-holder rotation is $-90°$, at matrix $[0\ \bar{1}\ 1]$ zone axis, a schematic figure of all possible interfaces with {1 1 1} vectors is drawn. By comparing the projection directions in Figure 13 left with these in Figure 14 right, we can directly know that the normal of the interface should be $(1\ 1\ \bar{1})$. Here the foil thickness is set to 100 nm, which should be adjusted according to multiple images at different orientations, or precisely determined by CBED method.

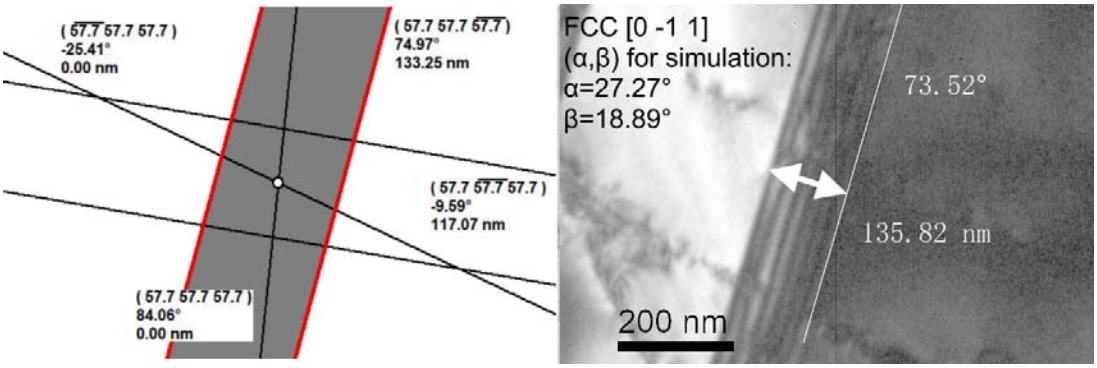

Figure 13 Experimental and simulated projection of interfaces at zone axis $[\ 0\ \bar{1}\ 1]$ of FCC matrix