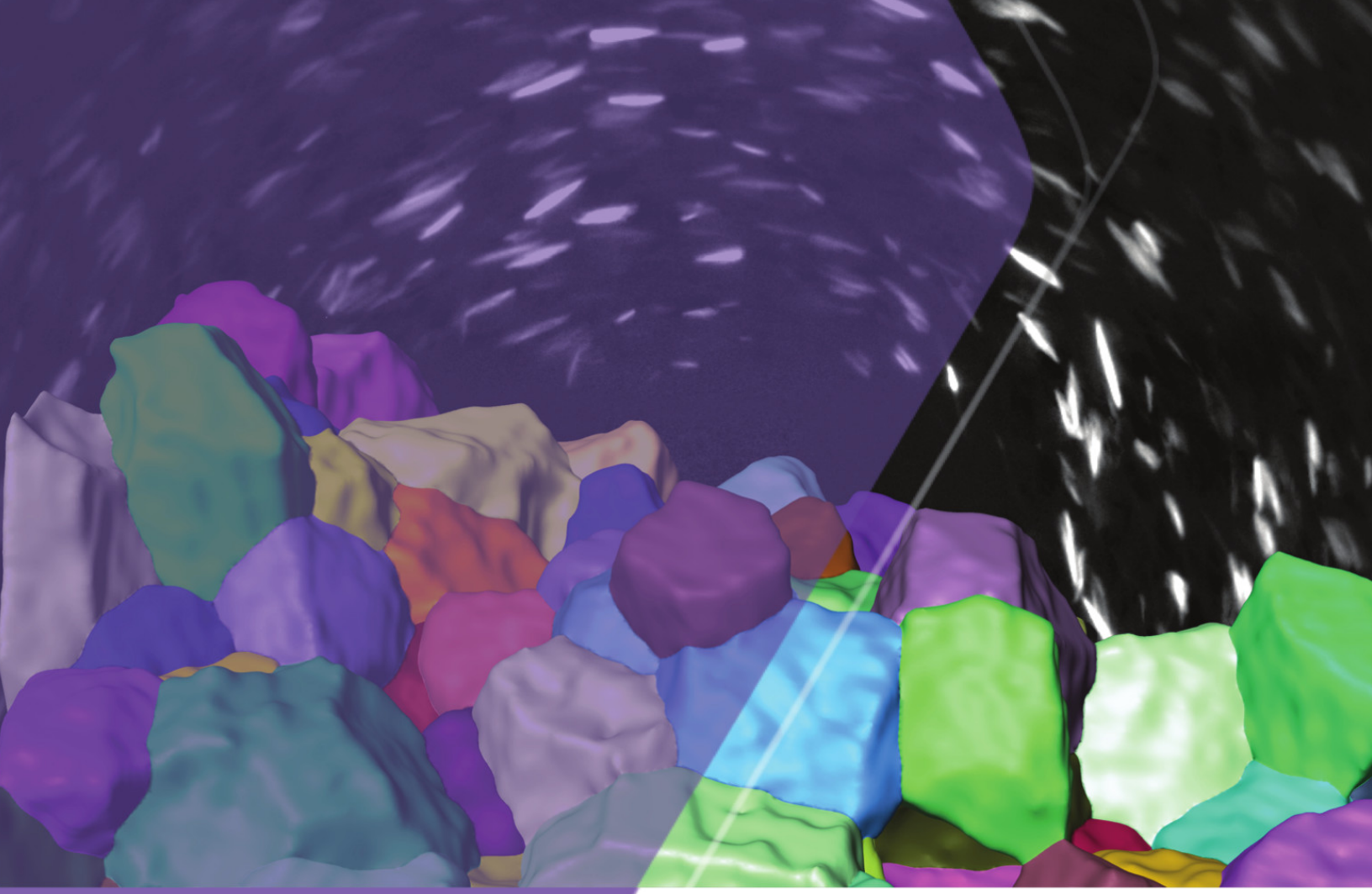

Release Notes

GrainMapper3D™ 3.1

Non-destructive 3D Grain Mapping Solution for Laboratory Diffraction Contrast Tomography

xnovotech

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LabDCT Pro Support

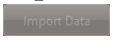
GrainMapper3D 3.1 is the dedicated reconstruction software enabling the analysis for both ZEISS Xradia Versa LabDCT Pro and Xradia CrystalCT. DCT data can now be collected either in Laue focusing geometry using the DCT 4X objective of the ZEISS Xradia 620/520 Versa or in projection geometry using the Flat Panel detector of a ZEISS Xradia CrystalCT or a ZEISS Xradia 620/520 Versa with flat panel extension. In order to support analysis for both imaging modalities a license upgrade has to be performed.

Data Import

The following changes have been made to the DCT and absorption data import.

Abort of Data Import The import of both DCT and absorption data can now be aborted during the import on the **Project** tab and **Absorption Mask** tab, respectively. The 

button changes to 

and then to 

once the process completes. Click 

if you need to abort the data import process before the process completes. Once the imported data is persisted to disk, the data import can no longer be aborted.

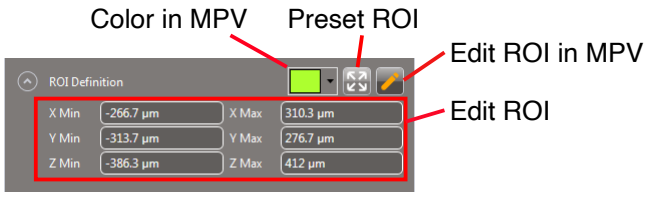
DCT Data Import The DCT projections in the **Project** tab are now always displayed in the **Scan Order**, even though images are reordered for the background estimation according the selected **Image Order** under the **Advanced DCT Import Options**. This allows to compare the background correction using the **Advanced Image Order** or the **Scan Image Order** for one and the same projection in the preview directly.

The **Noise Reduction** method (*i.e.* **Denoising** or **Hot Pixel** correction) is now also applied to the reference projection. This improves the segmentation of faint foot prints of the direct beam illumination through the aperture of the *illumination mask* on the **Detector Mask** tab.

Absorption Data Import The **ROI Definition** for **Absorption Data Import** recipe on the **Absorption Mask** tab now supports predefined ROI sizes. Press **Preset ROI** (Figure 1) in order to select between different predefined ROI sizes, either:

- **Full Volume** to maximize the ROI to the extent of the entire absorption volume
- **Illuminated Volume** to have the ROI fit the illuminated volume
- **Default Region**, which is 10% larger than the Illuminated Volume

Figure 1 Editing the ROI Definition in the **Absorption Mask** Tab



Furthermore, the following fixes have been made to the absorption import:

- Fixed issue computing the illuminated absorption data ROI correctly when DCT data was not taken centered around the rotation axis of the absorption data but acentric. The wrong part of the absorption volume may have been imported, which resulted in an empty reconstruction.
- Fixed issue in the preview of absorption data containing more than 2500 slices not being displayed correctly.
- Fixed the line profile in the absorption preview not displaying data.

Reconstruction

The reconstruction algorithm implementation has been revised. Depending on the indexing scenario a reconstruction now performs up to *30-50% faster* compared to GrainMapper3D 3.0. In particular, the indexing performance was improved significantly for patterns with many spots (>1000 per pattern). Also, the user interface stays more responsive when reconstructing large volumes (>50 million voxels). Furthermore, the following two new features have been added.

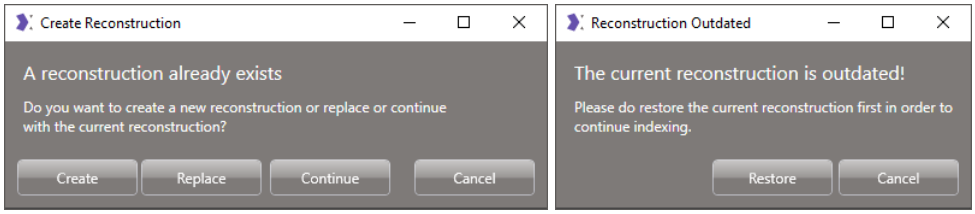
Boosting The advanced indexing option **Boosting** has been added to the **Completeness Tolerances** section (Figure 2). **Boosting** constrains the growing of new regions such that only solutions with a completeness higher than the fraction (specified by the boosting factor) of the existing completeness will grow. This reduces the effort spent on similar solutions and may speed up indexing by 100% or more, depending on the DCT data. The larger the boosting factor, the faster the reconstruction. To remove the **Boosting** option, press **Remove Option** next to it. To add **Boosting**, press **Add Options** and select **Boosting**.

Figure 2 Boosting Option

Continue Reconstruction A reconstruction can now be resumed. This feature allows to check for intermediate results on the **Grains**, **Inspection** and **Expert** tab. After pressing **Stop**, press **Run** again and select **Continue** in the popup dialogue (Figure 3a). The functionality requires that all settings (Segmentation, Calibration, Phase Definition, Region of Interest, Completeness Tolerances and Options) are identical, otherwise the reconstruction has to be restored first (Figure 3b). A reconstruction can only be resume if it was created with this release of the GrainMapper3D.

Figure 3 Managing a New *Reconstruction* Process

(a) Create, Replace or **Continue** a *Reconstruction* **(b) Restore** *Reconstruction* to Continue



Inspection and Self-Fitting

Combined HKL Selection For the forward simulation of diffraction spots in the **Inspection** tab, entering both a **Structure Factor** and a **d-spacing** will expand or reduce the list to only comprise hkl that fulfill the combined selection where both values are larger than those specified.

Combine Grain Selection The ability to combine several grain selections has been added both to the **Inspection** tab of GrainMapper3D and to the GrainMapper3D Viewer as detailed in Table 4.

Performance Improvements The performance when computing residuals has been significantly improved, in particular for dataset with a lot of spots per projection (>1000 per pattern). This mainly impacts collecting results after defining grains or performing a self-fitting.

Forward Simulation Fixed issue with forward simulation staying empty for large grains. When a grain was significantly larger than the illuminated FOV and its centroid was located outside of the FOV, the forward simulation failed to compute the outline of the grain shape.

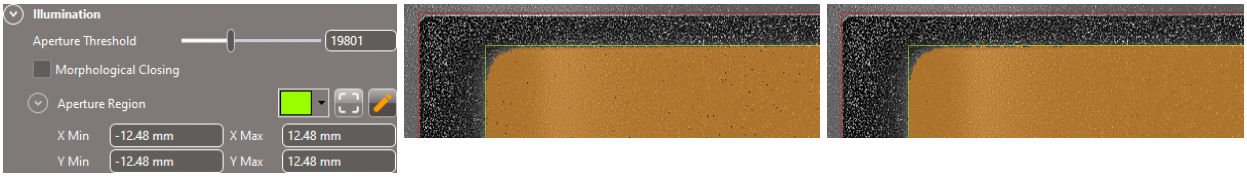
Other Enhancements

Radial Distance Filter A DCT segmentation filter based on **Radial Distance** from spot centroid to detector (in microns) center has been added.

Morphological Closing for Aperture Segmentation A properly segmented aperture region is of importance to the illumination model to compute the completeness. A noisy reference projection might introduce undesirable holes to the segmented mask. Check the **Morphological Closing** (Figure 4a) to apply a morphological closing to the aperture segmentation if the **orange** **Aperture Mask** overlay looks noisy at the boundaries or contains holes, see Figure 4b versus Figure 4c for an example.

Figure 4 Morphological Closing for Aperture Segmentation

(a) Morphological Closing **(b)** No Morphological Closing **(c)** Applying Morphological Closing



User Interface Changes

Recipe Parameters

The behavior for recipe parameters has been modified.

Remember Recipe Parameters Recipe parameters are now remembered when switching back and forth between different recipes. This mainly affects the **Detector Mask** and **Absorption Segmentation** recipes as there are several recipes to choose from.

Recipe Parameters Reset Recipe parameters can now be reset to their default values. Hover over a recipe to make the **Recipe Reset** option appear next to the recipe drop-down list symbol (Figure 5). Press to reset all recipe parameters to their default values.

Figure 5 Recipe Reset

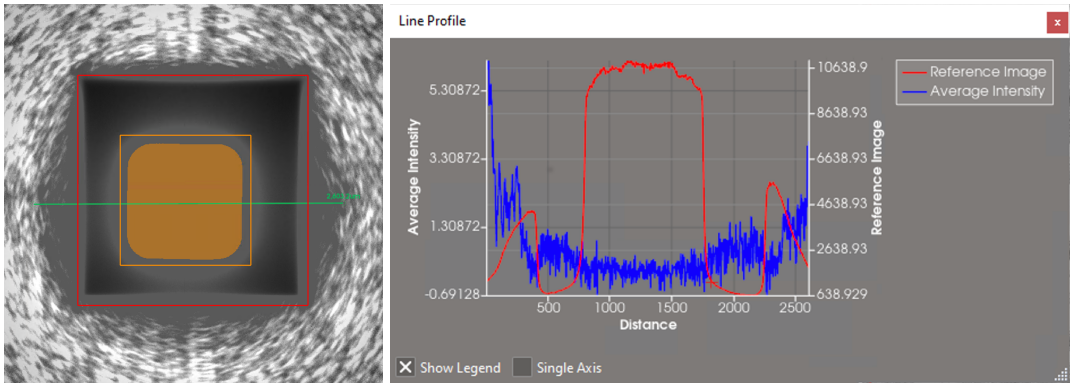
Other Changes

Line Profile Tool The **Line Profile Tool** now shows graphs for all image layers with intensity, see example in Figure 6. Here Figure 6a shows a line profile drawn across the beam stop and aperture region of the **Detector Mask** tab, while Figure 6b

shows the plot of the corresponding graphs for the layers in the plot, namely the *Reference Image* and the *Average Intensity*.

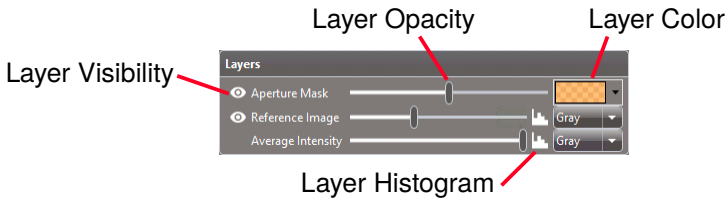
Figure 6 GrainMapper3D Line Profile Tool

(a) Line Profile in Detector Mask **(b)** Plot of Line Profile in Detector Mask



Layer Control A **Layer Histogram** to open the histogram of the corresponding intensity image layer has been added to the **Layer Control** (e.g. Figure 7).

Figure 7 **Layers** Control for DCT Detector Mask Visualization in the **Detector Mask Tab**



Import and Export of Grain Filter Recipes The **Grain Selection Recipes** can now be exported to and imported from JSON-file. Press to export the current project as a human readable JSON-file which can be imported with the import recipes wizard. Press to open the import recipes wizard, browse for the JSON-file and select to import the desired Grain Selection recipe (Figure 8).

Figure 8 Import Grain Selection Recipes

Absorption Preview The labels **Visible slice** and **Cropping** have been added to the sliders of the absorption import preview.

License ID Any label **User ID** has been renamed to **License ID**.

New Preferences A preference to set the preferred **Date and Time** format throughout the program has been added.

DCT Acquisition Wizard

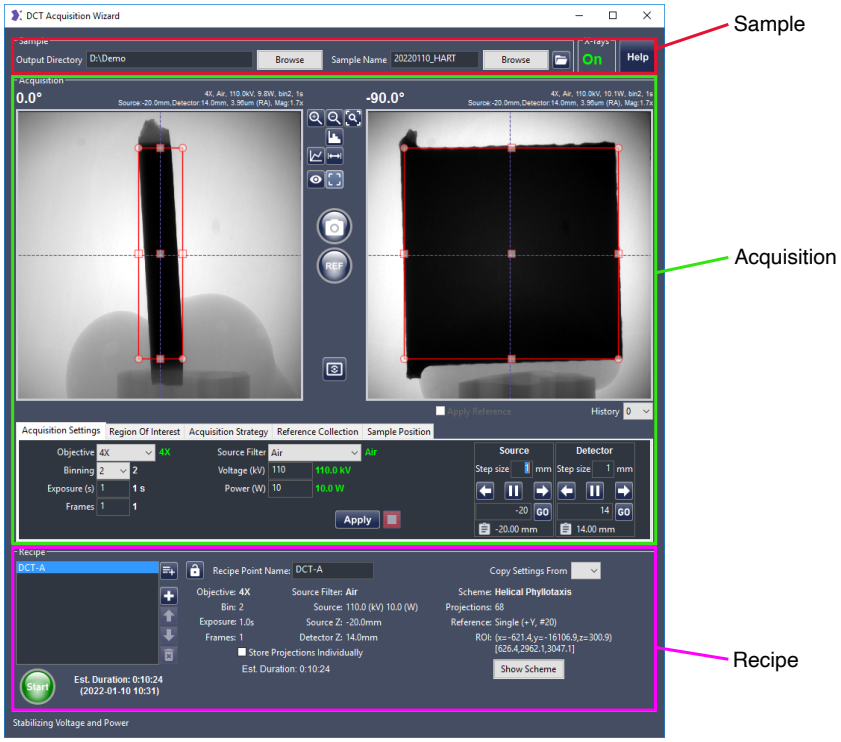
> The DCT Acquisition Wizard is only to be installed on the primary workstation by ZEISS Service.

New Features and Product Enhancements

Introduced with GrainMapper3D 3.0, the DCT Acquisition Wizard is the tool to set up an advanced acquisition DCT scan. The layout of the DCT Acquisition Wizard has been revised in order to accommodate new tools and features and to adapt the *look and feel* of the Scout-and-Scan control system more.

Figure 9 shows the updated layout of the **DCT Acquisition Wizard** with revised image display controls and the new tabs **Region of Interest** and **Reference Collection** in the **Acquisition Section**. The **Acquisition Options** tab has been removed.

Figure 9 Revised Layout of the DCT Acquisition Wizard

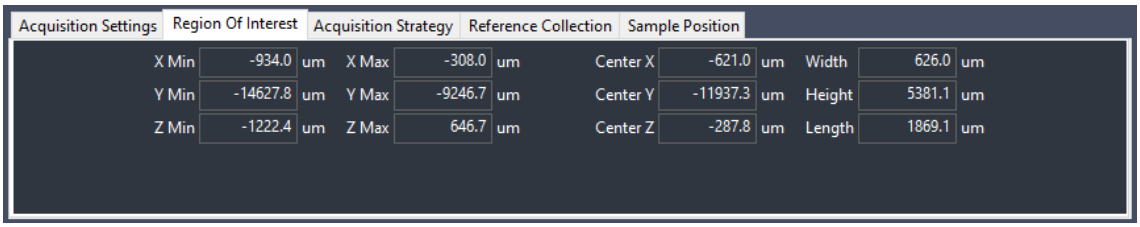


Region of Interest

The **Region Of Interest** (ROI) can now be defined in two different ways, either by dragging rectangles on top of the 0° and –90° absorption projections to cover the

desired sample ROI as illustrated in Figure 9, or using the new **Region Of Interest** tab (Figure 10) that allows direct manipulation of the acquisition ROI by editing either the boundaries of the ROI (left columns) or the ROI center and extent (right columns). The rectangles defining the ROI will update accordingly.

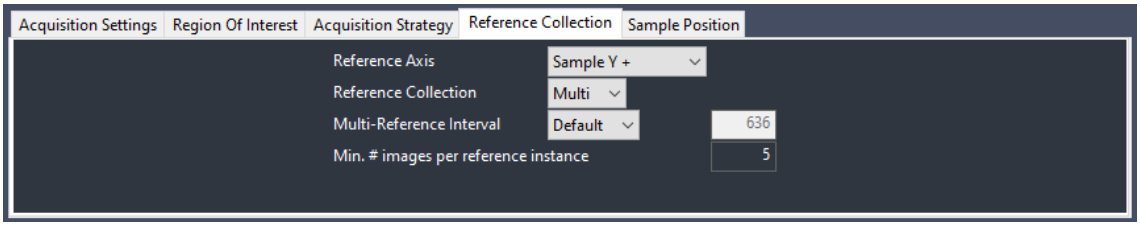
Figure 10 Defining the **Region of Interest** in the **DCT Acquisition Wizard**



Reference Collection

The **Acquisition Options** tab has been replaced by the new **Reference Collection** tab shown in Figure 11. The functionally detailed in Table 1 resembles the one of the **Reference for Scouts** tab within **Scout** view and the Reference Collection modes of the **Advanced Acquisition** tab within the **Scan** view of the Scout-and-Scan control system.

Figure 11 Typical **Reference Collection** tab



Reference Axis The default direction for moving a sample out of the FOV to collect a DCT reference is **Sample Y+** (sample moves down). If the sample is too tall to move out of the FOV as shown in Figure 12a, the **Reference Axis** can now be changed to **Sample Z+**, **Sample Z-**, **Sample X+** or **Sample X-** (*c.f.* Table 2) such that a proper reference can be collected as shown in Figure 12b.

Multi-Reference Collection When performing long scans exceeding 400 diffraction contract patterns or taking longer than 12h, collecting multiple reference instances may improve data quality.

Refer to sub-section *"Set the Reference Collection Mode"* of section *"Setting up an Advanced DCT Scan using the DCT Acquisition Wizard"* of the GrainMapper3D User's Guide for detailed instructions.

Figure 12 Example of Poor and Good **Reference Axis** for Plate-like Sample

(a) Poor Reference Axis Sample Y+ **(b)** Good Reference Axis Sample X+

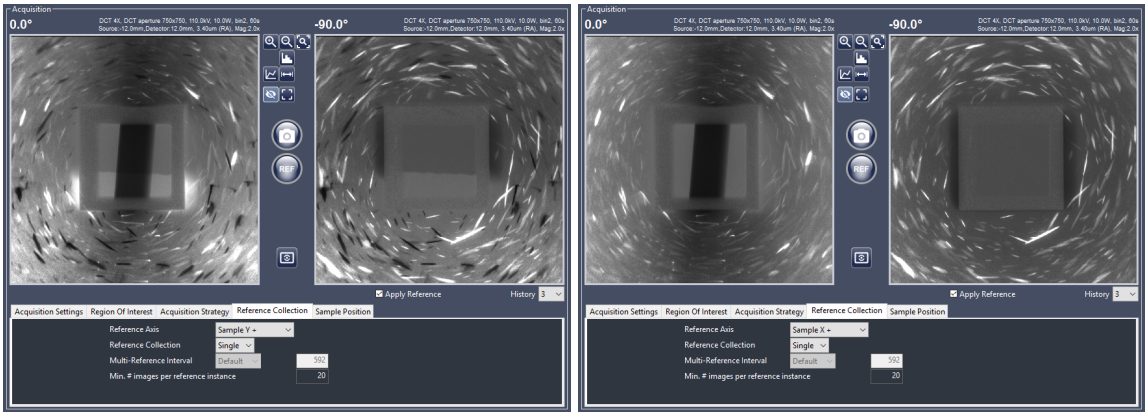


Table 1 Controls of the Reference Collection Tab

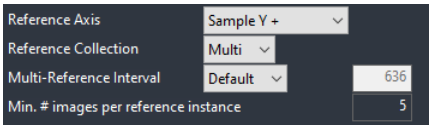
Control	Function
	**Reference Axis**, choose from the drop-down list box the sample reference axis **Sample Z+**, **Sample Z-**, **Sample Y+**, **Sample X+** or **Sample X-** to be used for the currently selected recipe point, refer to Table 2. **Reference Collection**, choose from the drop-down list box the type of reference to collect: • **Single**, to be performed before the scan starts • **Multi**, to be performed before the scan starts and every time the number of Projections specified by the **Multi-Reference Interval** has been acquired. • **None**. **Multi-Reference Interval**, enabled when selected **Reference Collection** mode is **Multi**. Choose from the drop-down list box between: • **Default** (25% of the total number of projections) • **Custom**, type a number into the text box **Min. # images per reference instance**, type the number of references to average.

Table 2 Reference Axis Parameters

Reference Axis	Sample Movement	Description
Sample X+	Moves the **Sample Theta** axis to 0°, and then moves the **Sample X** axis to its positive limit.	Useful for plate-like samples where the height exceeds the travel available to the Sample Y stage and the long side of the sample is aligned with the Sample Z axis.
Sample X-	Moves the **Sample Theta** axis to 0°, and then moves the **Sample X** axis to its negative limit.	
Sample Y+	Moves the **Sample Y** axis to the positive (“most downward”) limit.	Useful for samples where the tip of the sample can be moved out of the aperture FOV with the available Sample Y
Sample Z-	Moves the **Sample Theta** axis to -90°, and then moves the **Sample Z** axis to its negative limit.	Useful for plate-like samples where the height exceeds the travel available to the Sample Y stage and the long side of the sample is aligned with the Sample X axis.
Sample Z+	Moves the **Sample Theta** axis to -90°, and then moves the **Sample Z** axis to its positive limit.	

Other Enhancements

Import and Export of Recipe Points Press  next to the list of *recipe points* to import *recipe points* from an existing **.dctrcp* file. A file dialogue opens, locate the file and press **Open**. The imported recipe points will be appended to the list of recipe points. When performing a scan, the DCT Acquisition Wizard now stores a copy of the used *recipe* in the scan folder.

Safer Sample Movements Handling larger samples within close distances can be challenging. Besides utilizing the *collision avoidance* with ZEISS SmartShield, the DCT Acquisition Wizard now allows to immediately stop any motion from within the user interface, in particular when collecting the two perpendicular projections at 0° and –90° or a reference projection.

Visual Light The visual light inside the instrument is now turned on after a scan is complete or aborted.

User Interface Changes

General Controls The layout and appearance of the general controls of the **Acquisition Section** listed in Table 3 has been updated to accommodate the added functionally.

Image View The image view now supports zooming of the image. To zoom in or out to a desired level of zoom, focus a view and roll the mouse wheel away from you to zoom in on, or toward you to zoom out of, the image. Alternatively, right-click into the view and select **Zoom In**, **Zoom Out** or **Reset Zoom** from the drop-down or use the corresponding buttons , , or as described in Table 3.

The image view now has crosshairs to easily see the image center also when zoomed in (Figure 9). Right-click into the view and toggle on/off **Show Crosshair** from the drop-down to show/hide the crosshairs.

A measurement tool has been added. Handles have been added to the line of the line profile tool. Click and hold onto a handle of the line to drag the line to another position.

When a reference has been collected, transmission values are now displayed as percentages rather than as fractions in the histogram or line profile.

Power Range Whenever changing the **Voltage**, the available **Power** range will be displayed underneath the text input field.

Help Click Help in the upper right of the **Sample** section to access the GrainMapper3D User's Guide on the primary workstation.

Projection Navigation When a acquisition is in progress, the **Projection Navigation** slider shown in Figure 13 allows you to navigate the acquisition in progress. Clearing the **Show Last** check box allows you to use the slider to navigate the acquired projections.

Figure 13 Projection Navigation Slider and **Show Last** Check Box

Table 3 General Controls

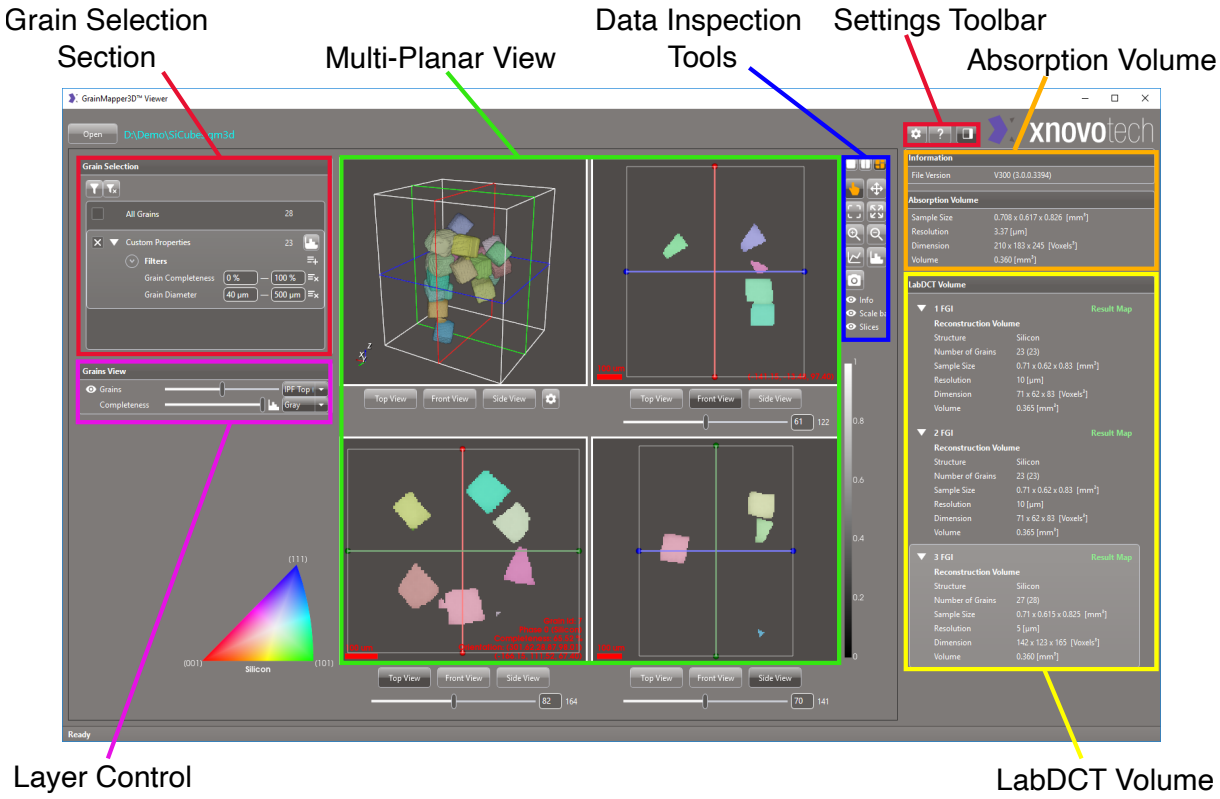
Control	Function
	Click **Zoom In** or **Zoom Out** to enlarge or shrink the data in the views. Click **Reset Zoom** to reset the zoom. Click **Histogram** to open the **Histogram Dialogue** of the view. Click **Line Profile** to enable the line profile tool. In a view press and hold left mouse button and draw a line. Release left mouse. Click **Measure** to enable the measurement tool. In a view press and hold left mouse button and draw a line. Release left mouse. Toggle the **Show Annotation** button to show or hide all annotations. Toggle the **Region of Interest** button to show or hide the rectangular ROI annotations.
	Click to collect two projections at Sample Theta 0° and -90°. The button changes to during imaging, which can be clicked if you need to abort. **The sample will be rotated to the 0° and -90° Sample Theta positions. Please check for potential risk of collision beforehand.**
	Click to collect a single reference projection with the currently selected reference axis (*c.f.* Table 1 and Table 2). The button changes to during imaging, which can be clicked if you need to abort. **The sample will be moved to the reference position specified. Please check for potential risk of collision beforehand.**
	Click to center the sample to the ROI center of the currently selected recipe point.

GrainMapper3D Viewer

New Features and Product Enhancements

Grain Selection The GrainMapper3D Viewer now supports the same grain selection capabilities as known from the Inspection tab of the GrainMapper3D. The available recipes for creating grain selections are listed in Table 4. In order to accommodate the functionality the layout of the main window has been changed as shown in Figure 14.

Figure 14 Layout of the GrainMapper3D Viewer



Documentation A dedicated GrainMapper3D Viewer User's Guide has been added. Press ? in the **Settings Toolbar** access the documentation.

Preferences The support of **Preferences** as listed in Table 5 has been added.

Table 4 Grain Selection Controls

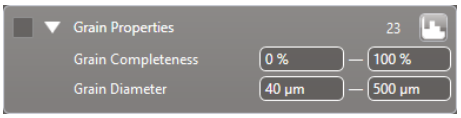
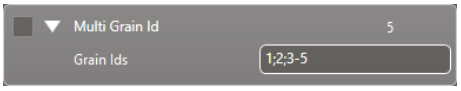
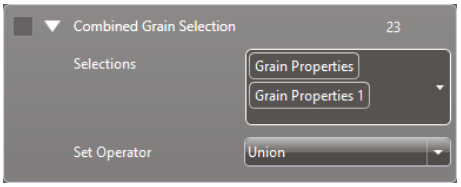
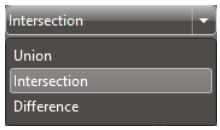
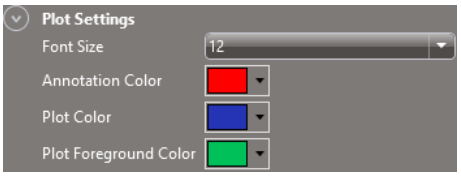
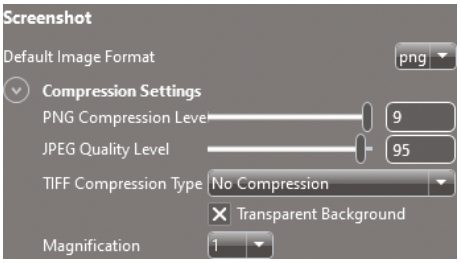
Control	Function
	Press **Add Selection** and choose a selection method from the drop-down. Select a selection from the grain selection list and press **Remove Selection**.
	**All Grains** selects all grains in the reconstruction.
	**Grain Properties** selects all grains with: • **Grain Completeness** inside specified range • **Grain Diameter** (ESD) inside specified range
	**Multi Grain Id** selects all grains with: • **Grain Ids** listed in the text field. Use '**;**' in order to enter multiple grain ids. Use '-' to select a range of grain ids
 	**Combined Grain Selection** enables combinations of grain selections: • In order to add a grain selection press the drop-down of the **Selections** parameter and select two or more selections in the list • **Set Operator** for grain selection combination, either: – **Union** of grains in all selections – **Intersection** of grains in all selections, or – **Difference** (selection1–selection2)

Table 5 Settings Toolbar and Preferences

Control	Function
	Press to open the **Preferences**. Press to get **Help**. Press to maximize the **Multi-Planar View** and hide the **Absorption Volume** and **LabDCT Volume** information.
	Set the **Font Size** on all 2D and 3D Plots. Select **Annotation Color** to change the color of the scale bar and info text in the plot. Choose **Plot Color** to change the color of *e.g.* Histograms. Choose **Plot Foreground Color** to change the color *e.g.* for the Line Profile.
	Choose a **Default Image Format** from the drop-down list to be **png**, **jpg**, **bmp** or **tiff** when creating a screenshot. Adjust compression settings if required. Screenshots will have the size of the current display. Choose a **Magnification** in order to enlarge the screenshot by given factor.

User Interface Changes

Besides the aforementioned changes to the main window layout *(*Figure 14), the Multi-Planar View (MPV) can now be maximized by pressing to collapse the right side bar containing information about the **Absorption Volume** and **LabDCT Volume**. If the opened file is a *GrainMapper3D Project File (*.gm3d)* containing several reconstructions these will all be listed in the **LabDCT Volume** info. From the displayed metadata, select the reconstruction you want to inspect by pressing it. The corresponding grain map will appear in the MPV.

GrainMapper3D™
Release Notes

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