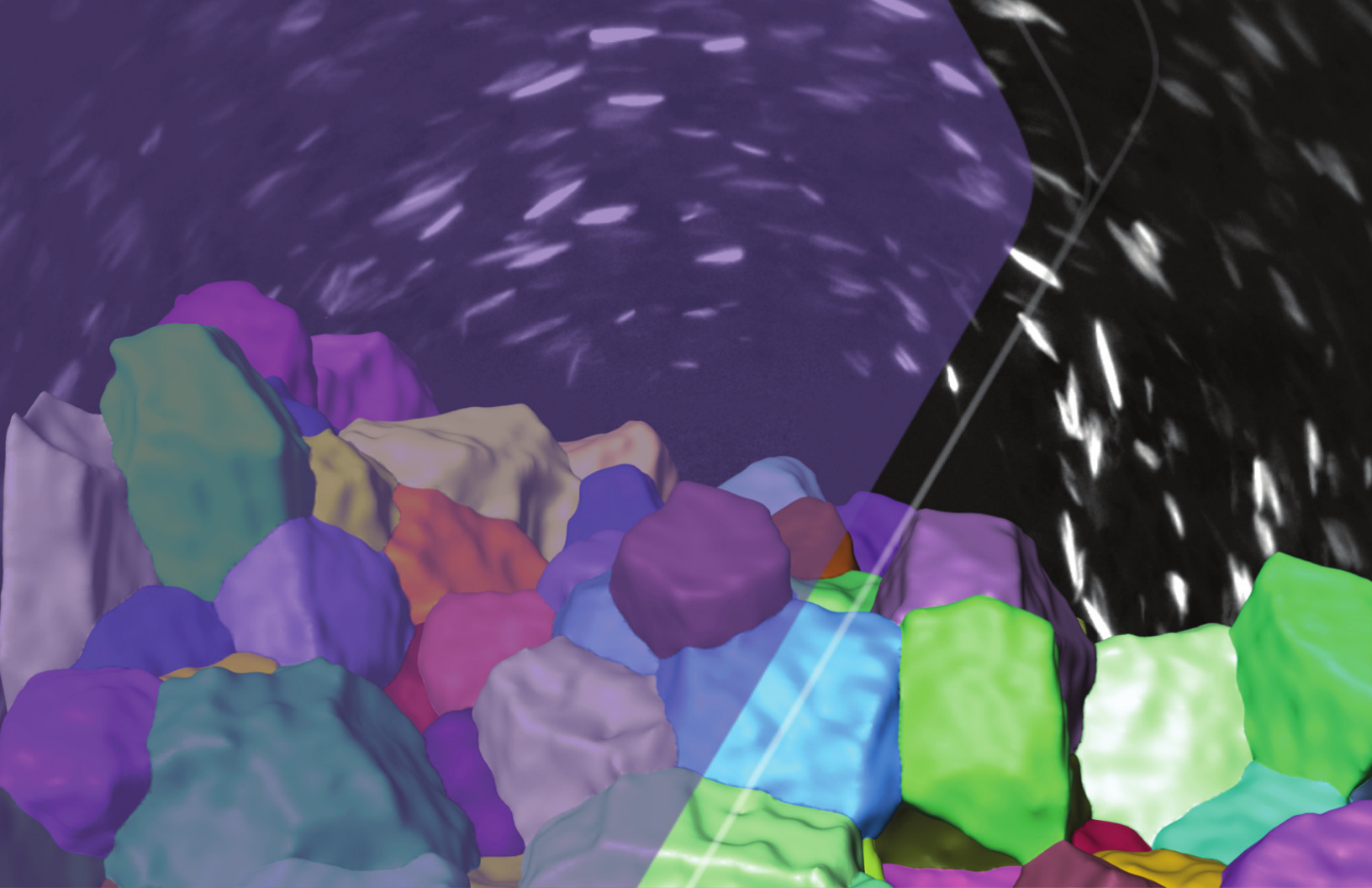




Release Notes

GrainMapper3D™ 4.1

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

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GrainMapper3D

New Features

GrainMapper3D 4.1 centers around tools enhancing the reconstruction capabilities for complex single- and multi-phase samples.

External Absorption Mask

GrainMapper3D Result File The *GrainMapper3D Result File* serves as an exchange format to provide a general interface for absorption masks created with external applications. To import a mask on the **Absorption Mask** tab, select in the corresponding section the **GrainMapper3D Result File** recipe (Table 1) from the drop-down and press **Browse** to locate the file. Using an external absorption mask gives access to more sophisticated segmentation tools, such as histogrammic segmentation or AI. Also, absorption masks with up to 255 labels are supported.

Figure 1 Illustration of Importing Multi-ROIs from Dragonfly 3D World ZEISS Edition

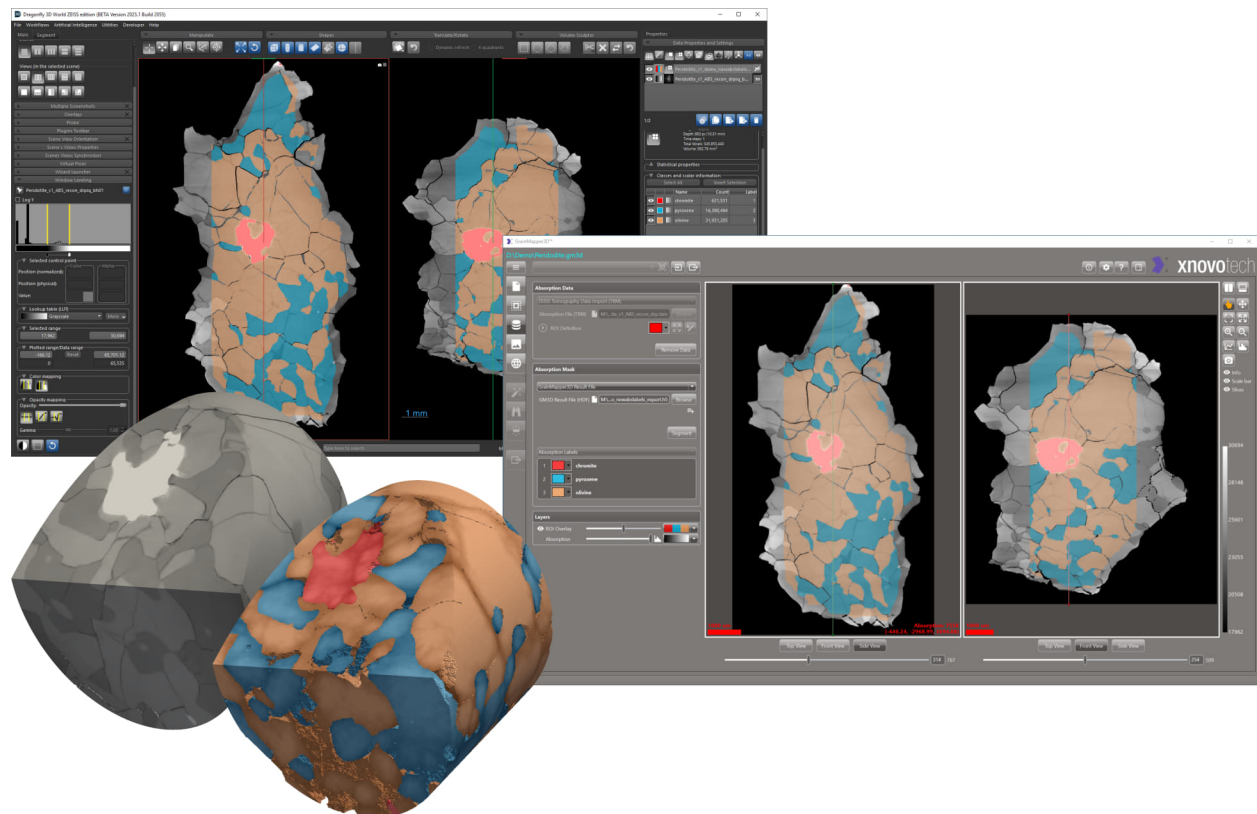
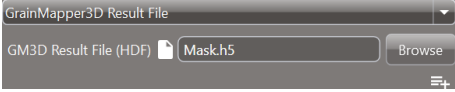


Table 1 Controls of Absorption Mask Tab

Control	Function
	GrainMapper3D Result File loads an Absorption Mask stored in a GrainMapper3D Result File. Press Browse to locate the result file in the file dialog. If the storage path of the project file changed, also refer to “Missing Files Dialog”.

Dragonfly 3D World ZEISS Edition 2025.1 Integration To facilitate workflows like depicted in [Figure 1](#), we have incorporated the option into Dragonfly to export a ROI or Multi-ROI to the GrainMapper3D Result File format, see [Figure 2a](#). Please note that the **TXM axis transformation** ([Figure 2b](#)) must be set correctly to avoid potential issues, if a non-standard convention was used when importing the absorption volume.

For more detailed instructions on how to import and segment an absorption volume in Dragonfly and export it back to GrainMapper3D, please refer to the chapter “Creating an Absorption Mask in Dragonfly 3D World ZEISS Edition” in the GrainMapper3D User’s Guide.

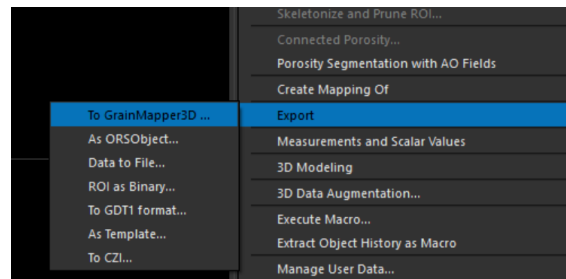
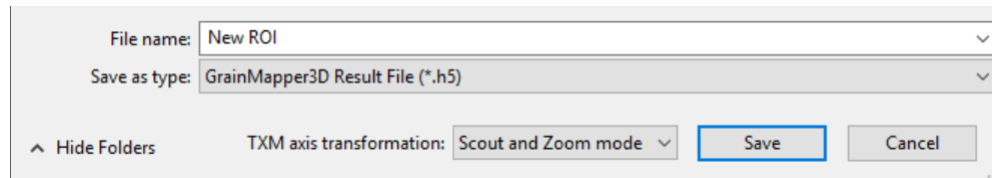
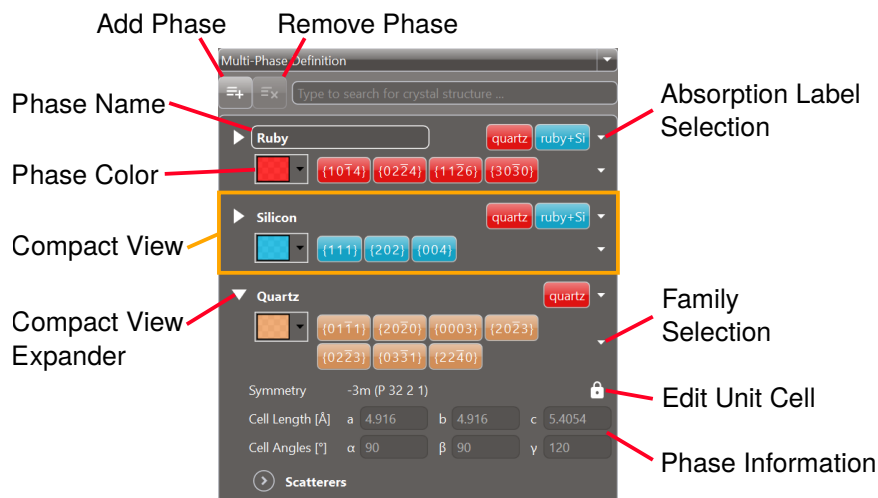
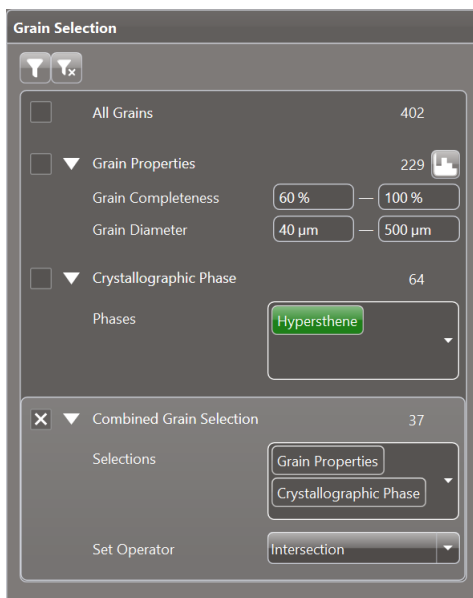
Figure 2 Export a ROI to GrainMapper3D**(a)** ROI Export Context Menu**(b)** GrainMapper3D Result File Export Options

Figure 4 Controls of **Multi-Phase Definition****Table 2** Family Selection Controls of Reconstruction Tab

Control	Function
	Family Selection drop-down allows to specify which families of hkl reflections to use for indexing. By default, the families of hkl reflections with highest structure factors are preselected until their multiplicities sum up to >30. Press to Compute completeness for each family of hkl reflections based on the current reconstruction of this phase. To change the selection of families of hkl reflections: - Click a family in the list to select or deselect it, - Press to Select all families, - Press to Select default families, - Press to Select recommended families, or - Press to Clear selection of families. To customize the family selection: - Click on the column header to sort the families of hkl reflections by multiplicity $M[\#]$, structure factor $F ^2/V_c$, d-spacing $d[\text{\AA}]$, completeness $c[\%]$, or recommendation. - Enter the smallest structure factor, d-spacing or completeness below the columns to expand or shorten the displayed list of families of <i>hkl</i> reflections. - Press to Revert to default list of families.

Unit Cell Fitting Once grains have been defined for a reconstruction, the fitting of cell parameters can then be performed on the **Expert** tab by using the **Fit Unit Cell** recipe in the **Advanced Post Processing** section, refer to [Table 3](#). The fitting procedure requires a grain selection comprising only reliable grains of a single phase. For multi-phase systems, this can be achieved by creating a **Combined Grain Selection** which intersects an adequate **Grain Properties** selection with a single **Crystallographic Phase** selection, for example, as shown in [Figure 5](#).

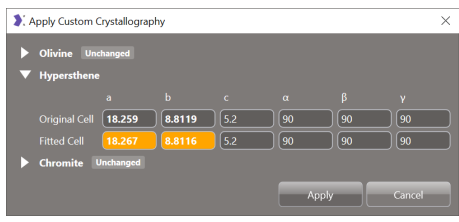
Figure 5 Grain Selection of Single Phase



If the fitting was successful, the **Apply Crystallography** button appears in the **Residual Summary** section. When clicked, the **Apply Custom Crystallography** dialog to review the changed cell parameters appears, refer to [Table 3](#). Confirming the changes navigates to the **Reconstruction** tab, where the new cell parameters are applied.

Please note that altering the unit cell parameters affects the structure factors as distances between scatterers and hence the electron density changes. Also, changing the cell parameters may significantly affect crystallographic orientation and consequently completeness. After fitting or editing unit cell parameters, it is advisable to recheck the completeness of the families of hkl reflections for the new reconstruction and adjust the family selection if applicable.

Table 3 Controls of Expert Tab (new)

Control	Function
	Fit Unit Cell performs a fitting of unit cell parameters, grain orientations and grain centroids of selected grains from one phase at the time, minimizing residuals between observed diffraction spot centroids and forward simulated ones. Specify Spot Distance to restrict the matching between forward simulated and observed spot centroids to a given distance.
	Apply Custom Crystallography dialog opens when pressing Apply Crystallography after running Fit Unit Cell: - The Apply Crystallography button only appears if the unit cell is updated during fitting. Changed unit cell parameters are then highlighted in orange. - Press Apply to use the fit unit cell parameters. - Press Cancel to cancel.

Product Enhancements

Reconstruction

Pseudo-Symmetry Solver Many crystal structures exhibit pseudo-symmetry. For instance, minerals such as quartz and pyrite. When indexing a diffraction contrast pattern to determine the crystallographic orientation, the symmetry of the pattern appears to be higher and a unique solution can not be assigned, but two or more indexing solutions appear to fit, as they show approximately the same level of completeness. This can lead to indexing artifacts in the resulting grain map, like speckle. Typically, these speckled grains expose a fixed misorientation relationship, which in some cases may erroneously be interpreted as a twinning relationship.

Although families of hkl reflections may not be geometrically distinguishable under the pseudo-symmetry operation, they often differ in intensity as their structure factors can vary. Hence, when segmenting the patterns, this variation leads to a tangible difference of statistical nature. To overcome pseudo-symmetry, in the past the appropriate selection of families of hkl reflections had to be specified manually. Now, the indexing algorithm automatically accounts for potential pseudo-symmetric solutions. The most probable orientation solution is determined by applying the symmetry operations listed in [Table 4](#) and considering the relevant hkl reflections.

Recommended Reconstruction Volume The new **Recommended Volume** preset ROI option on the **Reconstruction** tab selects the minimum box to fit the intersection

Table 4 Pseudo-Symmetric Operations

Laue Class	Bravais lattices	Apparent Laue Class	Symmetry Operation
4/m	tP, tI	4/mmm	[100] \ 180°
$\bar{3}$	hP, hR	6/mmm (if hexagonal setting)	[001] \ 60° and [100] \ 180°
$\bar{3}m$	hP	6/mmm	[001] \ 60°
6/m	hP	6/mmm	[100] \ 180°
$m\bar{3}$	cP, cF, cI	$m\bar{3}m$	[001] \ 90°

of the illuminated volume and the absorption mask. For advanced scans with helical phyllotaxis sample motion, half of the height of the aperture field of view at the top and bottom of the scan are excluded to reduce effects of partial illumination.

Convergence Summary When a crystallographic phase is associated only with specific absorption labels, the convergence summary now only computes the average completeness for involved labels, rather than for all labels.

Unified Detector Mask Recipe

All previous **Detector Mask** recipes containing different combinations of **Illumination** and **Signal Region** have been merged into a single one. The **Illumination** and **Signal Region** for the **Aperture**, **Beam Stop** and **Outer Bounds** are now specified by a drop-down menu with available options listed in [Table 5](#). When importing flat panel data the recipe selects **Circular Outer Bounds** automatically, whereas for DCT 4X data it defaults to **No Outer Bounds**.

The **Signal Mask** is shown in the DCT Data View as a **yellow** layer, together with the **Aperture Mask** as an **orange** layer on top. The signal used for segmentation appears unmasked, as illustrated in [Figure 6](#).

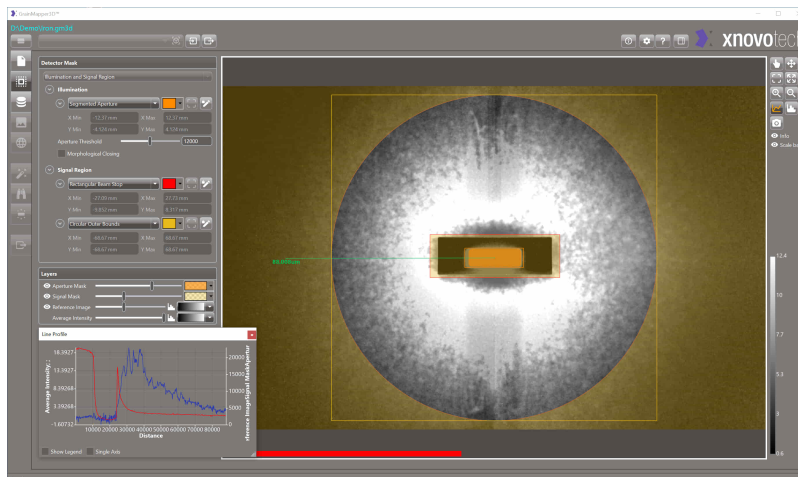
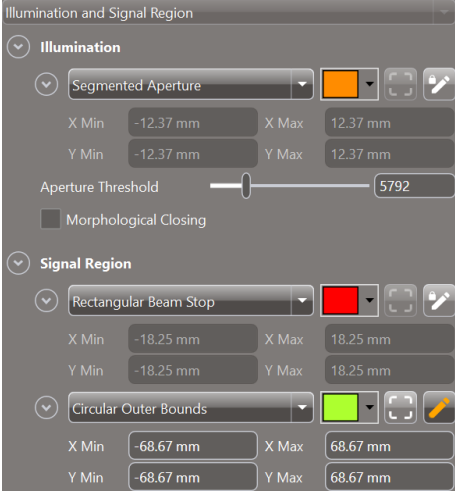
Figure 6 Typical **Detector Mask** Tab Showing Flat Panel Data with **Circular Outer Bounds**.

Table 5 Unified **Detector Mask** Recipes

Control	Function
	Illumination and Signal Region of the DCPs. - Press  to edit either the aperture, beam stop or outer bounds regions. - Press  to select one of the preset region sizes. - Specify the boundaries either by dragging the green box or by typing appropriate values. Illumination region, select from drop-down: Segmented Aperture, if the aperture illumination is visible through the area covered by the beam stop and can be segmented out. - Drag the Aperture Threshold slider or type in the desired threshold value. - Check Morphological Closing to remove holes in the segmented aperture region. Rectangular Aperture, if the aperture illumination is visible but can not be properly segmented. Same as Beam Stop, otherwise. Signal Region inner bounds, select from drop-down: Rectangular Beam Stop, if the region blocked by the beam stop is of rectangular shape. Circular Beam Stop, if the area to be masked fits better within a circle. Signal Region outer bounds, select from drop-down: Rectangular Outer Bounds, if the detector signal towards the edges is noisy and/or very weak. Circular Outer Bounds, if the detector signal towards the edges is noisy and/or very weak and fades radially (default for the Flat Panel detector). No Outer Bounds, otherwise (default for the DCT4X objective). - For Rectangular or Circular outer bounds, the presets for the Flat Panel detector are: - Default Outer Bounds. - Outer Bounds enclosing 50, 60, 70, 80, 90, or 100% of the detected intensity.

User Interface Changes

Multi-Planar View Layout

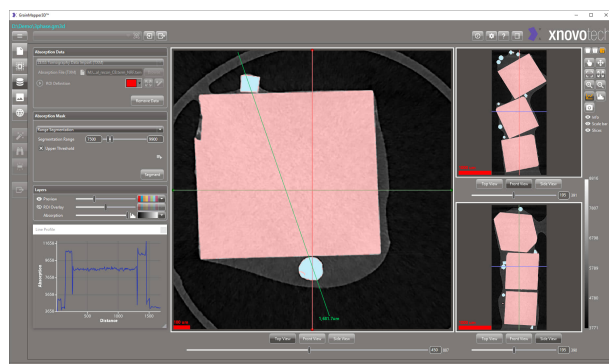
The layout of Multi-Planar Views (MPVs) can now be arranged in more flexible ways, and a focus mode that hides away individual view controls has been added, see [Table 6](#). Two alternative MPV layouts are illustrated in [Figure 7](#).

Table 6 Revised MPV Controls

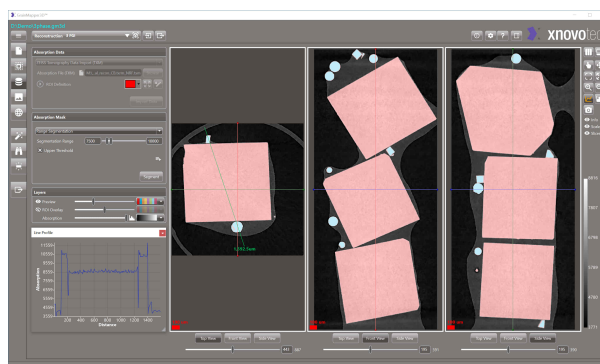
Control	Function
	Display Multi-Planar View for volumetric data.
	Press  to Change Scene Layout . The relevant version of the displayed menus will unfold and allow selecting different Split View Layouts .
	Press  to Hide View Controls below views.
	Press  to Show View Controls below views.

Figure 7 Different MVP Layouts

(a) Default MVP Layout



(b) Alternative MVP Layout Option



Import Recipes

The dialog to import recipes from another *project file* has been revised. The dialog now has a **Recipes Selection Toolbar** to filter and select recipes by type and it shows the currently loaded *project file* on top, see [Figure 8](#).

[Figure 9](#) summarizes the functionality of the toolbar. When opening the import recipes dialog, the **Recipes Type Filter** is set to the current active tab, e.g., when

being on the segmentation tab and opening the dialog, only segmentation recipes will be shown. To import all recipes of another *project file*, press first **Remove Filters** and then **Select All**.

Figure 8 Import Recipes Wizard

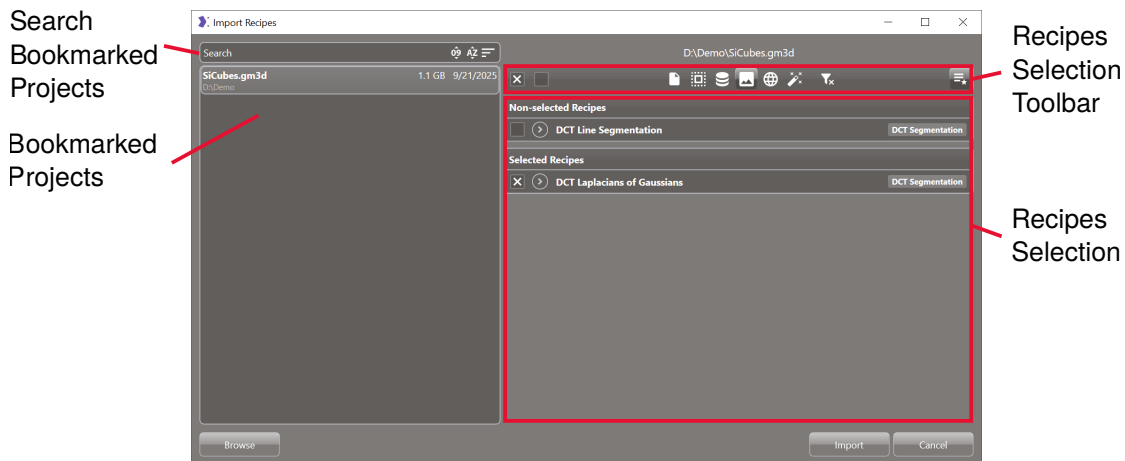
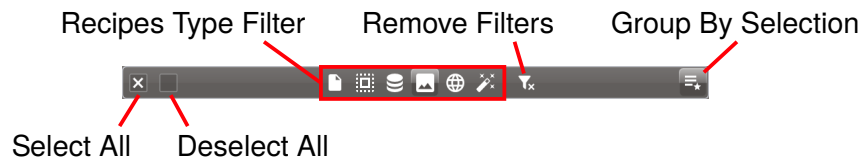


Figure 9 Recipes Selection Toolbar



Other Changes

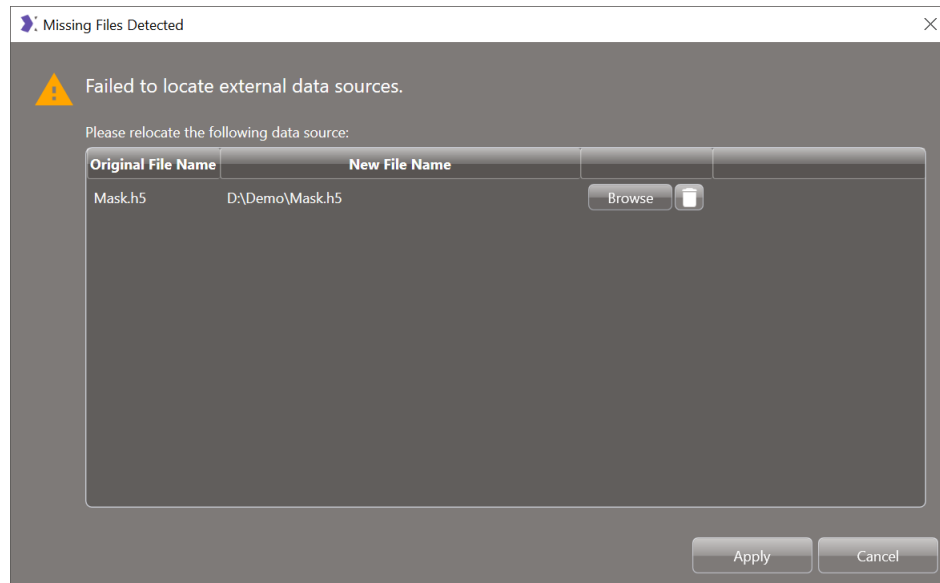
Missing Files Dialog The GrainMapper3D *project file* is self-contained. However, when using external absorption masks, the mask is always loaded from the *result file*. It is only imported temporarily and is not part of the *project file*. This allows to work with different external absorption masks within the same project file.

If the file containing the mask can not be found the **Missing Files Detected** dialog shown in [Figure 10](#) will appear. For each entry in the list, press **Browse** and locate the new file location in the file dialog. Then press **Apply** to accept changes.

Please note, that there are no safety checks whether the file specified is the file that was used for the processing step. Specifying the wrong file may corrupt the already processed results.

DCT Data Import An issue has been resolved where data could not be imported if the *project file* was stored directly on the top-level directory (e.g., D:\Untitled.gm3d). For data collected with Scout-and-Scan 11 or prior, an issue where sample positions were not loaded correctly has been fixed.

Figure 10 Missing Files Detected Dialog



Absorption Data Import An issue has been resolved where cropped absorption tomography data created with ZEN navx or ZEISS ART could not be imported. In addition, binned and cropped data created with Scount-and-Scan Reconstructor 16.x and prior can no longer be imported due to an anomaly in the sample mean position.

Export Absorption Mask The option to store absorption data or absorption mask into the *GrainMapper3D Result File* has been added.

Histogram Layers When opening the histogram from the **Data Inspection Tools**, the histogram of the top-most visible layer will be shown by default, and the drop-down can be used to show the histogram of another layer.

GrainMapper3D Viewer

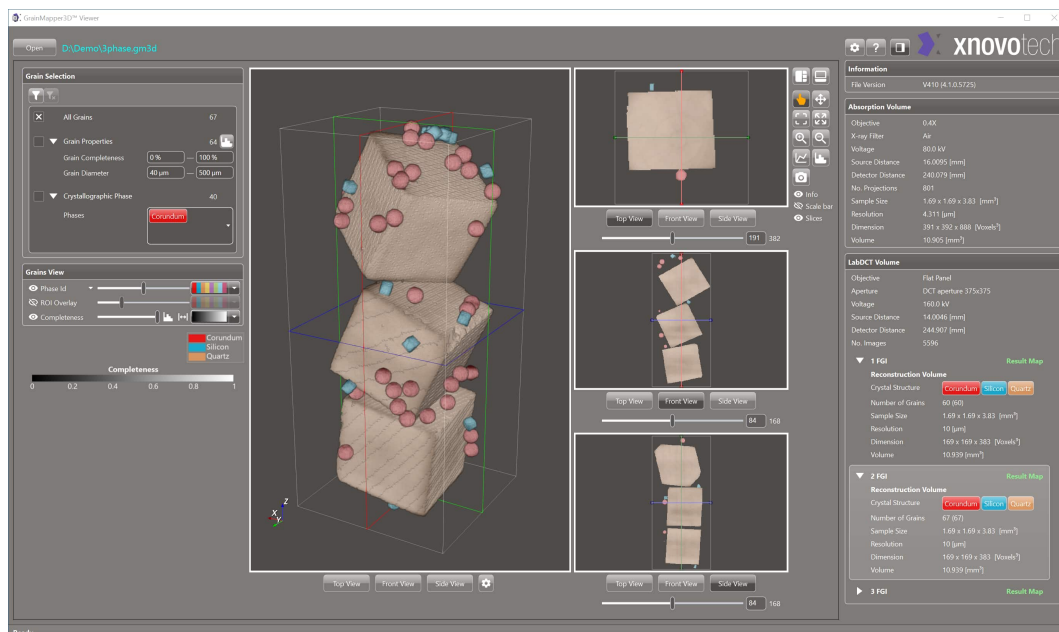
GrainMapper3D Viewer 4.1 features a few updates in line with GrainMapper3D 4.1 updates, namely:

User Interface Changes

Multi-Planar View Layout

The layout of the Multi-Planar Views (MPVs) can now be arranged in more flexible ways around the 3D view, for example as shown in [Figure 11](#). A focus mode has been added that hides individual view controls. Refer to [Table 6](#) for a description of the revised controls.

Figure 11 New 3-1 Scene Layout



DCT Acquisition Wizard

New Features and Product Enhancements

Continuous Imaging

Known from the Scout-and-Scan and ZEN navx Control System, continuous imaging allows to rapidly locate the sample and find suitable acquisition settings interactively. Now the DCT Acquisition Wizard got this feature to ease the process of setting up DCT recipe points, too. [Figure 12](#) shows a typical screen for continuous imaging, where the layout changes to a single projection view. The sample can be centered by double-clicking the object in the projection. [Table 7](#) summarizes the control. Please note that it is still recommended to take two perpendicular projections to define the ROI of a scanning scheme.

Figure 12 Typical Continuous Imaging Screen

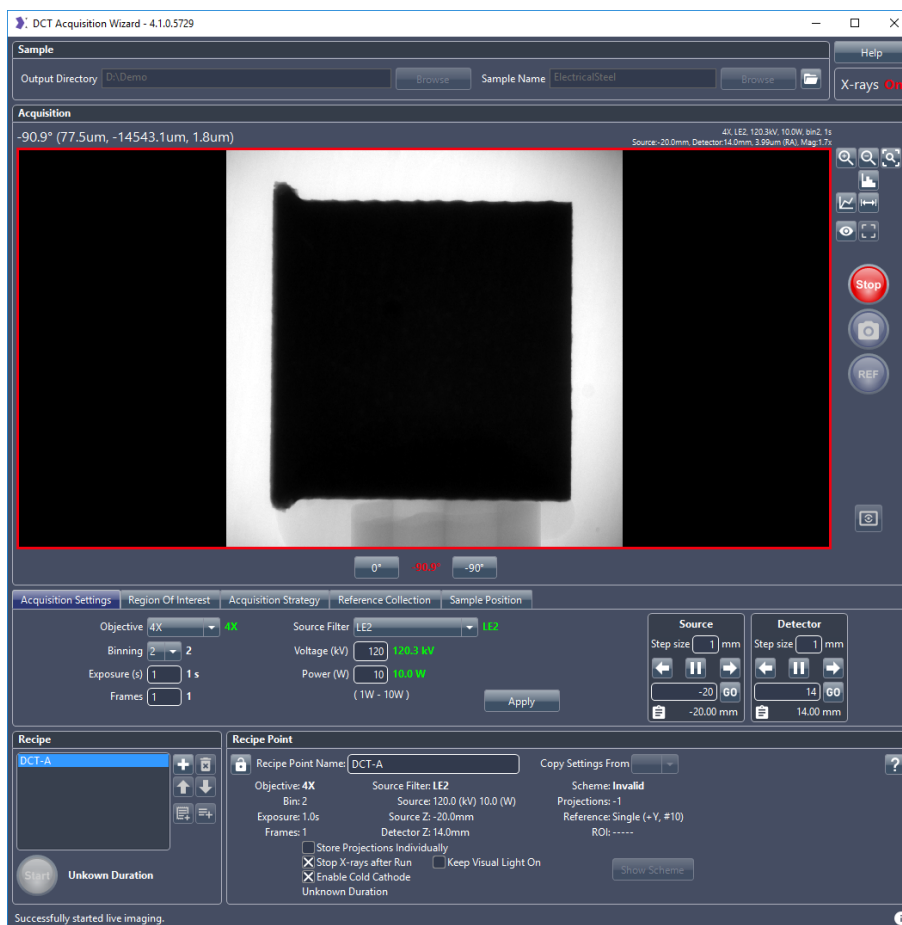
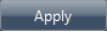
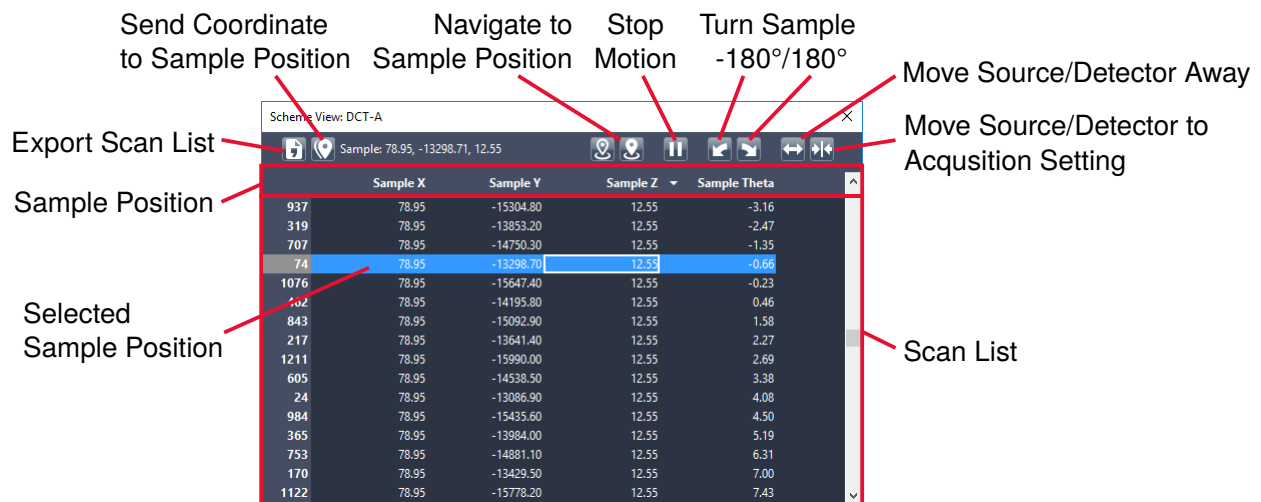


Table 7 General Controls (new)

Control	Function
	Click to start continuous imaging mode. Press  or  to rotate the sample. Choose acquisition settings and press  to accept.
	The button changes to  during continuous imaging. Click to stop continuous imaging.

Scheme View

The dialog listing the sample positions of a recipe point has now been superseded by the **Scheme View** shown in [Figure 13](#). The revised dialog allows to sort sample positions by clicking on the table column header of the sample axis. In addition, the dialog got a toolbar that allows to navigate to sample positions and inspect the sample movements. The navigation controls are explained in [Table 8](#). For samples with irregular shapes, e.g. plate like, this allows to check how close the source and detector can be safely positioned without risking collision at critical angles. Select one or multiple sample positions in the **Scan List** and press **Navigate to Sample Position** to see how the sample moves and adjust working distances accordingly. The navigation tool will traverse the sample positions and can also be used during continuous imaging.

Figure 13 Scheme View

Default Number of Projections

The **Projections** and **Equivalent Projections** of the **Acquisition Strategy** tab now feature a drop-down menu that specifies how the number should be determined.

Table 8 Scheme View Navigation Toolbar

Control	Function
	Scheme View Toolbar Click  to export the scan list to a CSV-file. Click  to send the selected sample position to the motion controls of the Sample Position tab. Click  to move the sample to the selected sample position in the X/Z plane but not vertically. Click  to move the sample to the selected sample position. Click  to abort any motion. Click  or  to turn the sample to -180° or 180° around the rotation axis of the ROI, respectively. Press  to move Source and Detector out by 5 mm. Press  to move Source and Detector to the positions specified in the acquisition settings. If acquisition settings differ from current state, a dialog will ask to confirm apply acquisition settings first.

Refer to [Table 9](#) for details on the available options. Consequently, the user input check boxes have been removed. The new **Default** option calculates the number of (equivalent) projections automatically based on the detector distance.

Cold Cathode Support

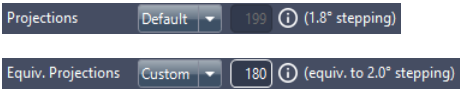
For Xradia 520 Versa, the **Enable Cold Cathode** check box has been added below the **Stop X-rays after Run** in the **Recipe Point** section. The check box is selected by default (recommended), which enables an Cold Cathode mode, an X-ray source mode of operation that increases the X-ray source's life span.

Other Enhancements

User Interface Responsiveness The internal mechanics of the DCT Acquisition Wizard have been overhauled. Previous versions lacked some responsiveness, e.g. when typing into text boxes or using the histogram control to adjust image contrast. These shortcomings have been addressed in favor of a better user experience.

User Interface Appearance When applying **Objective**, **Source Filter**, **Voltage (kV)** or **Power (W)** changes, their current status will now blink **red** during the change. Also, the **X-rays** status indicator will blink when changing status and has adapted the same **On/Off** colors like the microscope control system. In addition, the appearance of some controls on high-DPI screens have been improved.

Table 9 Controls of the Acquisition Strategy Tab

Control	Function
	Choose Projections or Equivalent Projections type from the drop-down, either: • Default, to use recommended number depending on the detector distance (hover ⓘ for tabulated values), • Custom, and enter custom number in the text box, or • User, to set vertical or horizontal number of steps and step sizes for the scanning scheme manually. The number of Projections corresponds to a full sample rotation without the last angle and without translation. The number of Equivalent Projections corresponds to the number of vertical steps to move the sample through the vertical aperture FOV.

GrainMapper3D™

Release Notes

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