

Release Notes

GrainMapper3D™ 4.0

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



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GrainMapper3D

New Features

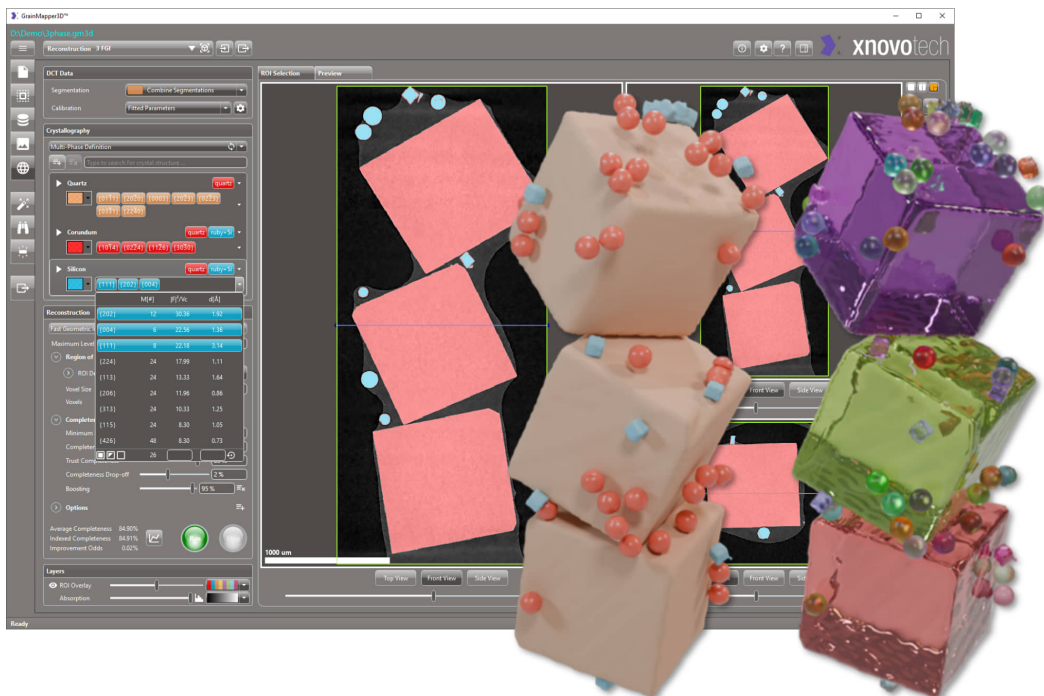
Multi-Phase Indexing

This release of the GrainMapper3D enables the reconstruction of DCT data for more than one crystallographic phase simultaneously.

A multi-phase reconstruction can be carried out in two ways: either by using absorption labels to define the boundaries between the different phases, in cases where the absorption contrast is large enough to distinguish the phases, or by reconstructing multiple phases within the same absorption label, in cases where the absorption contrast of the associated crystallographic phases overlap. In the latter case, the indexing solution of the crystallographic phase with the highest completeness is assigned to each voxel, which makes the selection of HKL families for each phase a vital step.

The **Crystallography** section has been revised and now offers an additional **Multi-Phase Definition** recipe to configure several phases at once as illustrated in [Figure 1](#). The new controls that enable the multi-phase reconstruction workflow are detailed in the following.

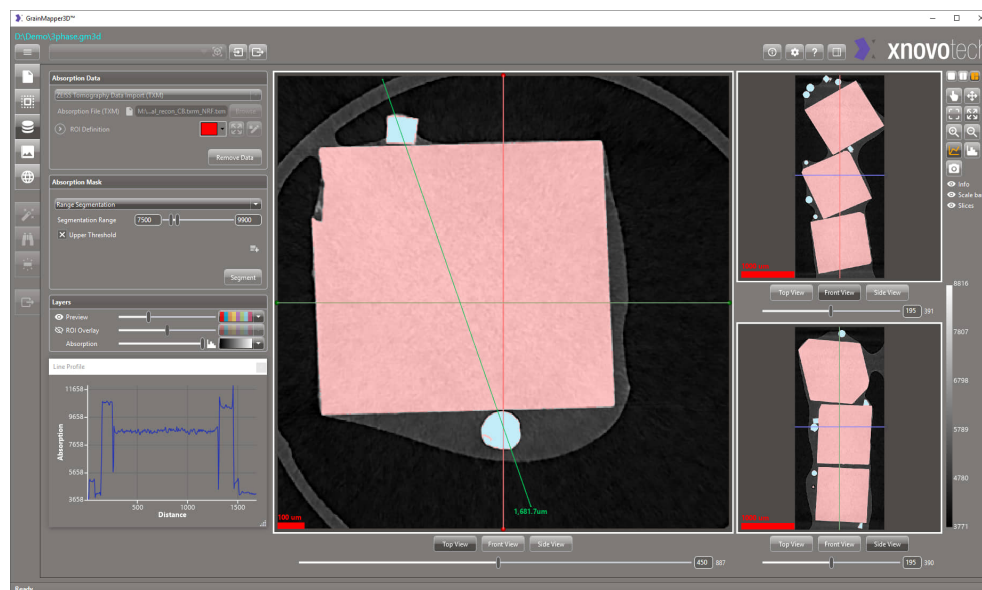
Figure 1 The New Multi-Phase Crystallography Support



Absorption Labels

For multi-phase samples where the phases can be distinguished by absorption contrast, it is now possible to assign **Absorption Labels** when defining an absorption mask. To define absorption labels select the **Range Segmentation** from the drop-down in the **Absorption Mask** section of the **Absorption Mask** tab (Figure 2). Values between the custom defined lower and upper thresholds are considered to be part of *Absorption Label 1*. Check the **Upper Threshold** box to make values above the upper threshold part of *Absorption Label 2*. Please note that the absorption labels are only displayed if the upper threshold is checked. The multi-label absorption segmentation is also shown in the segmentation preview.

Figure 2 Typical Screen for Threshold Determination Using a **Line Profile**



Once the data is segmented with more than one label, the absorption label control shows up (Figure 3). Use the control to customize the names and colors of the absorption labels. The changes to the controls on the Absorption Mask tab are detailed in Table 1.

Figure 3 Absorption Labels

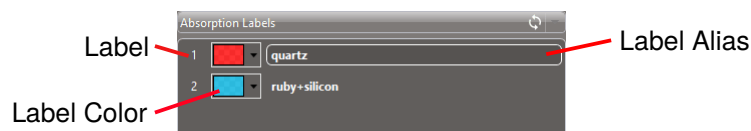

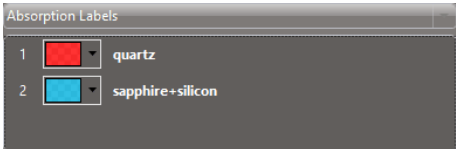



Table 1 New and Revised Controls of **Absorption Mask** Tab

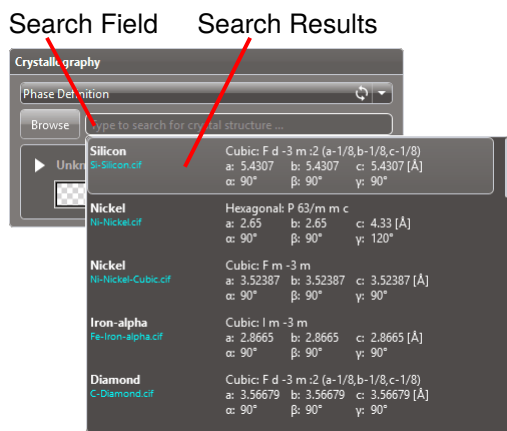
Control	Function
	<p>Range Segmentation performs a threshold segmentation of the absorption volume based on a user specified lower and upper threshold.</p> <ul style="list-style-type: none"> Check Upper Threshold to create a second absorption label for intensities above the upper threshold
	<p>Absorption Labels allows to customize name and appearance of absorption labels. Click the label name to edit it. Use the color picker drop-down to change label color.</p>
	<p>Preview of the Absorption Data: Use the slider to change opacity of the preview. Use the histogram to enhance image contrast of the preview. Use the drop-down to change color of the preview.</p>

Defining Multi-Phase Crystallography

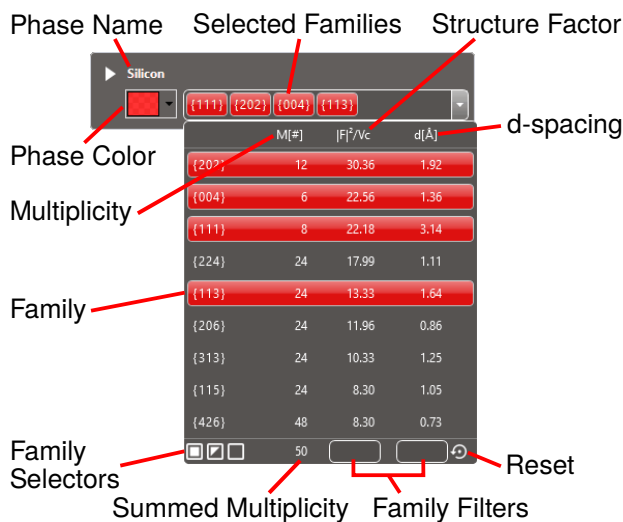
The crystallographic controls have been revised in support of the multi-phase workflow. They offer a unified way of how to set up the single **Phase Definition** and the added **Multi-Phase Definition** recipe as shown in [Figure 4](#) and [Figure 6](#)

Figure 4 Controls of **Phase Definition**

(a) CIF Finder Tool



(b) Selection of HKL Families



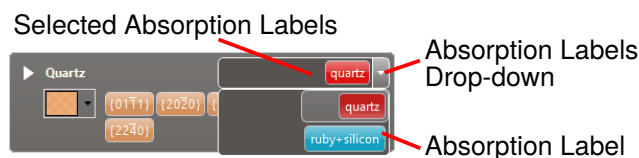
CIF Finder Tool The new **CIF Finder Tool** shown in [Figure 4a](#) allows to quickly find crystallographic information as needed. Enter the phase or file name of the CIF

into the **Search Field** and click the **Search Result** in the result drop-down list to use the CIF found.

Selecting HKL Families The selection of **HKL Families** control (Figure 4b) has been revised and can now be expanded to select arbitrary HKL by entering a structure factor or d-spacing for the **Family Filters**. In addition to that, the structure factor is now normalized by the cell volume to make it comparable between different phases. When selecting lattice planes, the sum of their multiplicity is displayed in the column footer to easily keep track of the total number of reflectors.

Assigning Absorption Labels Assigning absorption labels to crystallographic phases only applies if more than one absorption label exists (Figure 3). Click the **Absorption Label Selection** drop-down button (Figure 5) of the crystallographic phase, and select from the drop-down list the **Absorption Label(s)** to associate with the phase. A phase can be assigned to one or more absorption labels.

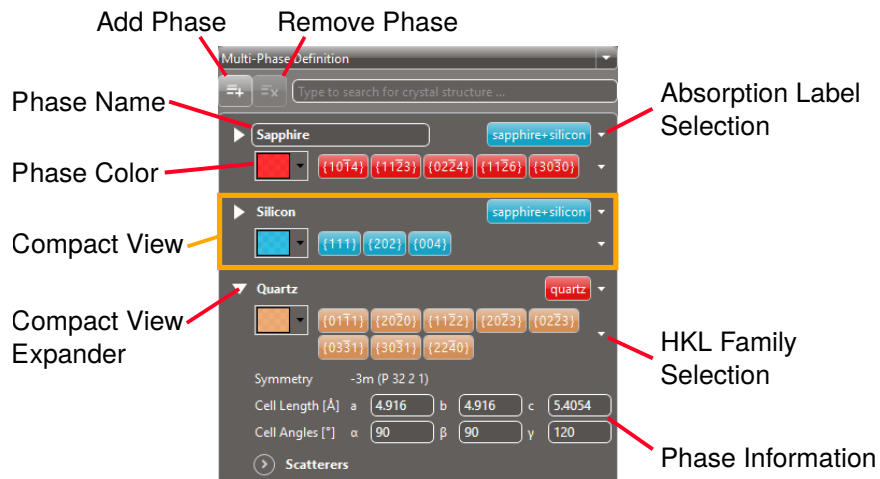
Figure 5 Typical **Absorption Label Selection** control



If no selection is made and multiple absorption labels are available, the **Absorption Label Selection** displays *No ROI Constraint*, and the phase will be assigned to all absorption labels.

Multi-Phase Definition To import multi-phase crystallographic information select **Multi-Phase Definition** in the drop down menu of the **Crystallography** section of the **Reconstruction** tab (Figure 6).

Figure 6 Controls of **Multi-Phase Definition**



Then import the crystallographic information for all the crystallographic phases present in the sample using the **CIF Finder Tool** or locating the CIF from hard disk drive by pressing or dragging the CIFs from the *Windows Explorer* into the multi-phase list below. For each phase, the **Phase Name** can be edited, the **Phase Color** can be changed, and the phases can be dragged around to change the order. To remove a crystallographic phase from the list, select it and press . Refer also to [Table 2](#).

Table 2 New and Revised Controls of the Reconstruction Tab


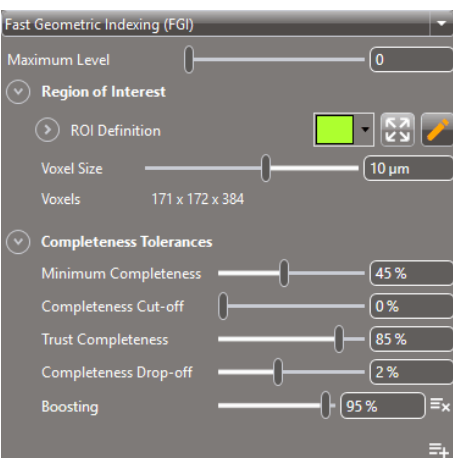
Control	Function
	<p>HKL Families drop-down allows to specify which families of reciprocal lattice planes to use for indexing. By default, the HKL families with the highest structure factor are preselected until their multiplicity sums up to more than 30.</p> <p>To change the selection of HKL families:</p> <ul style="list-style-type: none"> • Click the item in the list to select or deselect a specific HKL family, • Press to Select all HKL families, • Press to Select default HKL families, or • Press to Clear HKL families selection. <p>Click on the column header to sort the HKL families by multiplicity M[#], structure factor $F ^2/Vc$, or d-spacing $d[\text{Å}]$. Enter the smallest structure factor or d-spacing below the columns to expand or shorten the displayed list of HKL families.</p> <p>Press to Revert to default list of HKL families.</p>
	<ul style="list-style-type: none"> • Completeness Tolerances fine tunes the Fast Geometric Indexing (FGI): <ul style="list-style-type: none"> – Completeness Cut-off only fills the reconstruction with completeness values larger than the cut-off. Must be smaller than the minimum completeness.

Table 2 New and Revised Controls of the Reconstruction Tab (*continued*)

Control	Function
	<p>Phase Definition imports the crystal structure from a CIF. To select the CIF, either:</p> <ul style="list-style-type: none"> • Press Browse to locate a file, • Drag the CIF from the <i>Windows Explorer</i> into the phase field, or • Enter a file or phase name into the search field to search the CIF database and click on the search result to select it.
	<p>Multi-Phase Definition imports crystal structures from multiple CIFs to be used for the reconstruction. To add one or multiple CIFs, either:</p> <ul style="list-style-type: none"> • Press Import phase from CIF and locate the files, • Drag the CIFs from the <i>Windows Explorer</i> into the phase list, or • Enter a file or phase name into the search field to search the CIF database and click on the search result to select it. <p>To remove a phase definition from the list, select the phase to be removed and press Remove Phase .</p> <p>Click the Phase Name to edit it per phase. Use the color picker drop-down to change the Phase Color per phase. Use the HKL Families drop-down to change the selection of lattice planes per phase. Use the Absorption Label drop-down to associate a crystallographic phase with one or more absorption labels (if applicable). The default is No ROI Constraint. Drag the phases around to change order.</p>

Grain Selection Filters





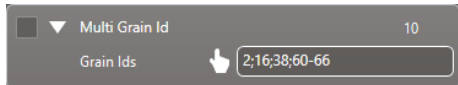


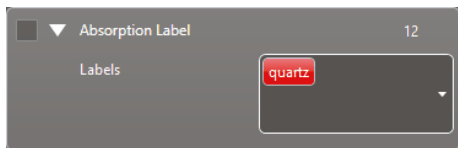
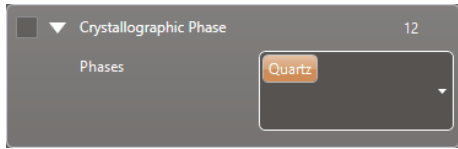
Additional **Grain Selection Filters** to select grains by **Absorption Label** or **Crystallographic Phase** have been added, see [Table 3](#). In addition, when hovering over a *grain selection*, the  symbol appears and allows to center the selection in the **Multi-Planar Grains View**. For faster picking of individual grains, the **Multi Grain Id** filter got a **Pick Grain Ids** tool  that allows to pick a grain of interest directly in either the **Multi-Planar Grains View** or the **Forward Simulation View**.

Table 3 Controls of Inspection Tab

Control	Function
	Hover over a grain selection and press  to center on the grain selection in the Multi-Planar View.
	Multi Grain Id selects all grains with Grain Ids listed in the text field: <ul style="list-style-type: none">• Use ‘;’ in order to enter multiple grain ids.• Use ‘-’ to select a range of grain ids. Press  to activate the Pick Grain Ids tool. When active,  , click on a grain of interest either in the Grains View or the Forward Simulation View to pick its grain id.
	Absorption Label selects all grains associated with the absorption labels specified. Click the drop-down to change selection of absorption labels.
	Crystallographic Phase selects all grains belonging to the phases specified. Click the drop-down to change selection of phases.

Circular Outer Bounds

It is now possible to remove the outer region from the signal region of a diffraction contrast pattern leaving a circular signal mask for detector mask recipes with **Circular Outer Bounds**. Using a detector mask recipe with circular outer bounds is recommended if the detector signal towards the edges is weak or noisy and the detector signal fades radially, which typically applies to DCT data collected for highly absorbing samples, see [Figure 7](#) for an example. The circular outer bounds are similar to the outer bounds both in terms of controls ([Table 4](#)) and looks ([Figure 7](#)), except the circle highlighted by the **Signal Mask Layer** can be larger than the smallest dimension of the detector as exemplified in [Figure 7](#).

Figure 7 Typical **Detector Mask** Tab Showing Flat Panel Data with **Circular Outer Bounds**.

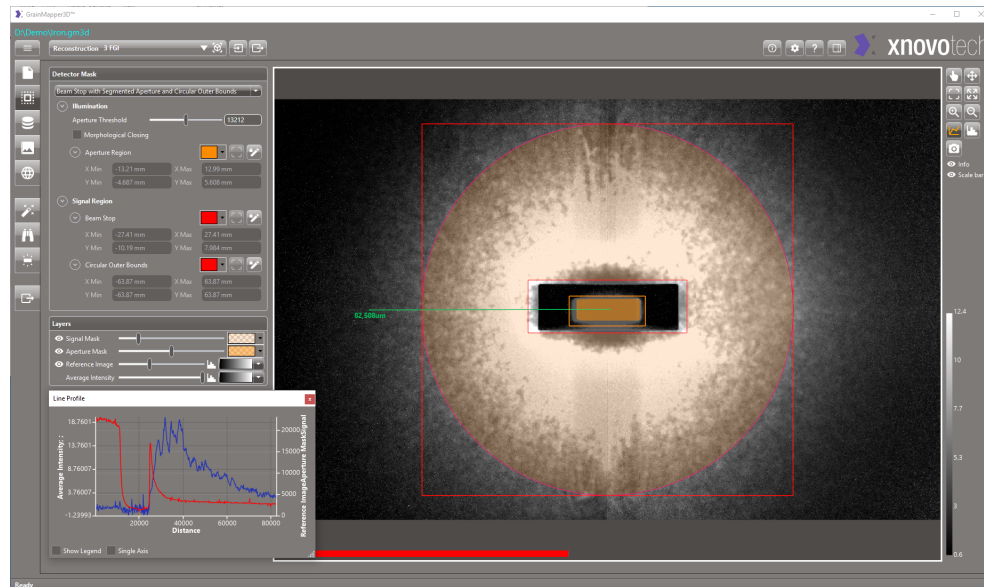



Table 4 New and Revised Controls of Detector Mask Tab

Control	Function
	<p>Define Circular Outer Bounds of the Signal Region if the detector signal towards the edges is noisy and/or very weak and fades radially, either:</p> <ul style="list-style-type: none"> • Press to edit the outer bounds • Press for preset values detector: <ul style="list-style-type: none"> – Default Circular Outer Bound – Circular Outer Bounds enclosing 50, 60, 70, 80, 90, or 100% of the detected intensity • Specify the boundaries of the circular outer bounds
	<p>Use the Layers control to visualize:</p> <ul style="list-style-type: none"> • Average Intensity of all DCPs (bottom, always shown) • Reference Image (middle) • Aperture Mask (top – Segmented Aperture only) • Signal Mask (top – Circular Outer Bounds only) <p>Use the eyes to turn visibility on/off. Use the sliders to change opacity of the layers. Use the histograms to enhance image contrast of the layers. Use the drop-down boxes to change colors of the layers.</p>

Dream3D Export

Besides exporting the reconstruction into a GrainMapper3D Result File, it is now also possible to export the reconstruction as a DREAM3D file. In the **Export** tab, select **Export DREAM.3D / NX File** from the export drop-down. The orientations are converted into the reference frame used by DREAM3D and stored as *Euler Angles* and *Quats*. Both DREAM.3D v6 and DREAM3D-NX v7 are supported. Refer also to [Table 5](#).

Table 5 Controls of Export Tab

Control	Function
	<p>Export DREAM.3D / NX File generates a result file readable by DREAM.3D v6^a or DREAM3D-NX v7^b.</p> <ul style="list-style-type: none">• Press Browse to specify a file output location.• Enter a unique Data Container in order to store several reconstructions into the same file.

^a<https://dream3d.bluequartz.net/>

^b<https://www.dream3d.io/>

Product Enhancements

Revised Indexing Implementation

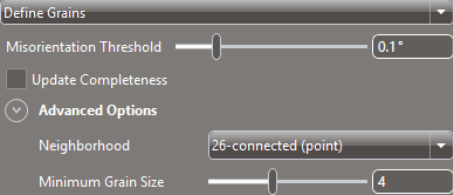
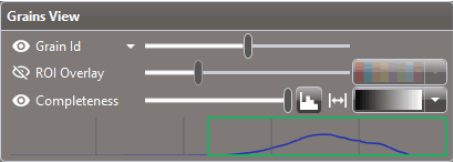
The **Fast Geometric Indexing** implementation has been completely revised to support indexing of multiple crystallographic phases. In particular for large *advanced acquisition* DCT data sets with more than 1000 patterns, GrainMapper3D 4.0 typically reconstructs the same problem in a third or less of the time compared to GrainMapper3D 3.2. As a part of this effort, the maximum number of voxels in the volume has been increased to 2048×2048×2048 down to a minimum permissible voxel size of 0.5 μm.

In addition, an extra **Completeness Cut-off** has been added to the **Completeness Tolerances**, refer to [Table 2](#) for how to use.

More Parameters when Defining Grains

The new **Advanced Options**, **Neighborhood** and **Minimum Grain Size** (refer to [Table 6](#)), allows better control over the **Define Grains** process. For instance, using a more restrictive neighborhood connectivity, *i.e.* 18-connected (point) or 6-connected (face), may help get rid of speckled or fuzzy grain boundaries, and increasing the minimum grain size may remove more small unreliable grains.

Table 6 Revised Controls of Grain Tab

Control	Function
	<p>Define Grains merges regions of adjacent voxels and assigns a new mean orientation and centroid position weighted by completeness.</p> <ul style="list-style-type: none"> • Misorientation Threshold merges adjacent voxels with smaller angular misorientation into the same region. • Check Update Completeness to recompute the completeness based on the newly assigned mean orientation. <p>Advanced Options for Define Grains:</p> <ul style="list-style-type: none"> • Neighborhood sets the voxel connectivity type, either: <ul style="list-style-type: none"> – 26-connected (point): Adjacent voxels share at least one of 6 faces, 12 edges or 8 corners (default), – 18-connected (edge): Adjacent voxels share at least one of 6 faces or 12 edges, or – 6-connected (face): Adjacent voxels share at least one of 6 faces. • Minimum Grain Size removes all grains smaller than the specified number of voxels and replaces by the most frequent neighboring orientation. If Update Completeness is not checked, the completeness will be NaN.
	<p>Use the Grains View control (shared with Inspection Tab) to visualize:</p> <ul style="list-style-type: none"> • Grain properties with the following color code options from the drop-down list (top): <ul style="list-style-type: none"> – Grain Id, (preset colors) – IPF Side (+X), IPF Front (+Y), IPF Top (+Z), (inverse pole figure colors) – Phase Id, (discrete colors) – Grain Completeness, Grain Diameter [um], or Grain Size. (continuous colors) • ROI Overlay (middle, discrete by absorption label), • Completeness map (bottom) <p>Use the eyes to turn visibility on/off. Use the sliders to change opacity of the layers. Use the histograms to enhance contrast by setting min/max. Use the ranges to turn clipping of the continuous colors on/off. Use the colorbar drop-down to change the colormap of a layer.</p>

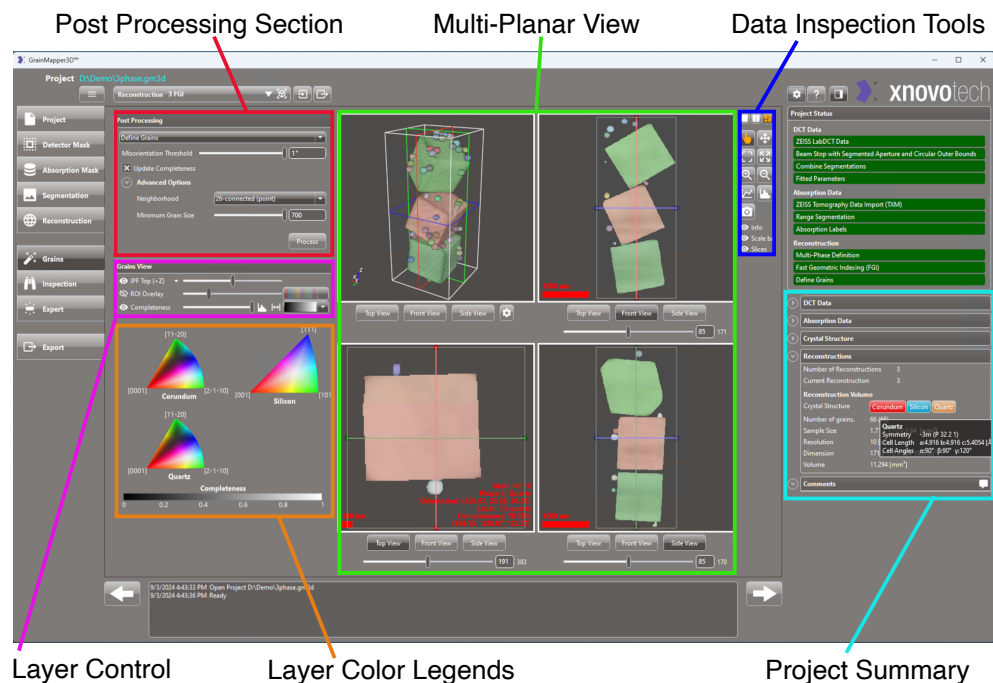
Enhanced Volume Rendering and Controls

A number of enhancements to the volume rendering and associated user controls have been added:

Improved High-DPI Support The support of high-DPI displays has been improved. All 2D and 3D views are now DPI-aware and will scale fonts, line widths and point sizes according to the display scale factor. In addition to that, **Point Size**, **Line Width** and **Font Size** on all plots can be adjusted in the preferential settings (refer to [Table 7](#), [Plot Settings](#)).

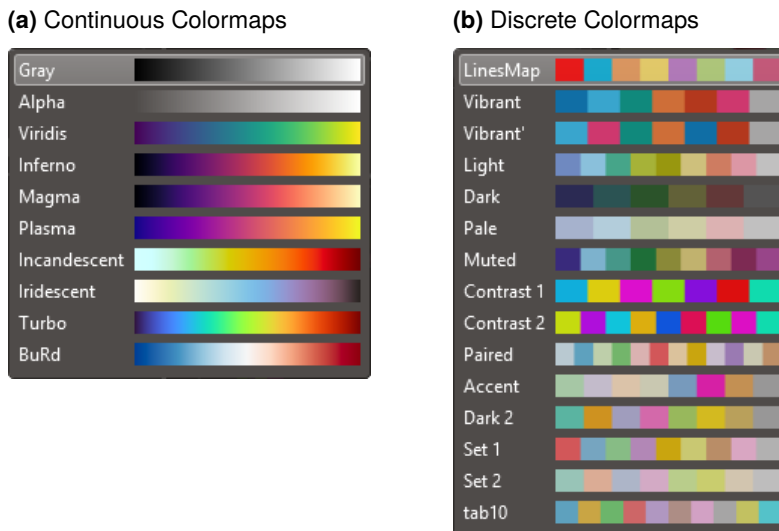
Volume Rendering Quality The way GrainMapper3D computes the color codes for the **Grains View** (refer to [Figure 8](#)) has been revised in order to support rendering of large volumes up to $2048 \times 2048 \times 2048$ voxels. As older graphic cards may not provide enough memory to hold this amount of RGBA data in their memory, the volume will be automatically resampled according to the available memory for visualization purposes. The **Volume Rendering Quality** can be adjusted in the [Preferences](#) ([Table 7](#)).

Figure 8 Grains View with Typical Layer Color Legends



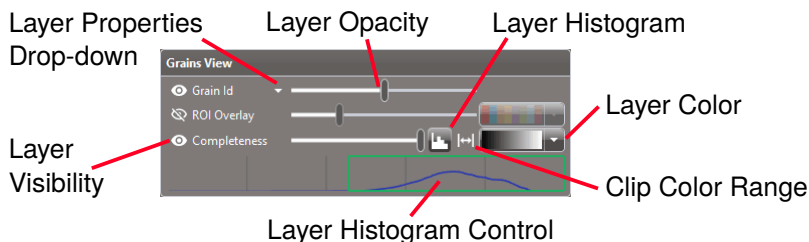
Revised Layer Controls All layer controls using either a discrete or a continuous colormap now have the colormap in the drop-down for intuitive feedback on which colormap is applied to which layer. Some more discrete and continuous colormaps have been added to the existing ones ([Figure 9](#)). Rather than using a pop-up histogram, the histogram can now be shown below the layer to interactively adjust color ranges, see [Figure 10](#). To set the preferential **Plot Settings**, refer to [Table 7](#).

Figure 9 Colormap Drop-downs of the Layer Control



The volume rendering **Layer Controls** in the **Grains View** (Figure 10) now allows enhanced color mixing and supports visualization by more grain properties, namely **Grain Completeness**, **Grain Diameter** and **Grain Size**. In addition, the color range of these properties can be adjusted and clipped. Refer to Table 6 for how to use. The (random) **GrainId Color Code** has been changed.

Figure 10 Grains View Control for Reconstruction Visualization



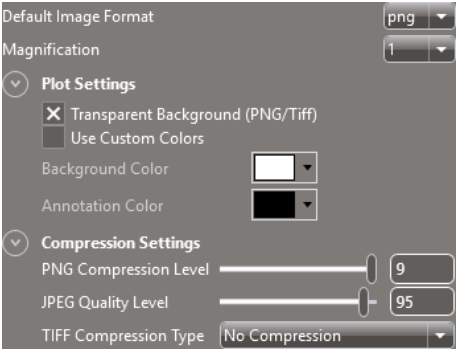
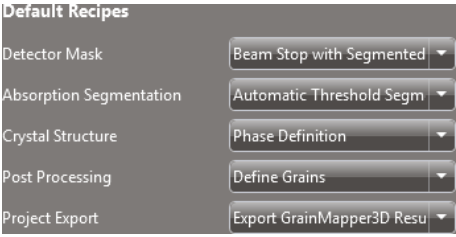


The **Layer Color Legends** now indicate color codes of all visible items in the volume view, see example in Figure 8. IPF color codes are only displayed for selected crystallographic phases. When creating screenshots, all colorbars will be saved.

Table 7 Preferences

Control	Function
<p>Performance</p> <p>Number of Cores: <input type="range" value="40"/> 40</p> <p><input type="checkbox"/> Remember Number of Cores</p> <p>Volume Rendering Quality: <input type="range" value="50%"/> 50 %</p> <p>Image Cache Size: <input type="range" value="25%"/> 25 %</p> <p>Clear Cache</p>	<p>Volume Rendering Quality can be adjusted from lowest to highest. If the volume dimensions are too large to fit into the graphics memory, they will be downsampled by this fraction.</p>

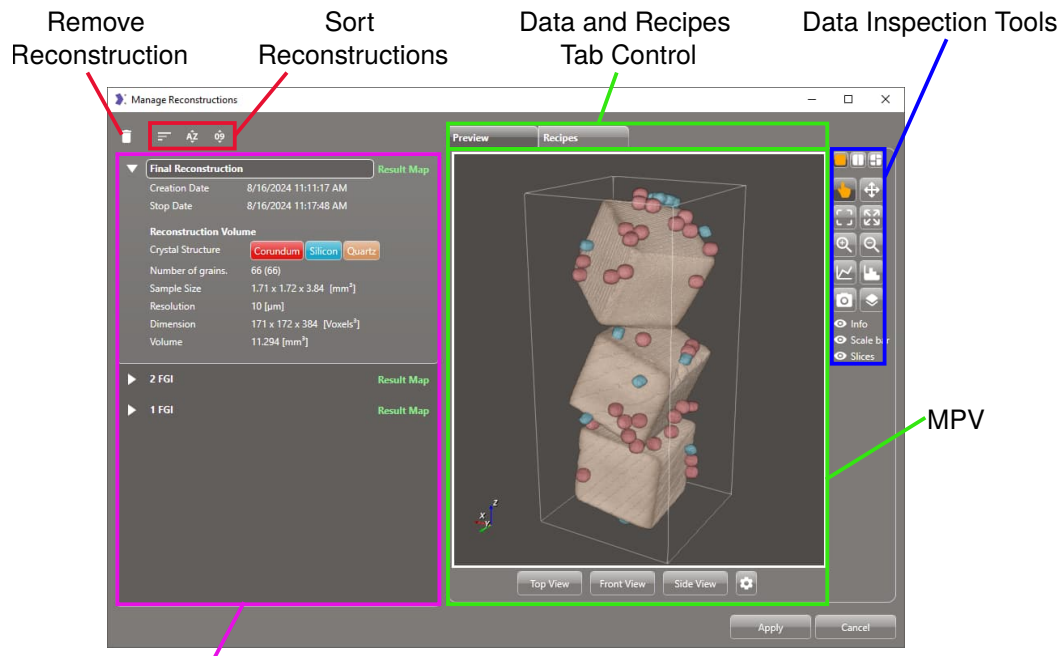
Table 7 Preferences (*continued*)

Control	Function
 The screenshot shows the 'Phase Colors' preference panel. It has a 'LinesMap' dropdown menu. Below it, there are two entries: 'Phase 0' with a red color swatch and 'Phase 1' with a cyan color swatch.	Choose or edit Default Phase Colors that will be assigned when adding a crystallographic phase on the Reconstruction Tab .
 The screenshot shows the 'Plot Settings' preference panel. It includes several dropdown menus: 'Image Info' (None), 'Display Coord. System' (Xnovo), 'Display Orientation' (Euler ZXZ (Bunge)), 'Point Size' (5), 'Line Width' (1.5), 'Font Size' (10), 'Annotation Color' (red), 'Plot Color' (blue), and 'Plot Foreground Color' (green). There is also a checkbox for 'Layer Histogram Control' which is currently unchecked.	Set the Point Size , Line Width and Font Size on all plots. Check Layer Histogram Control to open the histograms below the Layers like in Table 6 . If left unchecked, the histograms will be pop-up dialogues.
 The screenshot shows two preference panels. The top one is 'Plot Settings' with a 'Transparent Background (PNG/Tiff)' checkbox checked and 'Use Custom Colors' unchecked. It also has 'Background Color' (white) and 'Annotation Color' (black) dropdowns. The bottom panel is 'Compression Settings' with 'PNG Compression Level' at 9, 'JPEG Quality Level' at 95, and 'TIFF Compression Type' set to 'No Compression'.	Check Transparent Background to export png or tiff with transparent background. Check Use Custom Colors and use the color picker drop-downs to change the background and annotation color when creating a screenshot. Can be used in combination with Transparent Background .
 The screenshot shows the 'Default Recipes' preference panel. It contains several dropdown menus: 'Detector Mask' (Beam Stop with Segmented), 'Absorption Segmentation' (Automatic Threshold Segm), 'Crystal Structure' (Phase Definition), 'Post Processing' (Define Grains), and 'Project Export' (Export GrainMapper3D Resu).	Choose Default Recipes that will be used when creating a new project.

User Interface Changes

Phase Information The layout of the **Crystal Structure** section in the **Project Summary** has been adjusted to accommodate multi-phase information. So has the **Crystal Structure** fields in the **Reconstruction** section of the **Project Summary** ([Figure 8](#)), and the **Reconstruction List** of the **Reconstruction Manager** ([Figure 11](#)). For the latter, additional information about the crystallographic symmetry and unit cell will be displayed upon hovering.

Figure 11 Reconstruction Manager




Reconstruction List

HKIL Notation and IPF Color Codes Hexagonal and trigonal crystal systems now show Miller-Bravais indices ($hkil$), $-i=h+k$, for **Selection of HKL families** (e.g. Figure 6). Rhombohedral lattice systems remain in (hkl) notation. Annotations on IPF colors codes show the crystallographic directions instead of the lattice plane normals. These use the correct notation $[uvw]$ and Weber indices $[uvtw]$ in the hexagonal or trigonal case.

Furthermore, issues with the IPF color codes for R-3c:H and for triclinic have been resolved.

Data Export **Export HDF** was renamed to **Export GrainMapper3D Result File (HDF)**.

Reconstruction Manager The **Grains View** of the **Reconstruction Manager** (Figure 11) now allows to adjust color codes by pressing the **Layers Control**  in the **Data Inspection Tools** section.

Tooltips Several **Tooltips** have been revised for the better.

Other Changes

Default Recipes When creating a new project, the default recipes used can be customized in the **Preferences**, refer to Table 7.

Absorption Volume Import Absorption volume import of TXM volumes now also supports uint8 and float format. Both will be converted to uint16.

GrainMapper3D Viewer

GrainMapper3D Viewer 4.0 features a few updates in line with GrainMapper3D 4.0 updates, namely:

Product Enhancements

Grain Selection Filters

The same Grain Selection Filters have been added as described for GrainMapper3D. The only difference is that the grain picking tool for the Multi Grain Id filter only works on the MPV as the GrainMapper3D Viewer does not have a Forward Simulation View.

Enhanced Volume Rendering and Controls

All of the enhancements to the volume rendering and associated user controls described for GrainMapper3D also apply for GrainMapper3D Viewer.

User Interface and Other Changes

Extended Phase Information When hovering over the **Crystal Structure** fields in the **Reconstruction** section, additional information about the crystallographic symmetry and unit cell will be displayed as for GrainMapper3D.

HKIL Notation and IPF Color Codes All of the enhancements to hkil notation and IPF color codes described for GrainMapper3D also apply for GrainMapper3D Viewer.

GrainMapper3D™

Release Notes

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