

# Latest developments in advanced 3D EBSD/EDS data processing with ESPRIT QUBE



Free online webinar – May 5<sup>th</sup> 2020  
Bruker Nano, Germany



Innovation with Integrity

# Presenters



- **Dr. Laurie Palasse**

Senior Application Scientist EBSD

Bruker Nano Analytics, Berlin, Germany

- **Peter Konijnenberg**

Senior Data Scientist, Bruker Nano Analytics

MPIE Max-Planck-Institut für Eisenforschung, Düsseldorf

# Latest developments in ESPRIT QUBE

## Webinar outline



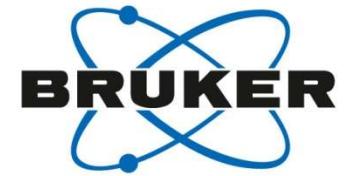
- Grain boundary network on experimental examples
- Analysis of 3D tomographic datasets with ESPRIT QUBE
- Q&A



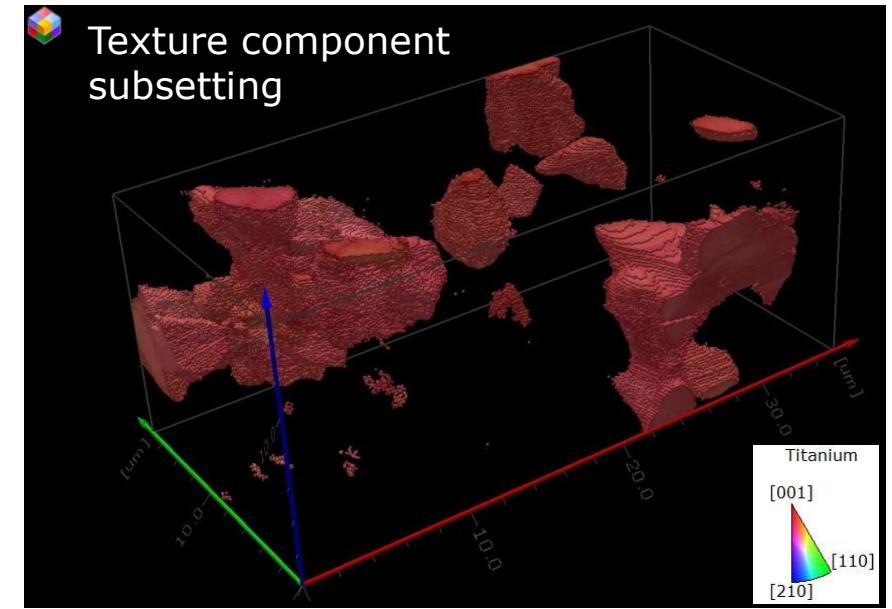
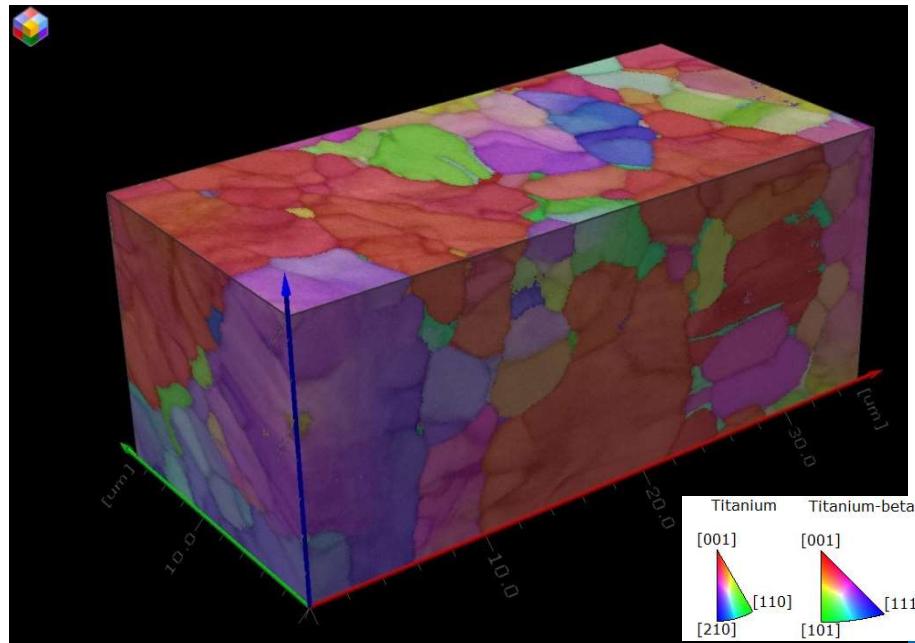
# Grain boundary network on experimental examples

# ESPRIT QUBE

## 3D data processing – Ti alloy example



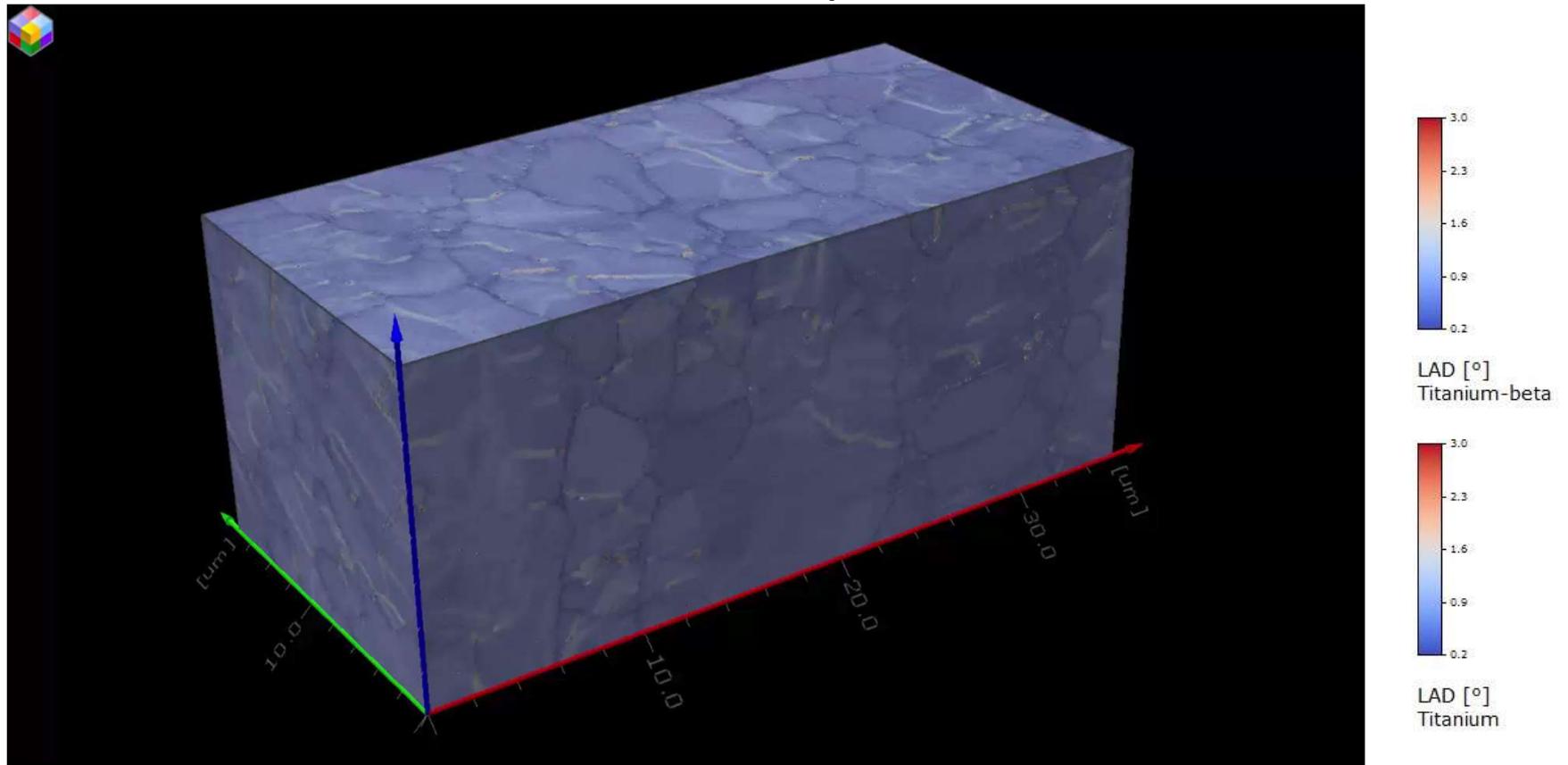
- Deformed Ti alloy (alpha and beta phases)
- Large data cube – 245 slices ( $35 \times 20 \times 20 \mu\text{m}^3$ )
- Serial sectioning using a PFIB-SEM (FEI) with non-static 3D
- Slice preparation time:  $\sim 2\text{min/slice}$
- 3D EBSD data acquisition time:  $\sim 7\text{min/slice}$



# ESPRIT QUBE

## 3D data postprocessing – Local Average Disorientation

3D EBSD on deformed Ti alloy – LAD visualization

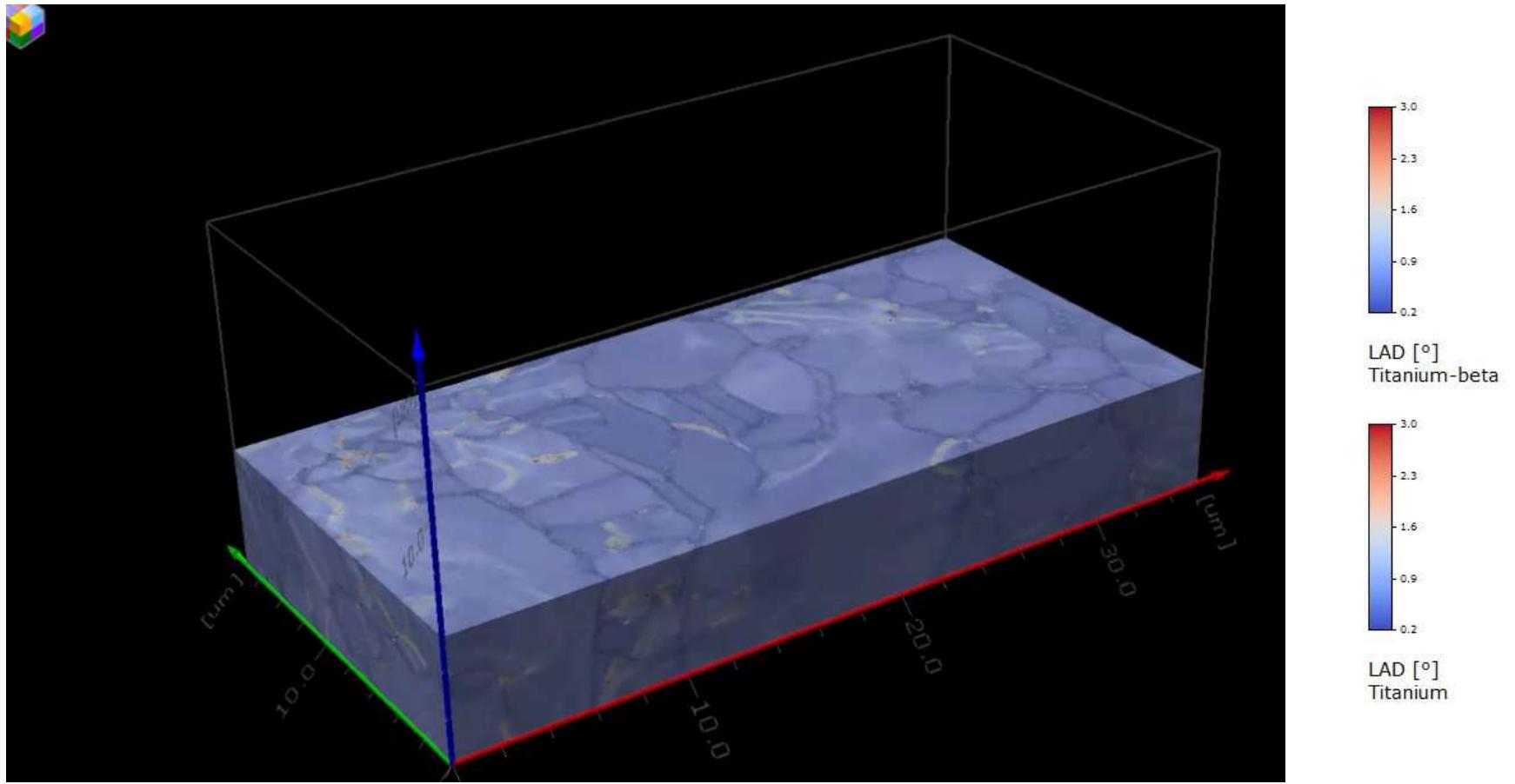


LAD after slice realignment & data filtering

# ESPRIT QUBE

## 3D data postprocessing – Local Average Disorientation

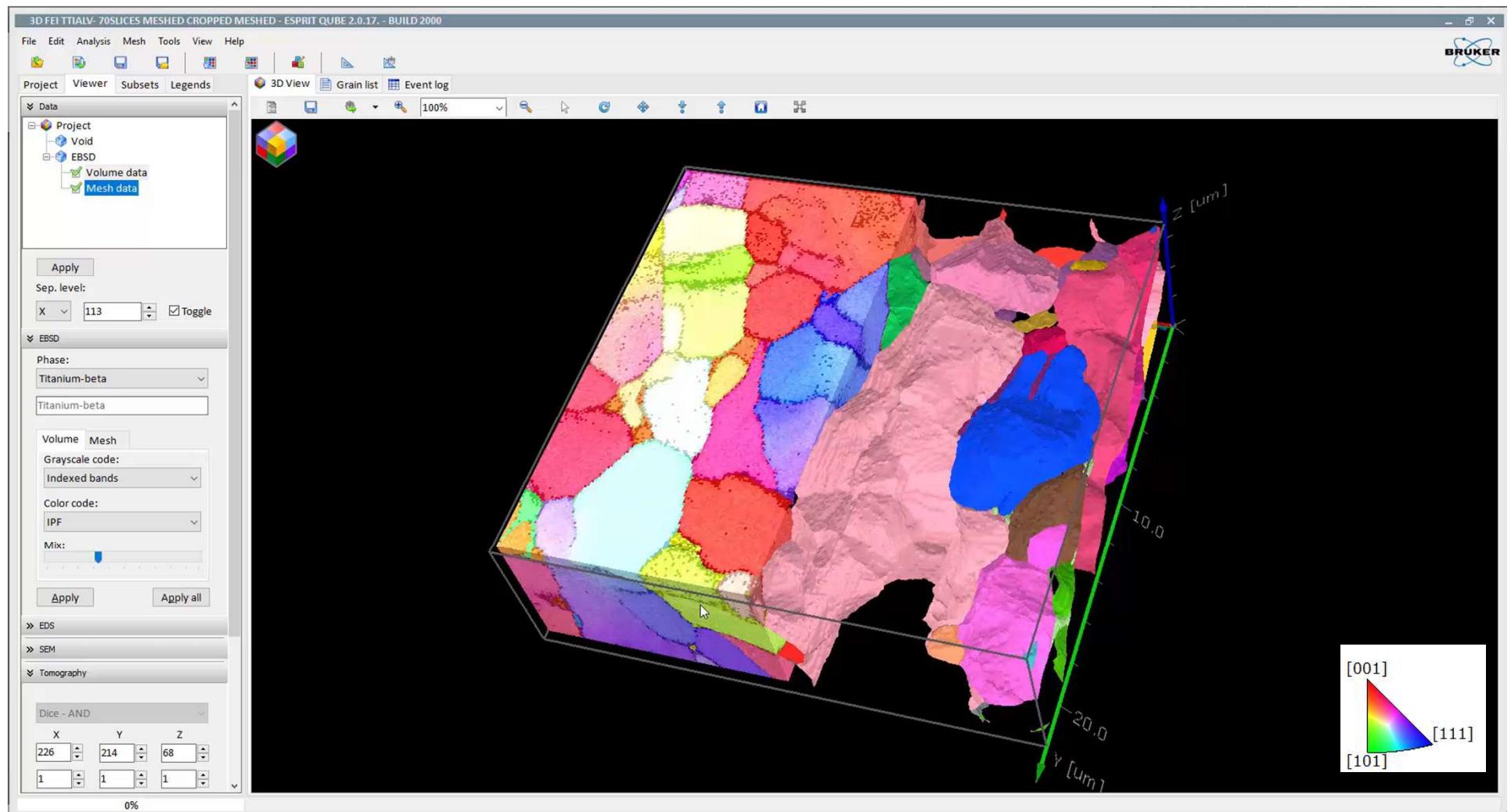
3D EBSD on deformed Ti alloy – LAD visualization



LAD after slice realignment & data filtering

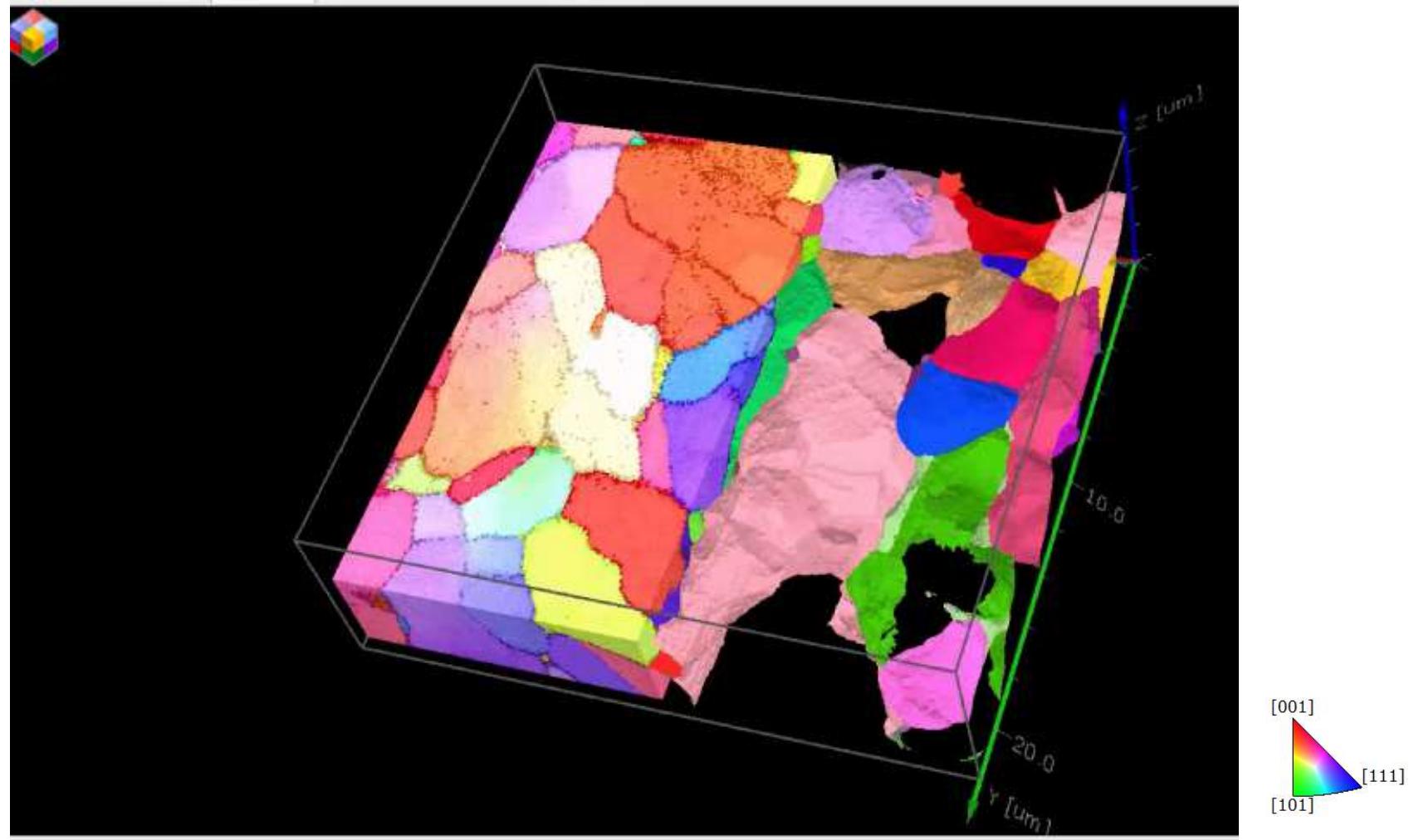
# ESPRIT QUBE

## Grain Boundary network – Ti alloy



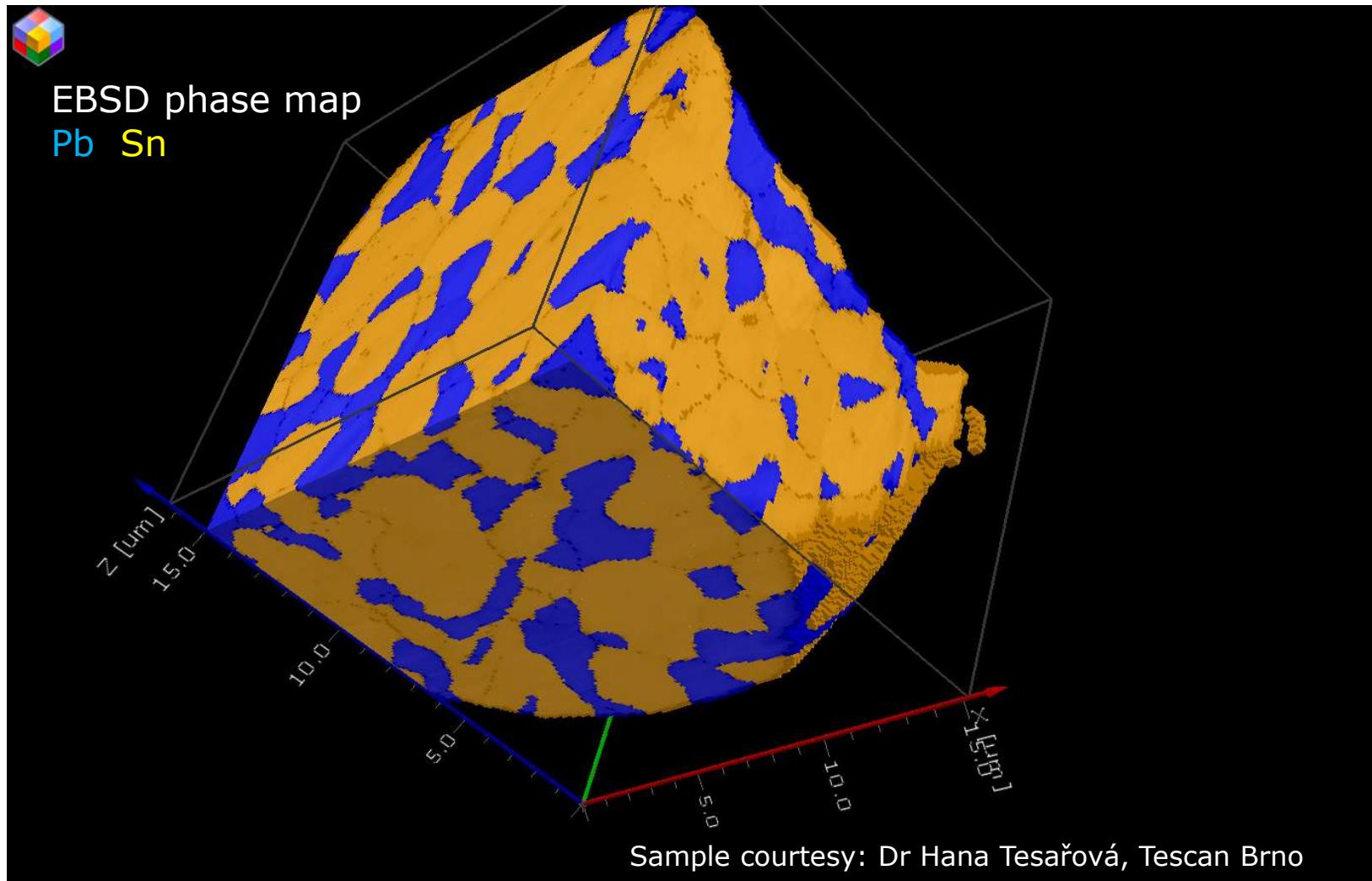
# ESPRIT QUBE

## Grain Boundary network – Ti alloy



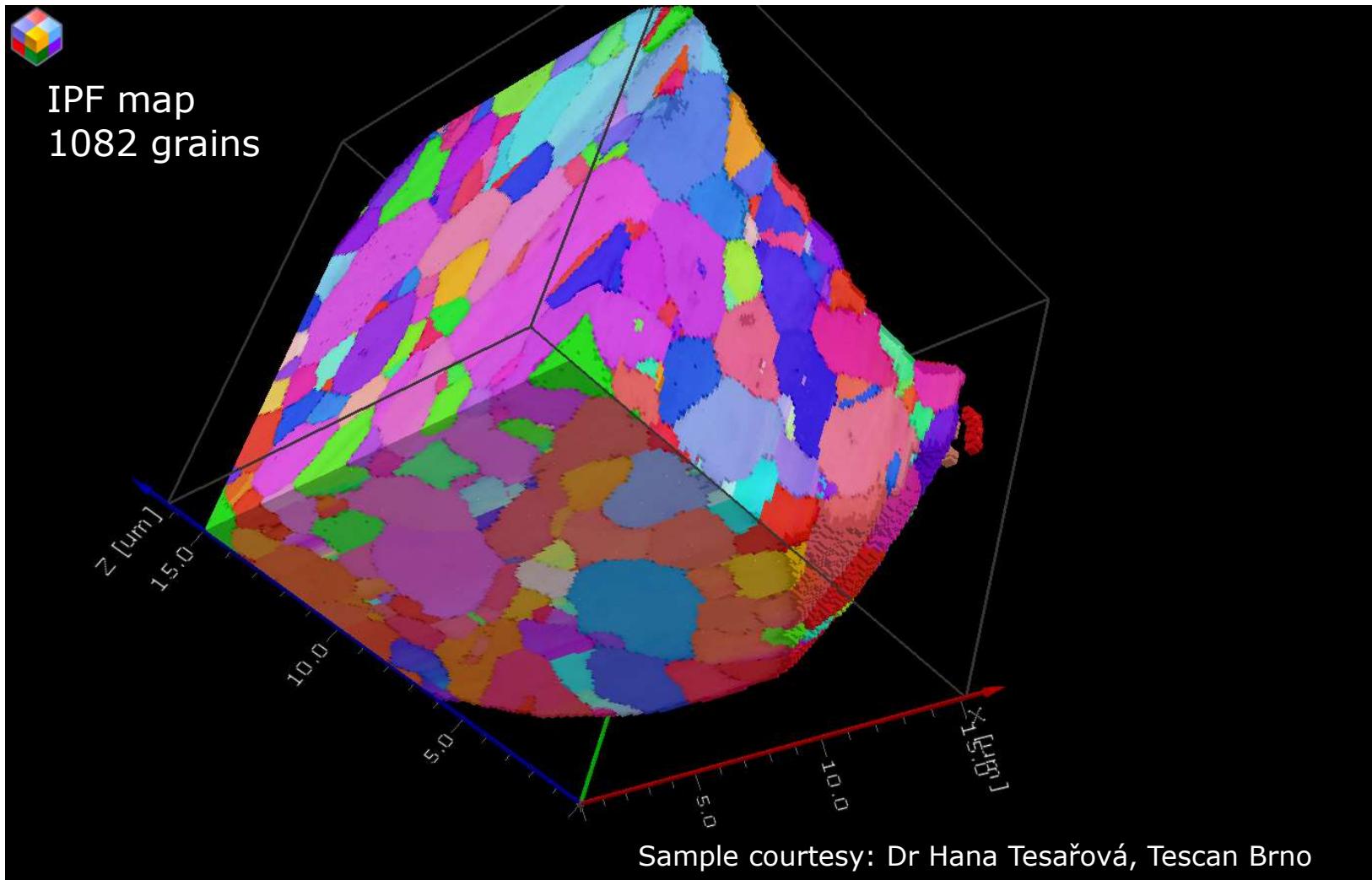
# ESPRIT QUBE

Grain Boundary network – PbSn powder metallurgy  
(solder ball) acquired with static 3D EBSD (Tescan)



# ESPRIT QUBE

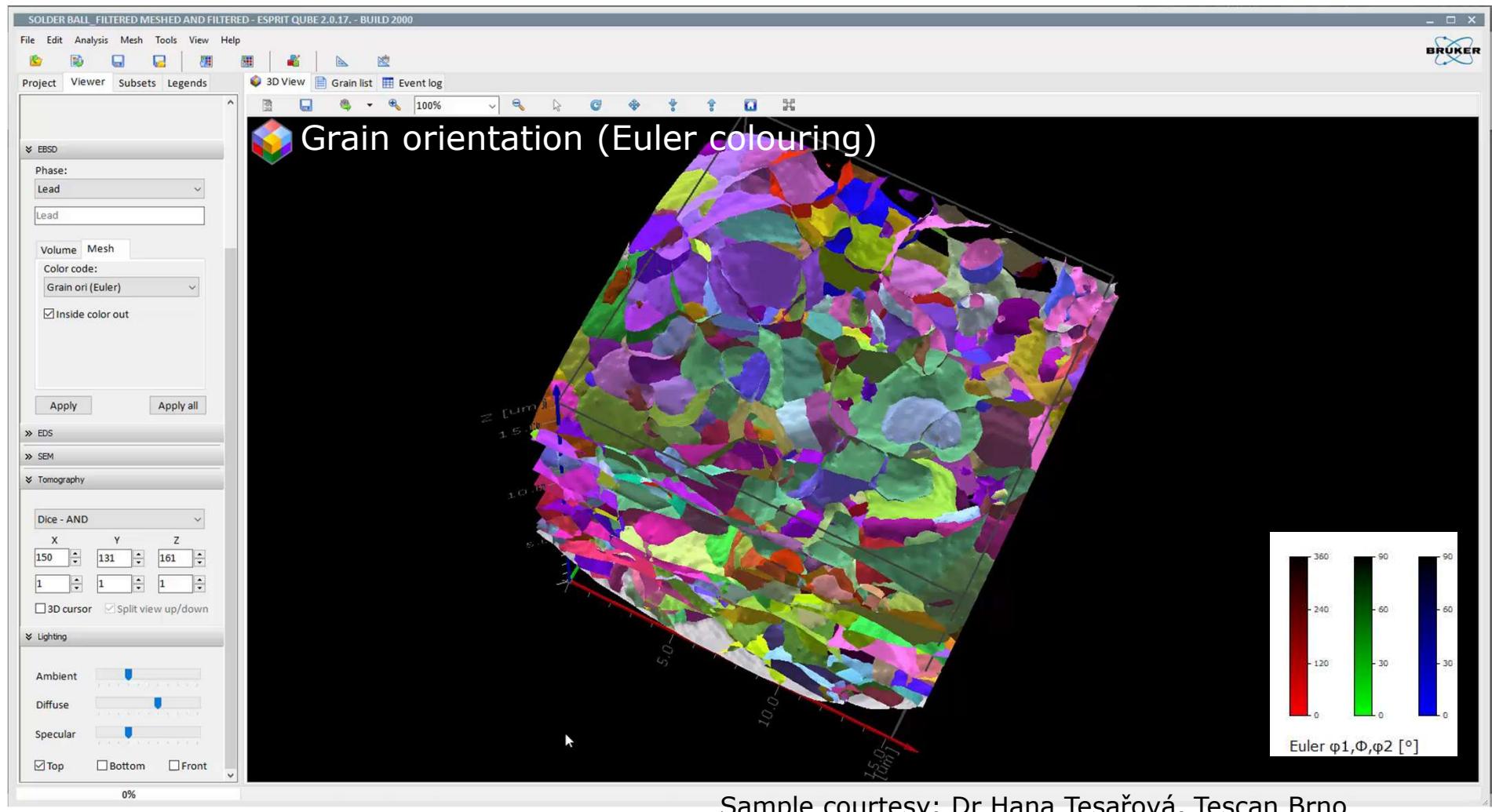
## Grain Boundary network PbSn powder metallurgy



# ESPRIT QUBE

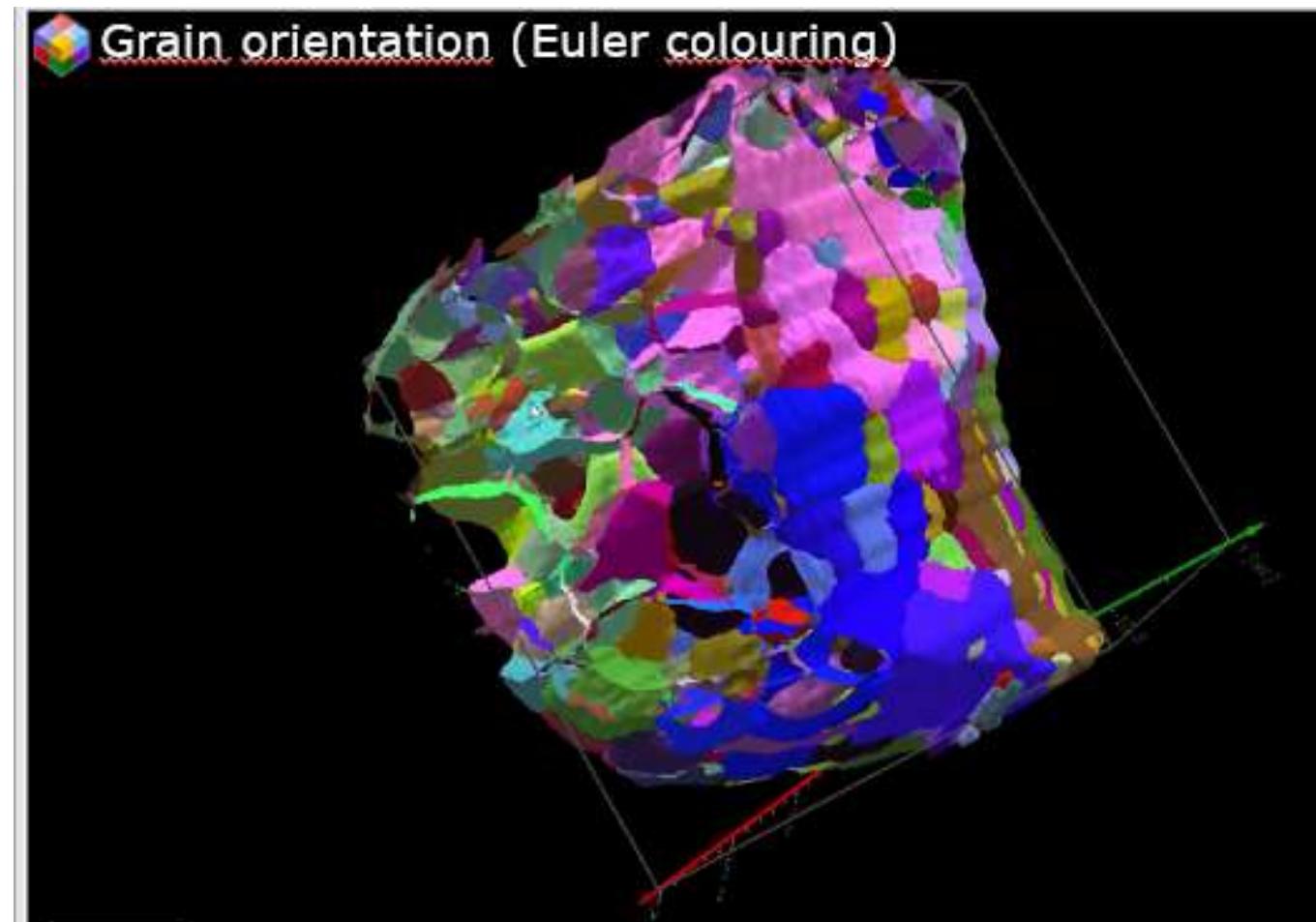
## Grain Boundary network

### PbSn powder metallurgy



# ESPRIT QUBE

## Grain Boundary network PbSn powder metallurgy



Sample courtesy: Dr Hana Tesařová, Tescan Brno



# Analysis of 3D tomographic datasets with ESPRIT QUBE

# ESPRIT QUBE

## Outline



- Introduction
- Data files
- Viewing and navigation
- Filters and geometry
- Analytical tools
- Subsets
- Surface meshes
- Data synergy
- Data monitoring

# ESPRIT QUBE

## Introduction 1(2)

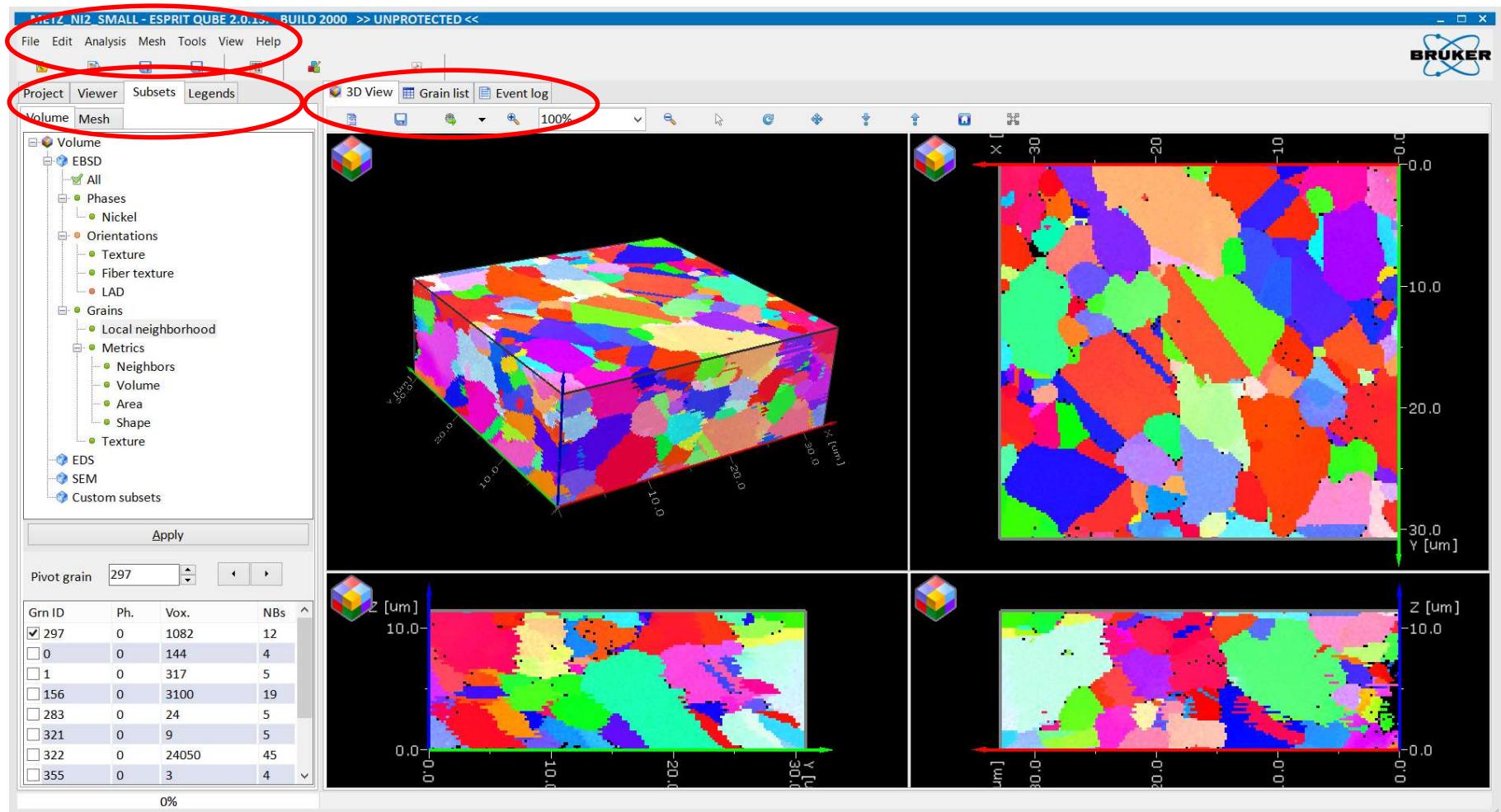


*What is QUBE ?*

- Reconstruction of tomographic data sets from analytical SEM
- Tailored for surface characterization techniques such as EBSD and EDS
- Integrative analysis of 3D data sets
- Customizable interactive processing pipeline
- Multimodal data sets

# ESPRIT QUBE

## Introduction 2(2)



Data set: courtesy of Dr. Nathalie Gey, LEM3



LABORATOIRE D'ÉTUDE DES MICROSTRUCTURES  
ET DE MÉCANIQUE  
DES MATERIAUX

# ESPRIT QUBE

## Data types and formats

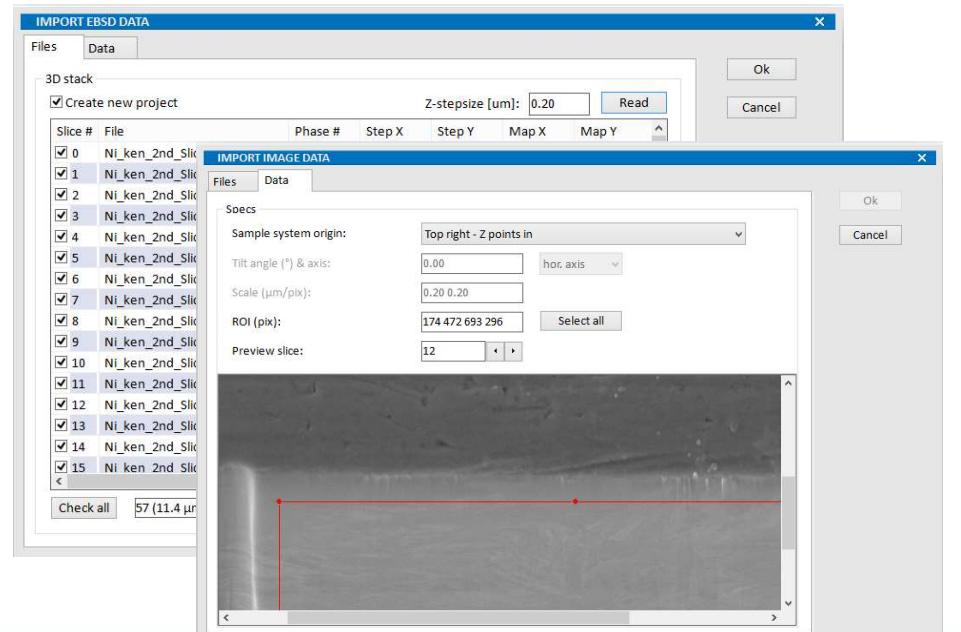


### *Import data sets:*

- Import of 2D slices, per data set
- EBSD: Bruker format (.bcf) and other common formats (e.g .ctf, .ang)
- EDS: Bruker (.bcf) (counts or conc.), as well as (.txt) files
- SEM Images: common bitmap formats (.bmp, .gif, .png, .jpg, etc)

### *Qube projects:*

- All 3 data types are saved into a single 3D project (.qml)
- .vti export
- Export of images, lists and intermediate results



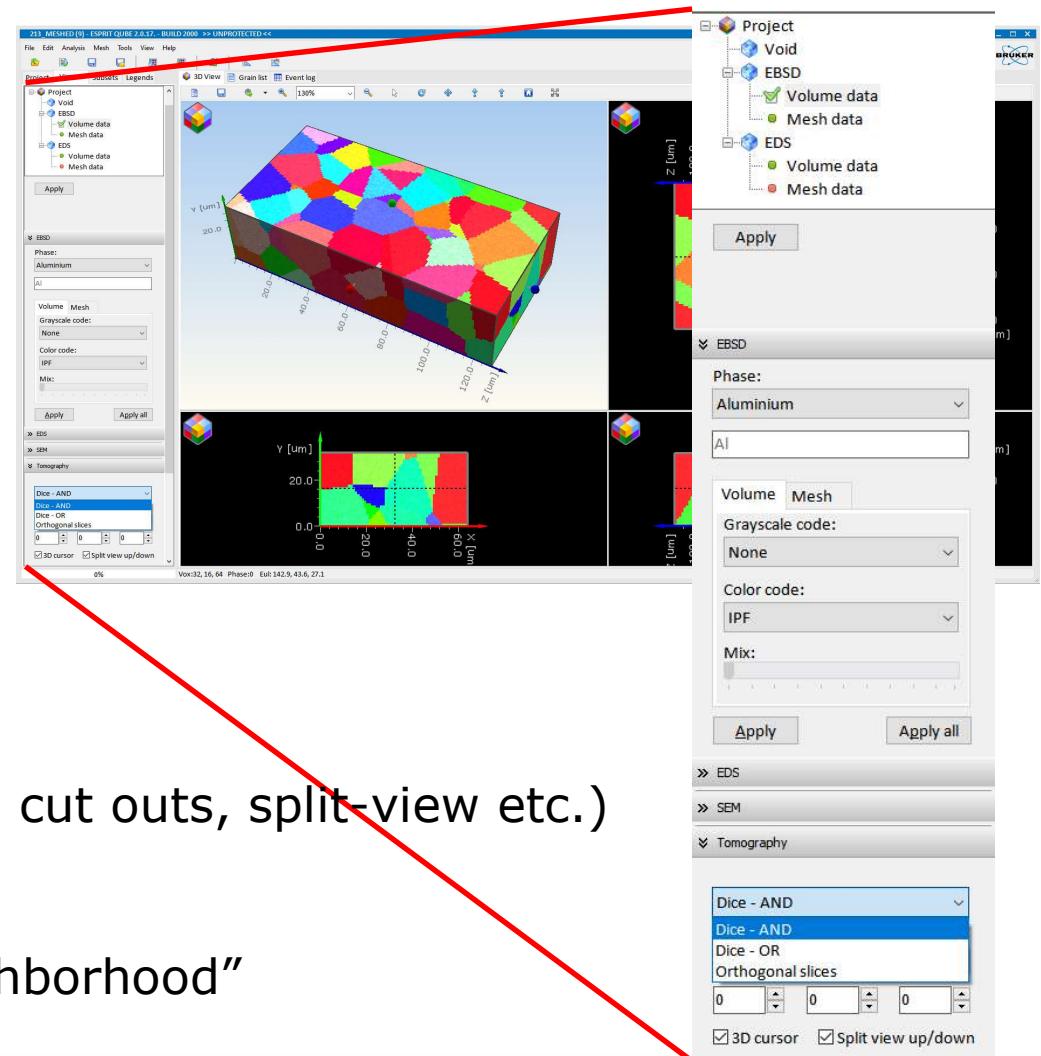
# ESPRIT QUBE

## Viewing & navigation



*Viewing:*

- “Real time” (wysiwyg)
- Extensive dedicated color codes for EBSD, EDS and bitmaps
- Semi transparency (scalar data)
- Multimodal views options



*Navigation by:*

- “Real time” (wysiwyg)
- Slice-wise: tomography (slicing, cut outs, split-view etc.)
- Voxel-wise: 3D cursor
- Segmentation-wise: “grain neighborhood”

File Edit Analysis Mesh Tools View Help



Project Viewer Subsets Legends

Apply

EBSD

Phase: Aluminium

AI

Volume Mesh

Grayscale code: None

Color code: IPF

Mix:

Apply Apply all

» EDS

» SEM

Tomography

Dice - AND

X	Y	Z
63	31	127
0	0	0

3D cursor  Split view up/down

Lighting

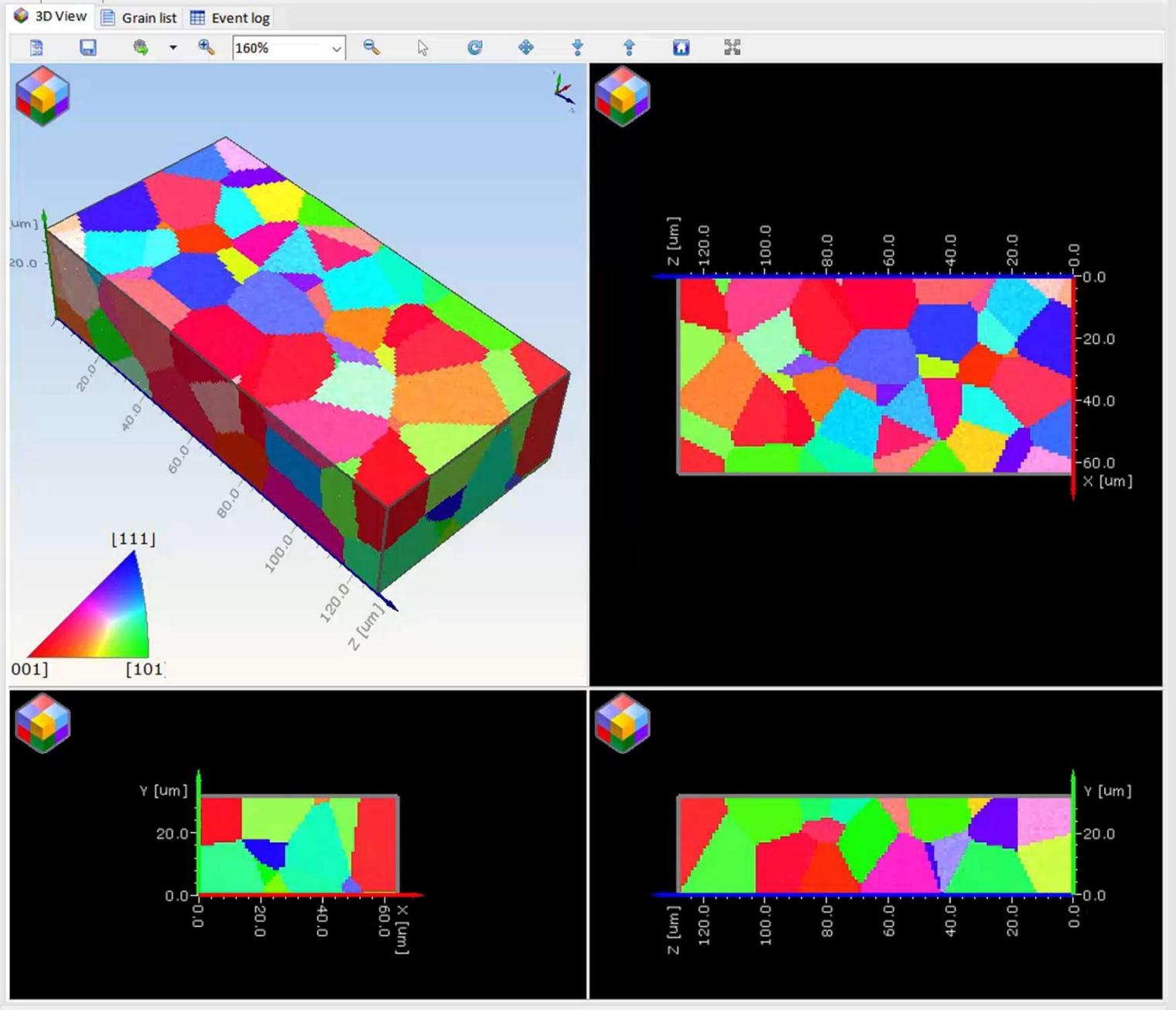
Ambient

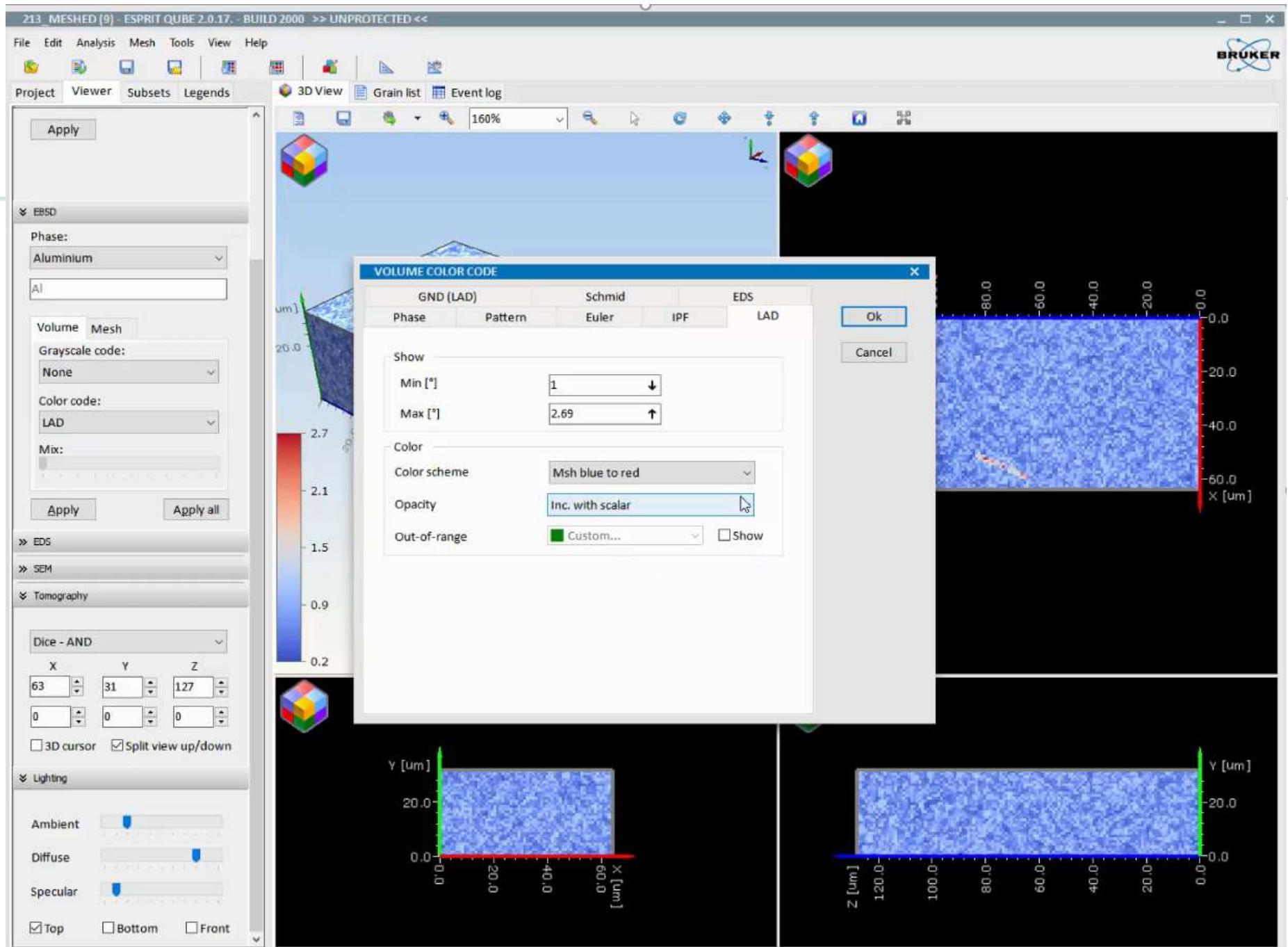
Diffuse

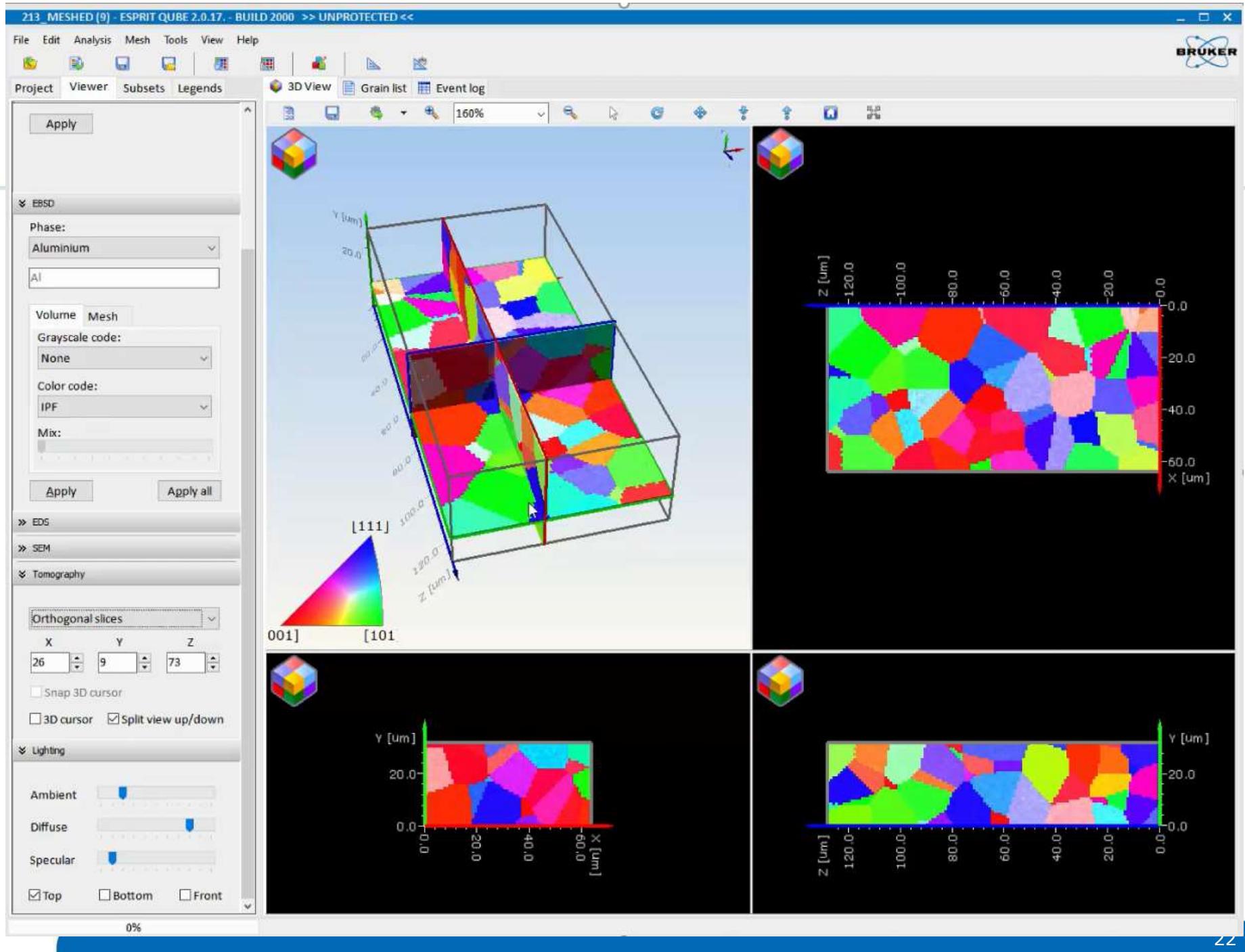
Specular

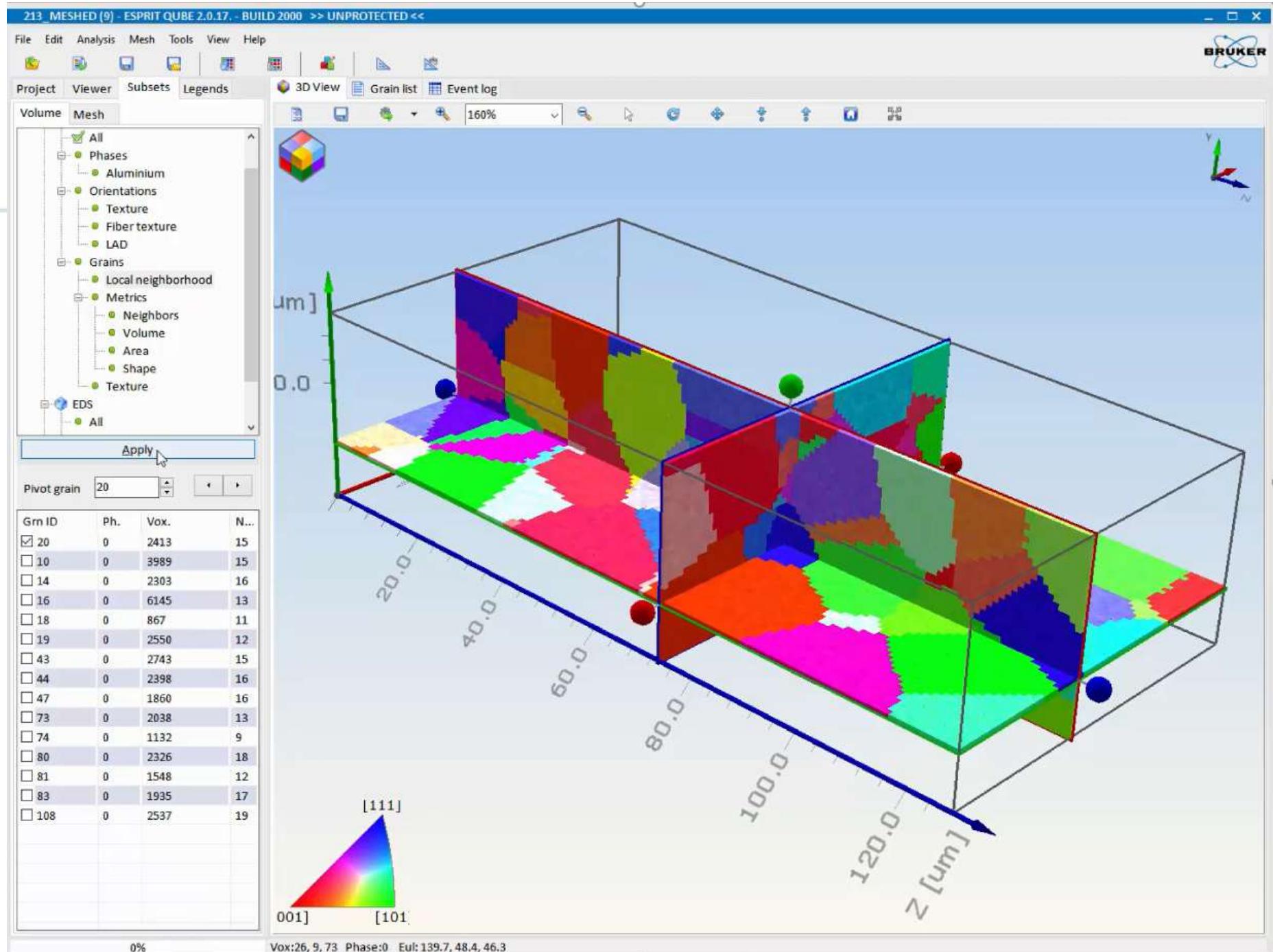
Top  Bottom  Front

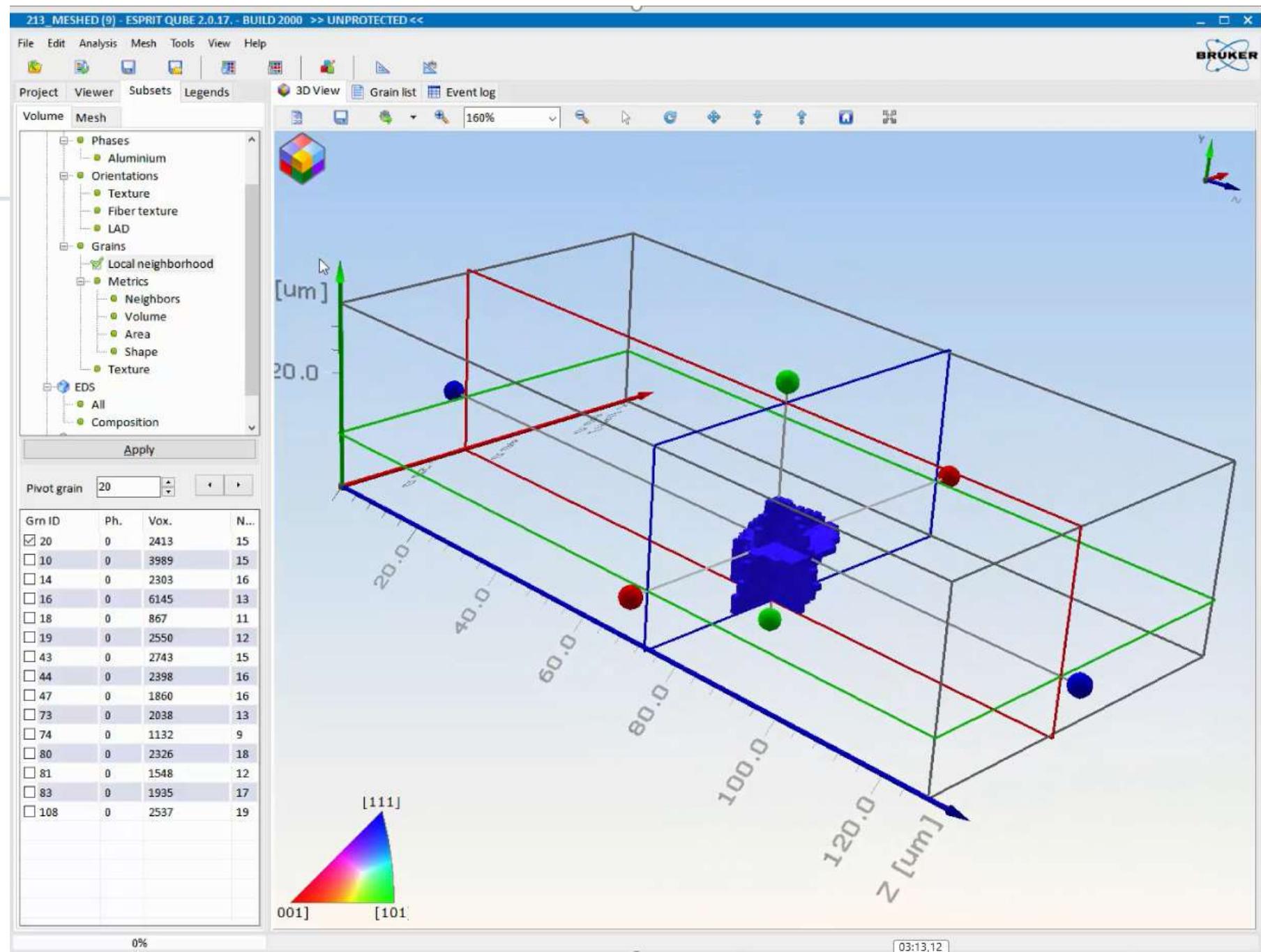
0%

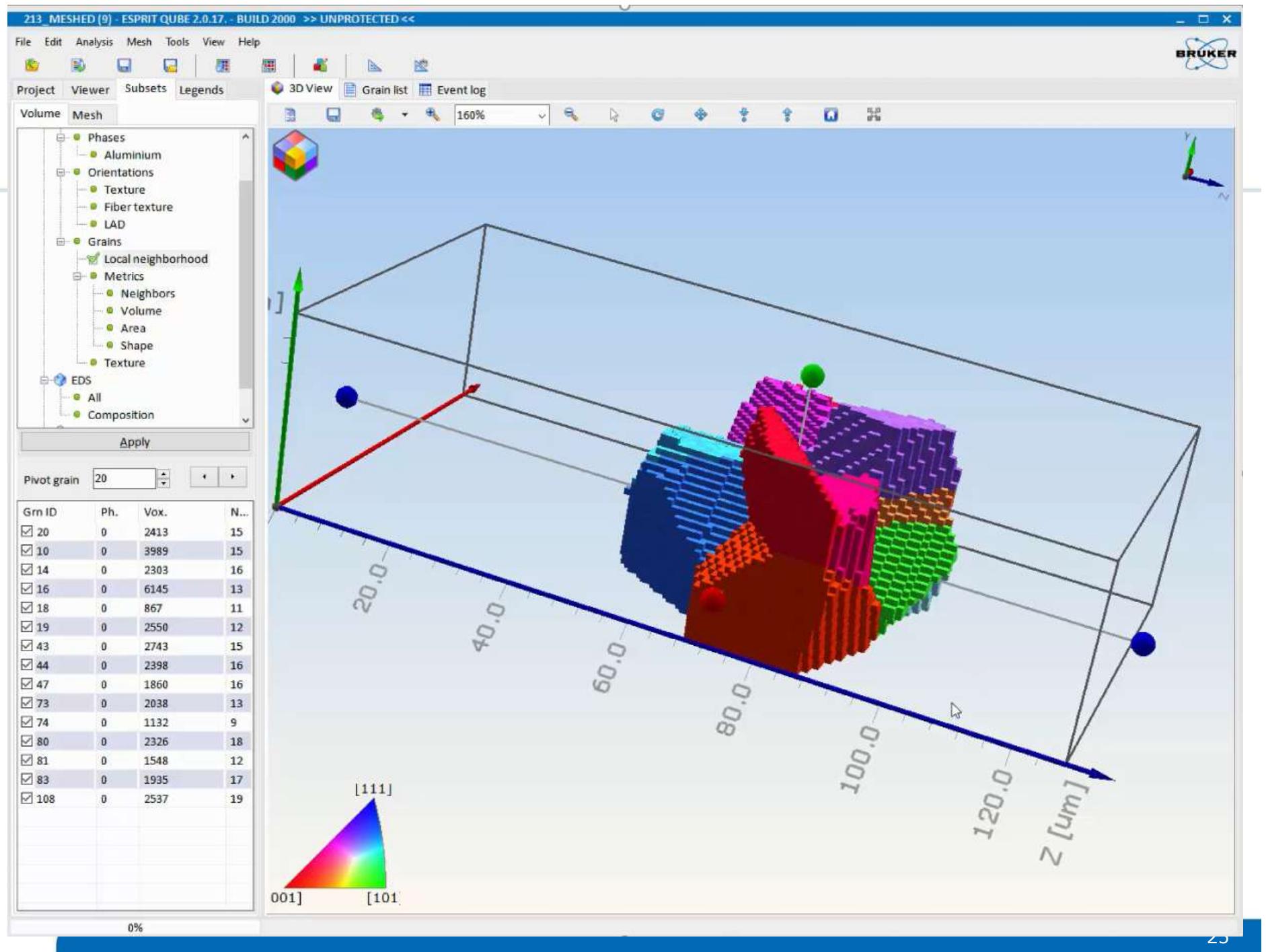












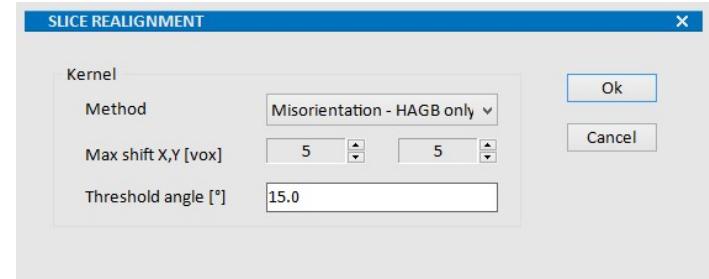
# ESPRIT QUBE

## Filters and geometry



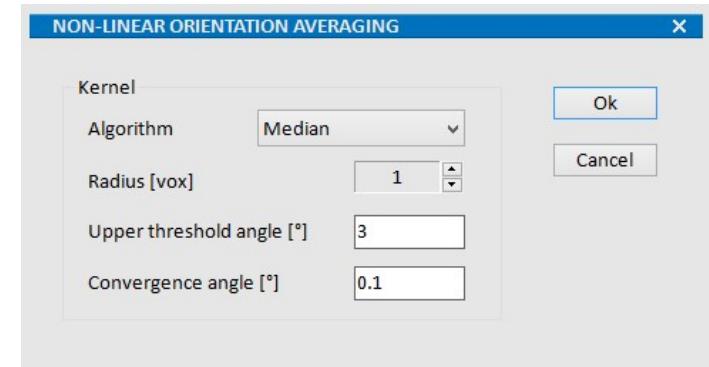
### *Geometry editing:*

- Cropping and slice deletion
- Slice registration
- Affects EBSD, EDS and SEM data sets



### *Data filtering:*

- Currently for EBSD (limited for EDS)
- Linear filters (Gaussian, box)
- Non-linear filters (Kuwahara, median)
- Despeckling (outliers)
- Clean up (stray voxels)

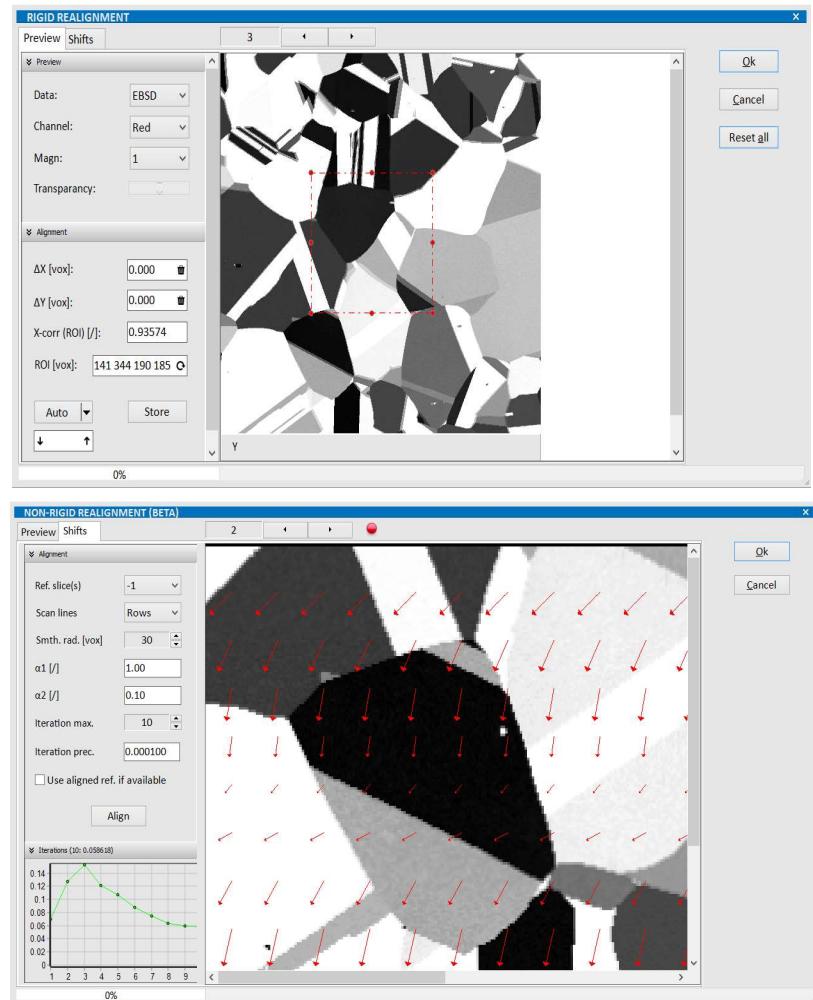


# ESPRIT QUBE Slice registration



*Slice registration:*

- Rigid realignment  
(manually)
- Rigid realignment  
(EBSD based)
- Non rigid realignment  
(Constrained smart align)
- Affects EBSD, EDS and  
SEM data sets



# ESPRIT QUBE

## Analytical tools



### *Analysis of EBSD data:*

- Grain segmentation (extensive EBSD grain list)

**GRAIN RECONSTRUCTION**

**Segmentation**

Critical disorientation angle [°]

Next neighbors to consider

**GB to disregard**

#	Phase	Axis	Angle [°]	Deviation [°]
1	0	111	60.00	8.0

**FILTER GRAIN LIST**

**Filter settings**

Grain volume <= [vox]:

Clean-up action:

Set to non-indexed, if no st

# ESPRIT QUBE

## Analytical tools

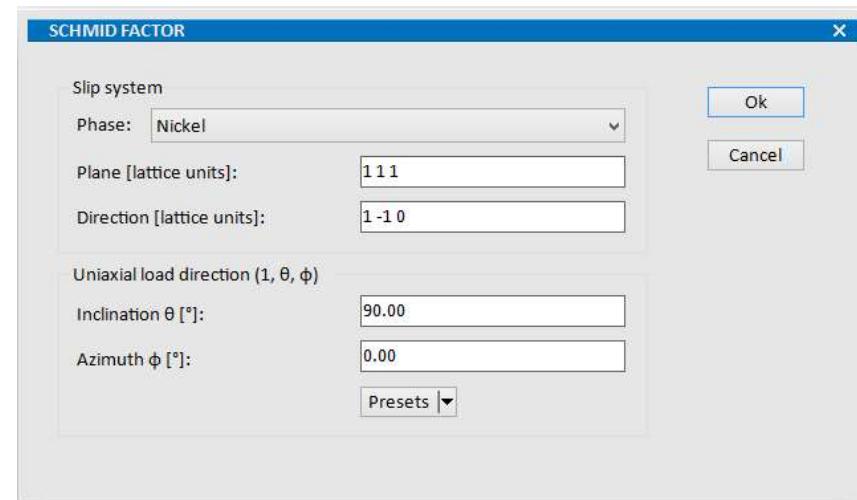


### *Analysis of EBSD data:*

- Grain segmentation (extensive EBSD grain list)
- Local average disorientation (LAD)
- Approximated GND density  
(based on LAD)
- Schmid factor
- Various subsets

### *Analysis of EDS data:*

- Subsets

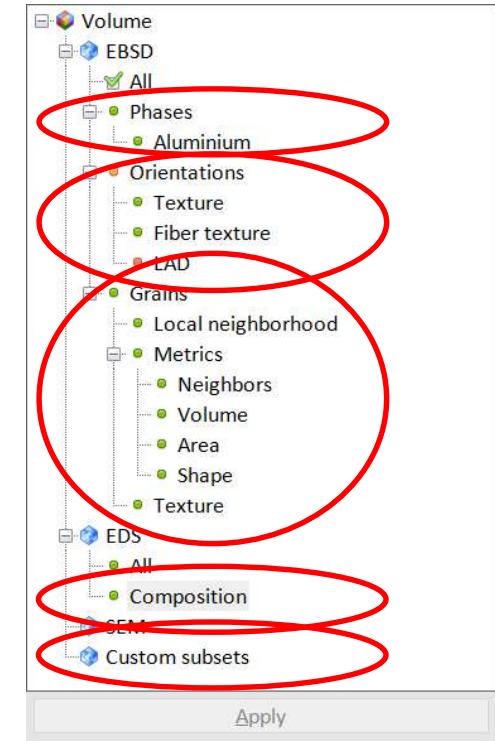


# ESPRIT QUBE Subsets



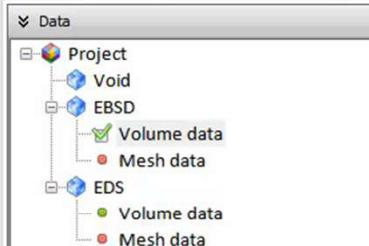
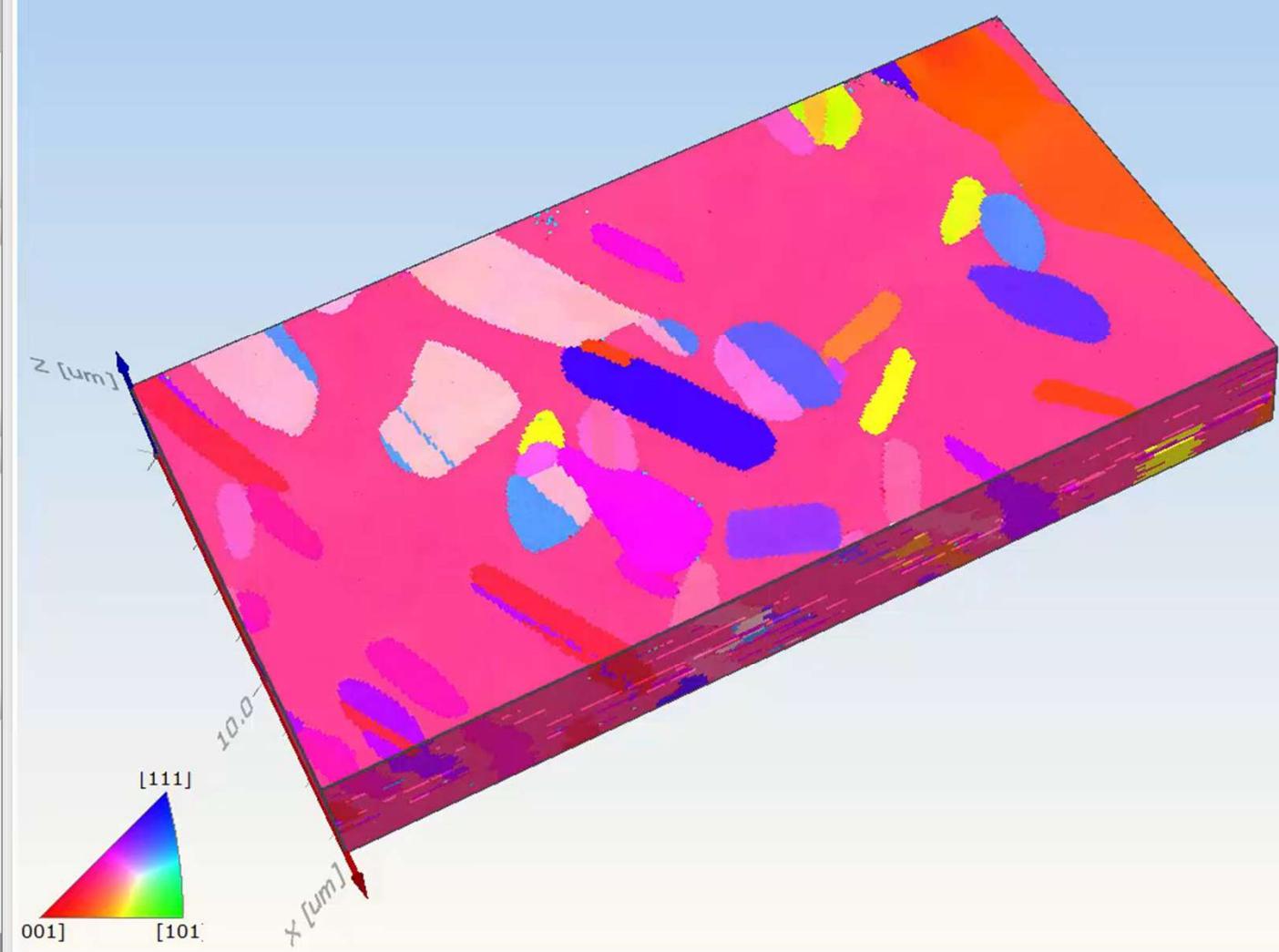
*EBSD volume subset options:*

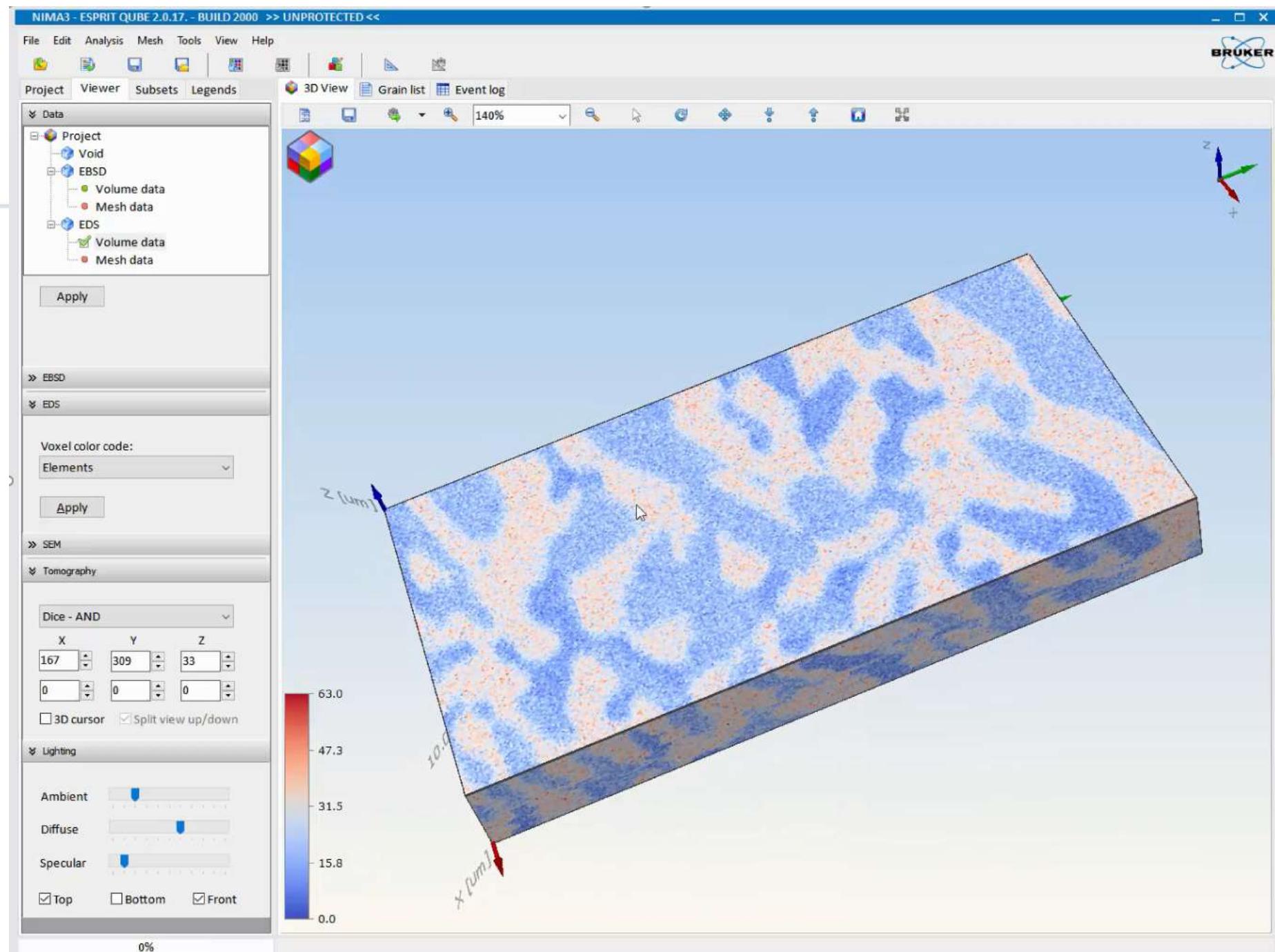
- Predefined subsets: phases, textures, LAD, grain metrics, grain texture, grain selections
- Custom subsets
- Subsets can be exported and imported
- Subsets can be applied across data sets (e.g. apply EBSD subset to EDS data set)



*EDS volume subset options:*

- Compositional subsets  
(user defined, picked from position or from .cif)

**File Edit Analysis Mesh Tools View Help****Project Viewer Subsets Legends****Apply****>> EBSD****>> EDS****Voxel color code:****Elements****Apply****>> SEM****>> Tomography****Dice - AND****X Y Z****167 309 33****0 0 0** **3D cursor    Split view up/down****>> Lighting****Ambient****Diffuse****Specular** **Top    Bottom    Front****0%****3D View   Grain list   Event log****140%**



NIMA3 - ESPRIT QUBE 2.0.17. - BUILD 2000 >> UNPROTECTED <<

File Edit Analysis Mesh Tools View Help

Project Viewer Subsets Legends

3D View Grain list Event log

**Data**

- Project
  - Void
  - EBSD
    - Volume data
    - Mesh data
  - EDS
    - Volume data
    - Mesh data

Apply

**EBSD**

**EDS**

Voxel color code: Elements

Apply

**SEM**

**Tomography**

Dice - AND

X	Y	Z
167	309	33
0	0	0

3D cursor  Split view up/down

**Lighting**

Ambient

Diffuse

Specular

Top  Bottom  Front

0%

**FILTER GRAIN LIST**

Filter settings

Grain volume <= [vox]:

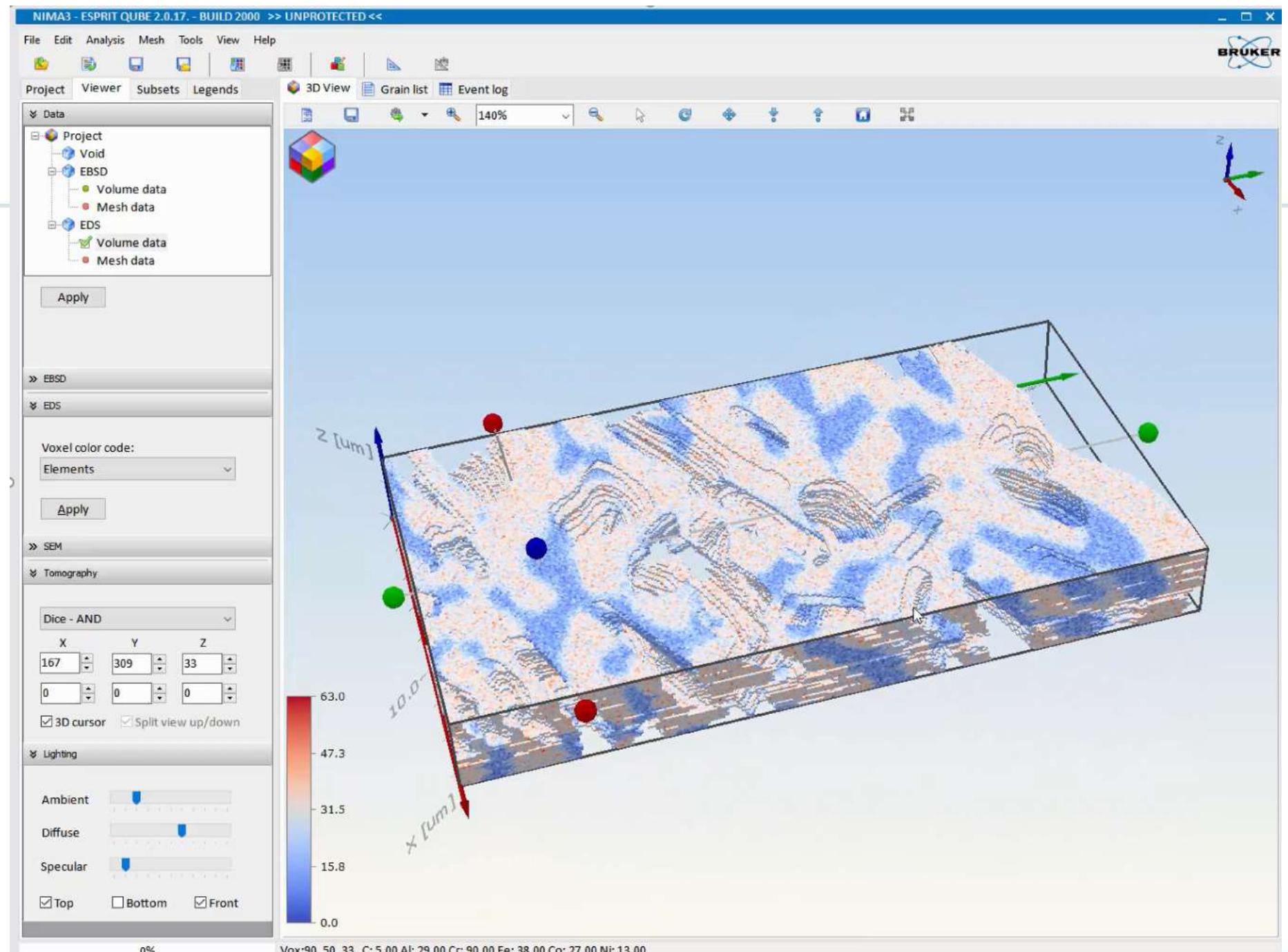
Clean-up action: Add to similar NB - retain ori -

Set to non-indexed, if no suitable neighbors available

Frequency [f]

Volume [vox.]

ID	Phase	Ori. mean [Re Im]	Ori. variance	Volume [vox]	Surface [um <sup>2</sup> ]	CMS [um]	Nei...	Bor...	Ellipsoid [um]	Ellipsoid vol...	Ellip...
2317	1	0.73 -0.37 -0.38 -0...	0.0000	1	0.06	4.05 9.35 2.15	4	0	0.00 0.00 0.00	0.00	0.00
2314	0	0.51 0.61 0.16 0.58	0.0000	1	0.06	13.25 9.15 2.15	5	0	0.00 0.00 0.00	0.00	0.00
2313	0	0.74 -0.37 -0.38 -0...	0.0000	1	0.06	5.45 9.15 2.15	4	0	0.00 0.00 0.00	0.00	0.00
2321	0	0.08 -0.09 -0.67 -0...	0.0000	1	0.06	4.65 9.55 2.15	5	0	0.00 0.00 0.00	0.00	0.00
2319	0	0.26 0.29 -0.88 -0....	0.0000	1	0.06	4.85 9.45 2.15	4	0	0.00 0.00 0.00	0.00	0.00
2318	0	0.40 -0.58 -0.46 0....	0.0000	1	0.06	4.15 9.35 2.15	5	0	0.00 0.00 0.00	0.00	0.00
2309	0	0.28 -0.92 0.12 -0....	0.0000	1	0.06	2.35 9.15 2.15	3	0	0.00 0.00 0.00	0.00	0.00
2308	1	0.56 0.79 0.04 0.24	0.0000	1	0.06	5.65 9.05 2.15	3	0	0.00 0.00 0.00	0.00	0.00
2306	0						0	0	0.00 0.00 0.00	0.00	0.00
2312	1						0	0	0.00 0.00 0.00	0.00	0.00
2311	0						0	0	0.00 0.00 0.00	0.00	0.00
2310	0						0	0	0.00 0.00 0.00	0.00	0.00
2322	0						0	0	0.00 0.00 0.00	0.00	0.00
2334	1						0	0	0.00 0.00 0.00	0.00	0.00
2333	1						0	0	0.00 0.00 0.00	0.00	0.00
2332	0						0	0	0.00 0.00 0.00	0.00	0.00
2337	0						0	0	0.00 0.00 0.00	0.00	0.00
2336	0						0	0	0.00 0.00 0.00	0.00	0.00
2335	0						0	0	0.00 0.00 0.00	0.00	0.00
2326	1						0	0	0.00 0.00 0.00	0.00	0.00
2325	0						0	0	0.00 0.00 0.00	0.00	0.00
2324	0						0	0	0.00 0.00 0.00	0.00	0.00
2330	1						0	0	0.00 0.00 0.00	0.00	0.00
2328	1						0	0	0.00 0.00 0.00	0.00	0.00
2327	0						0	0	0.00 0.00 0.00	0.00	0.00
2304	0						0	0	0.00 0.00 0.00	0.00	0.00
2285	1						0	0	0.00 0.00 0.00	0.00	0.00
2283	0						0	0	0.00 0.00 0.00	0.00	0.00
2281	0						0	0	0.00 0.00 0.00	0.00	0.00
2288	0	0.24 -0.53 0.64 0.51	0.0000	1	0.06	2.55 4.25 2.15	3	0	0.00 0.00 0.00	0.00	0.00
2287	1	0.71 -0.41 0.39 -0....	0.0000	1	0.06	2.35 4.25 2.15	3	0	0.00 0.00 0.00	0.00	0.00
2286	0	0.22 0.13 -0.51 -0....	0.0000	1	0.06	4.75 4.15 2.15	14	0	0.00 0.00 0.00	0.00	0.00
2275	0	0.12 0.05 -0.02 -0....	0.0000	1	0.06	0.25 3.45 2.15	4	0	0.00 0.00 0.00	0.00	0.00
2274	0	0.84 -0.26 -0.47 0....	0.0000	1	0.06	5.45 3.35 2.15	5	0	0.00 0.00 0.00	0.00	0.00
2273	0	0.06 0.08 -0.97 -0....	0.0000	1	0.05	0.05 3.35 2.15	3	1	0.00 0.00 0.00	0.00	0.00
2279	0	0.11 0.00 0.06 -0.99	0.0000	1	0.06	5.15 3.75 2.15	5	0	0.00 0.00 0.00	0.00	0.00
2278	0	0.58 0.52 0.46 -0.42	0.0000	1	0.06	5.35 3.65 2.15	6	0	0.00 0.00 0.00	0.00	0.00
2277	0	0.58 -0.12 -0.62 0....	0.0000	1	0.06	0.35 3.55 2.15	4	0	0.00 0.00 0.00	0.00	0.00
2289	0	0.39 -0.59 -0.46 0....	0.0000	1	0.06	3.85 4.25 2.15	4	0	0.00 0.00 0.00	0.00	0.00
2299	0	0.81 0.43 0.40 -0.02	0.0000	1	0.06	1.55 4.95 2.15	3	0	0.00 0.00 0.00	0.00	0.00
2298	1	0.52 -0.84 -0.13 0....	0.0000	1	0.06	1.85 4.75 2.15	3	0	0.00 0.00 0.00	0.00	0.00
2297	1	0.27 0.71 0.27 0.50	0.0000	1	0.06	5.15 4.55 2.15	6	0	0.00 0.00 0.00	0.00	0.00



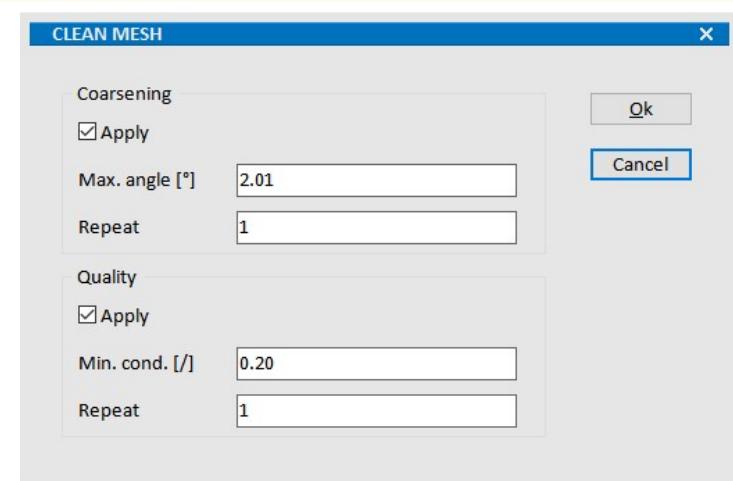
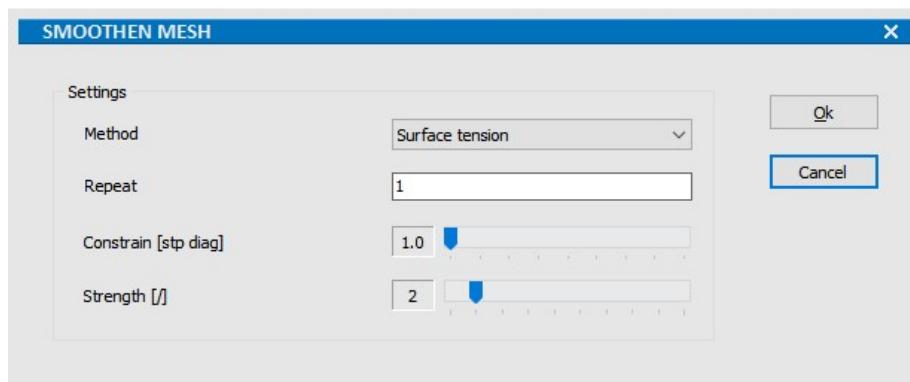
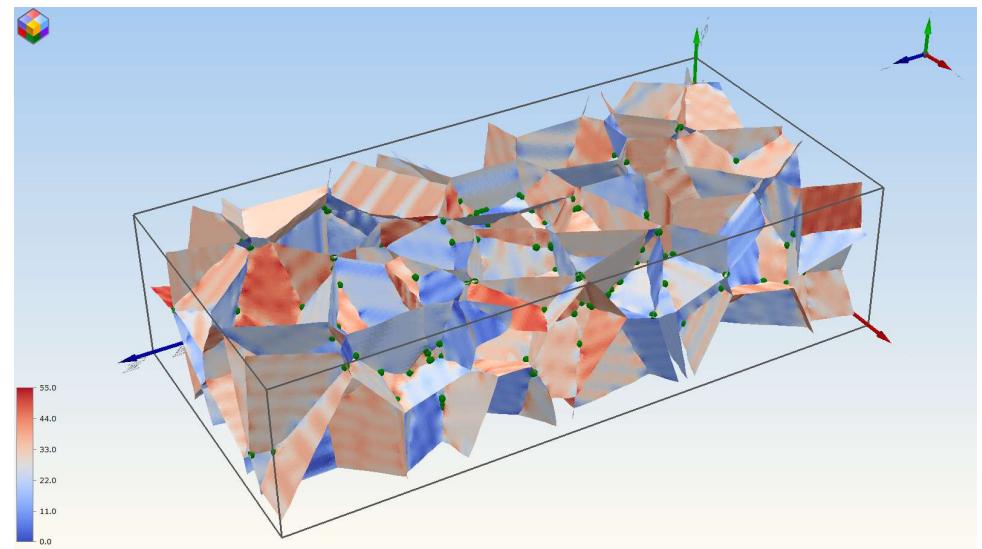
# ESPRIT QUBE

## Surface meshes



*Mesh structure generation:*

- EBSD grain boundary structure
- Dedicated color codes
- Smoothing
- Filtering



# ESPRIT QUBE

## Surface meshes



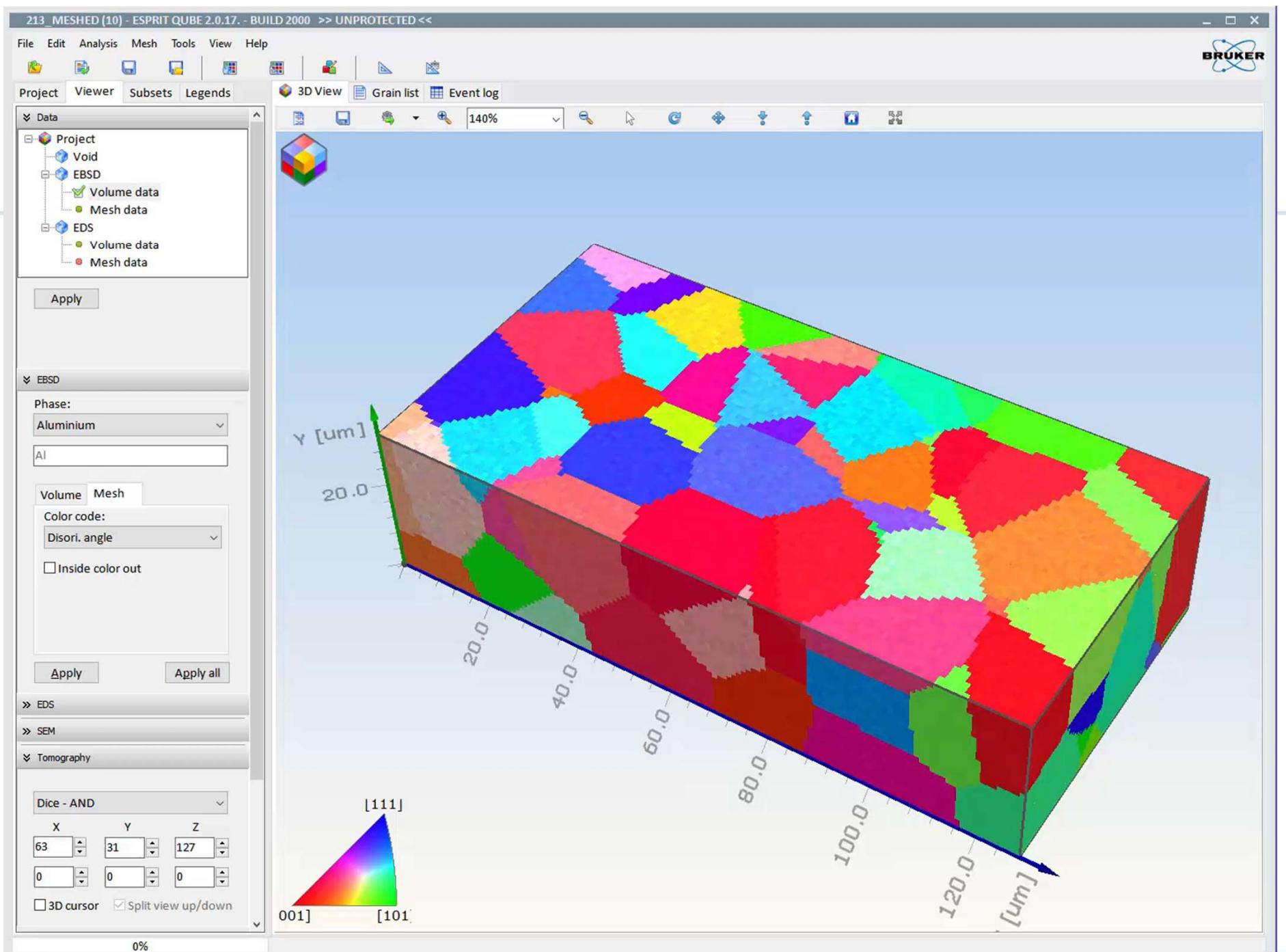
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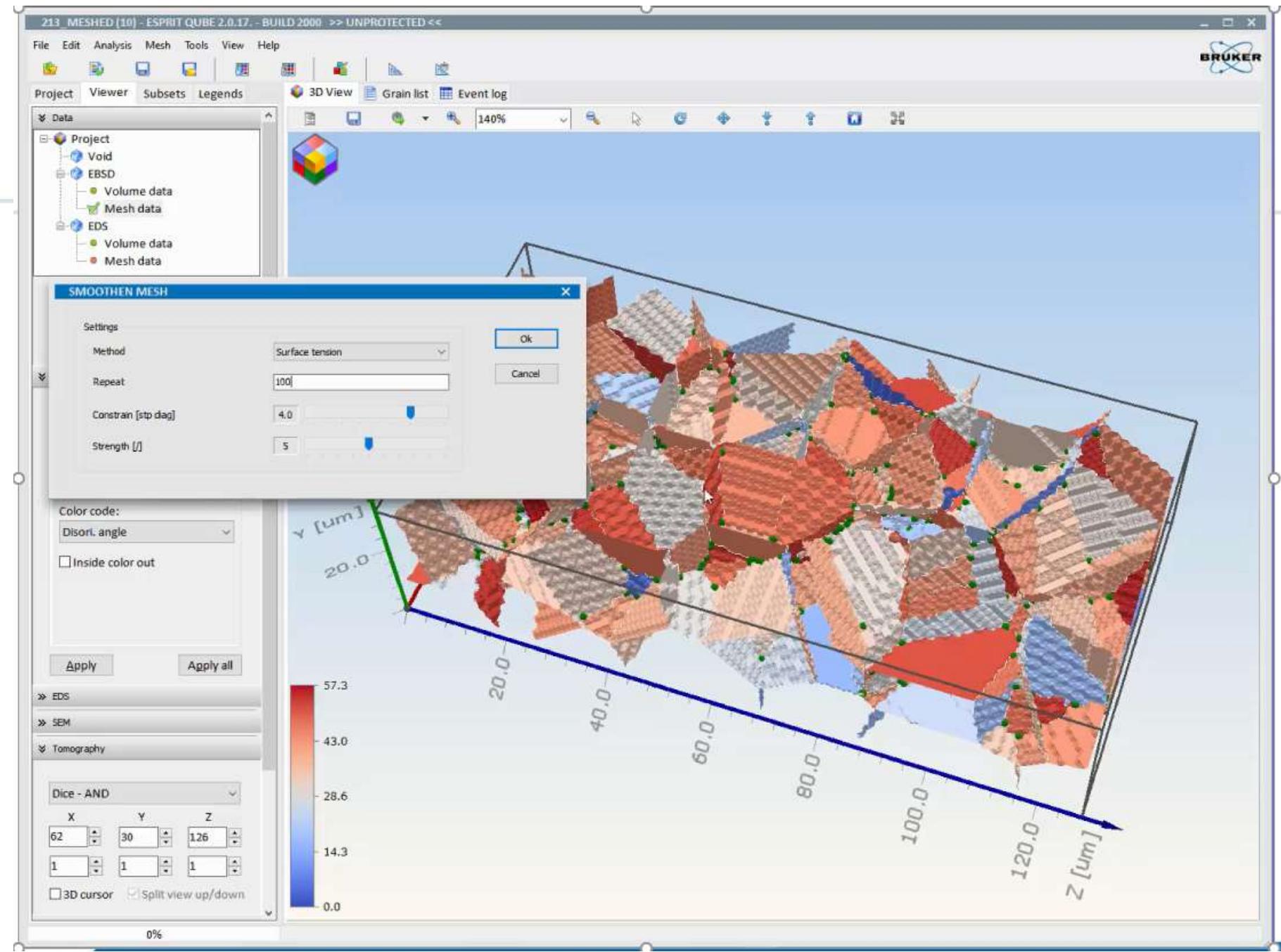
*Mesh structure generation:*

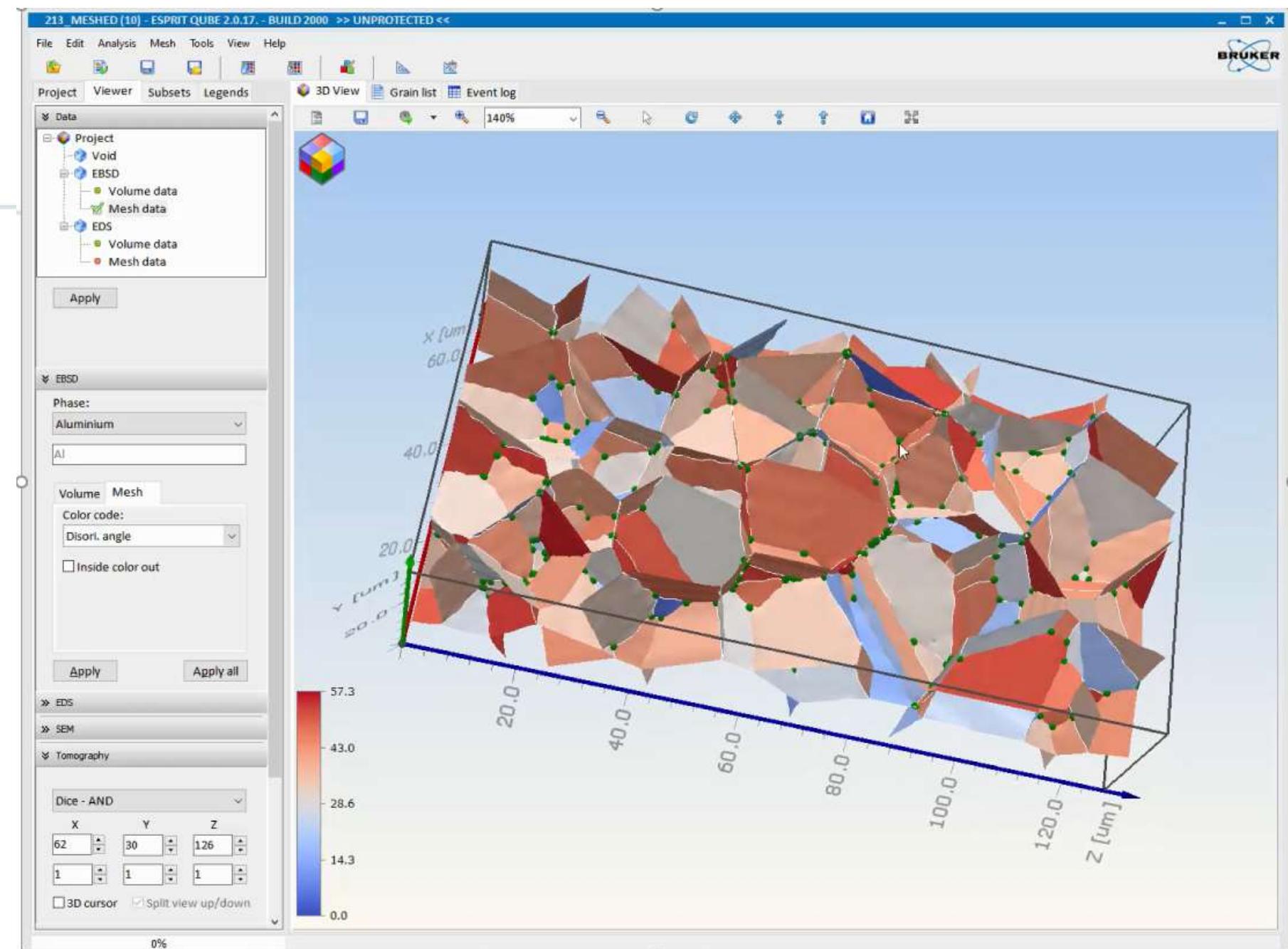
- EBSD grain boundary structure
- Dedicated color codes
- Smoothing
- Filtering

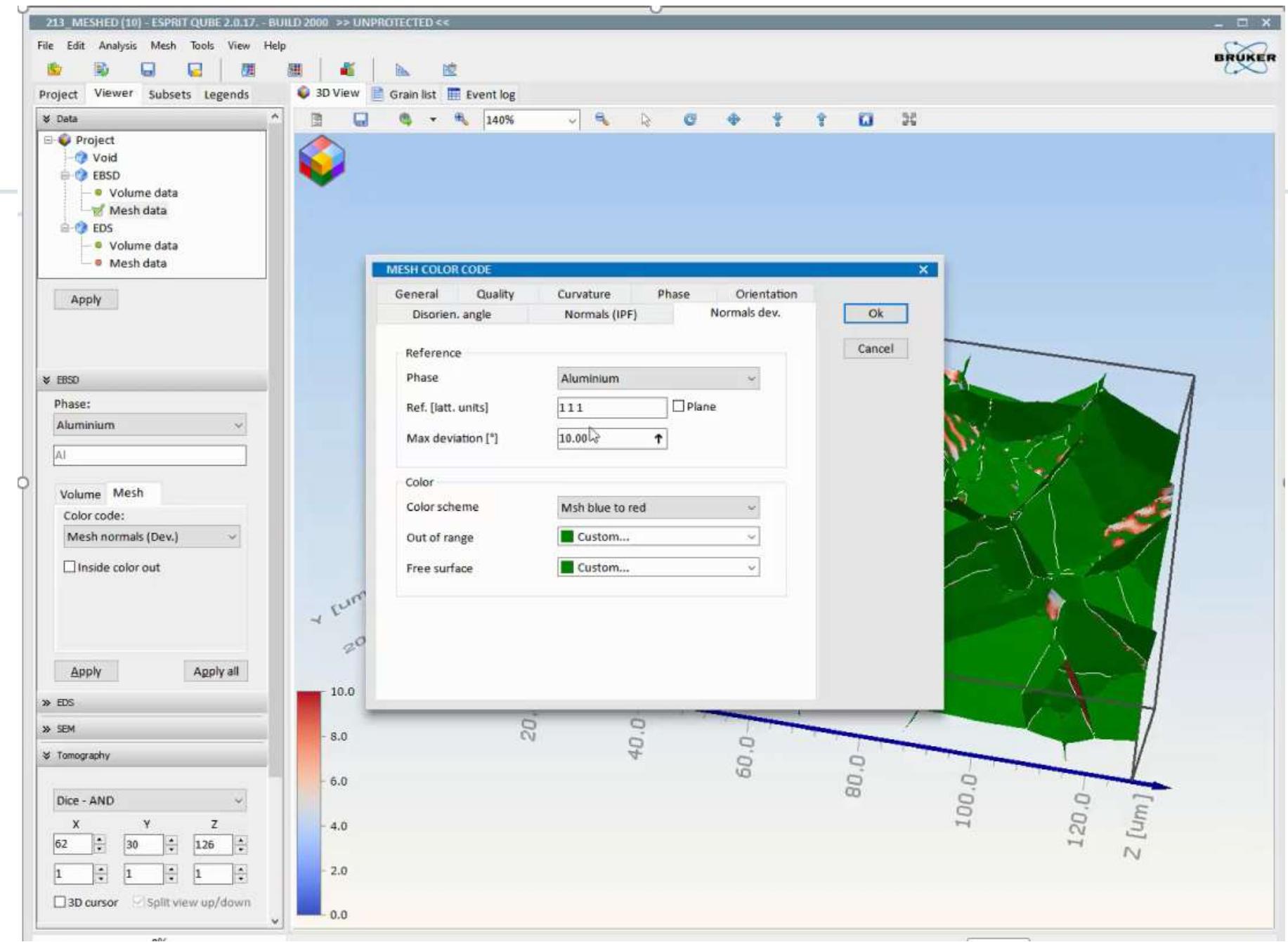
*Planned*

- EDS meshes
- Mesh subsets
- Boundary pole figures









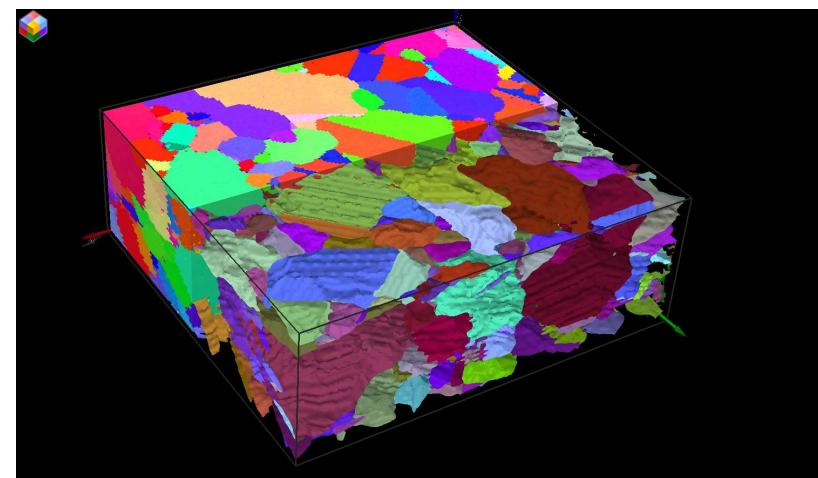
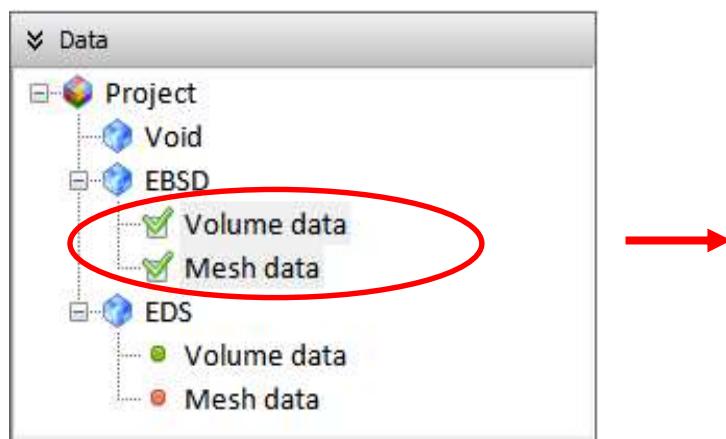
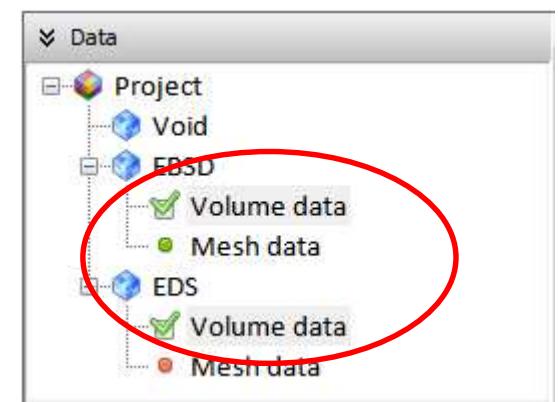
# ESPRIT QUBE

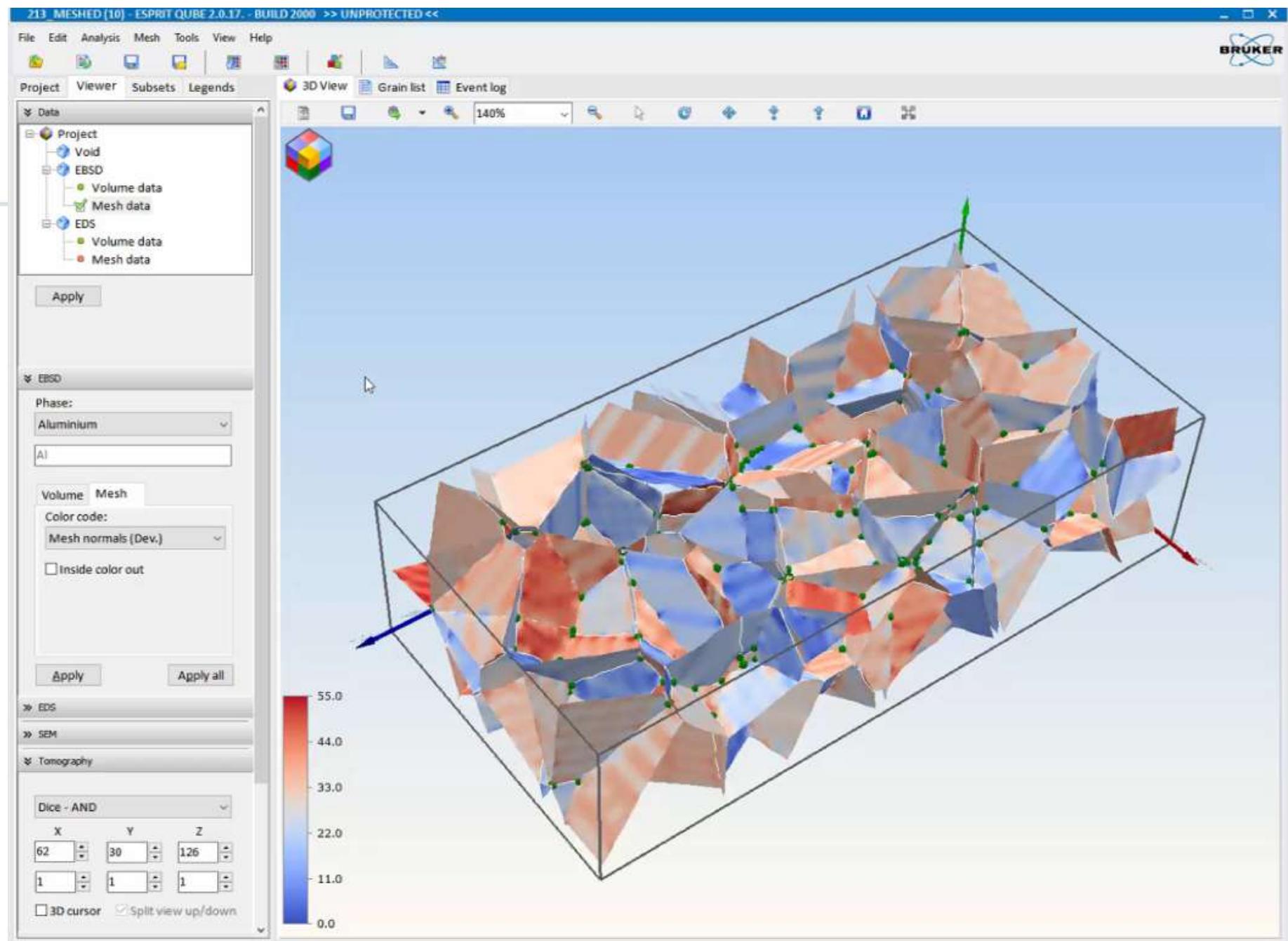
## Data synergy

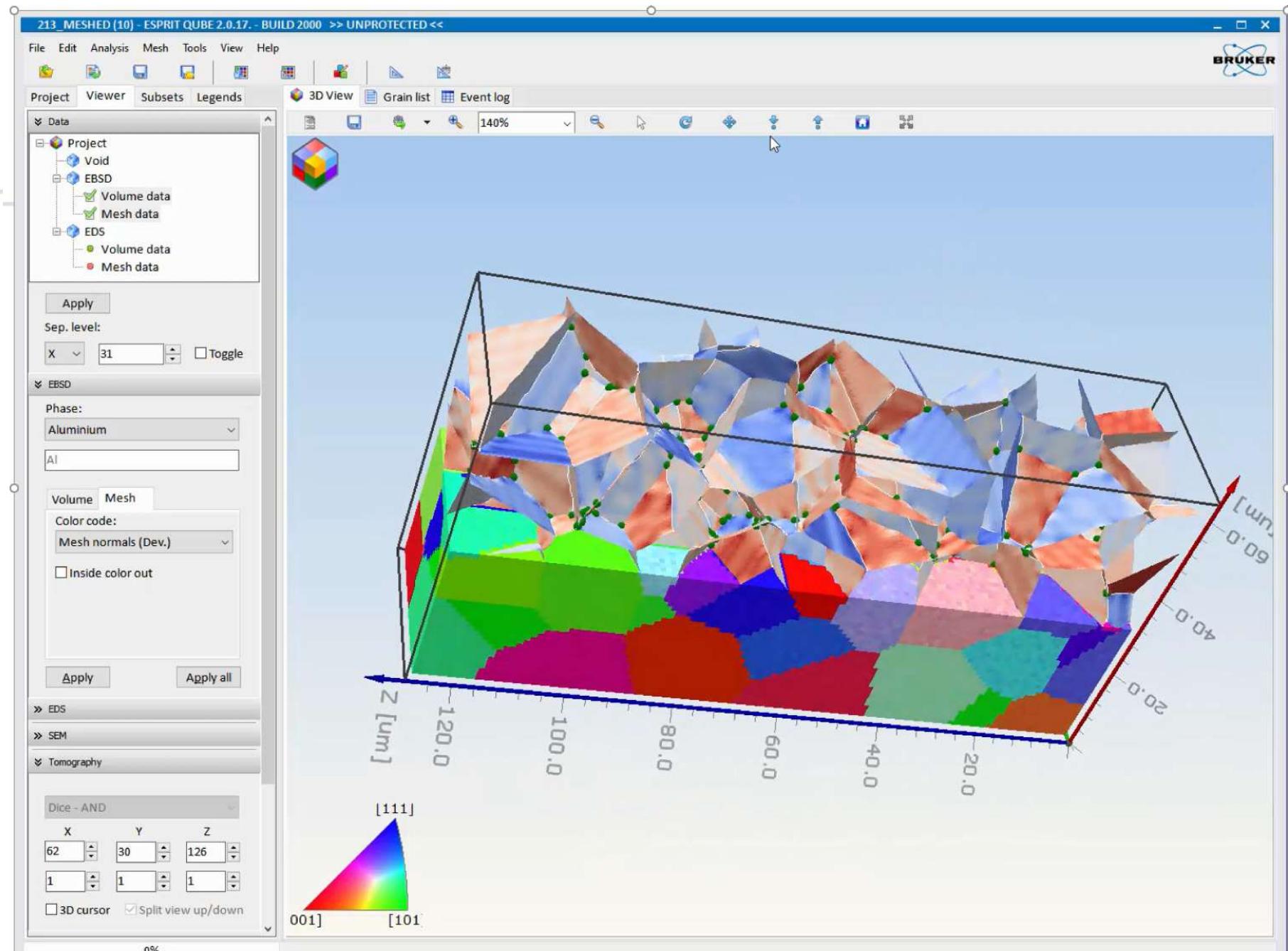


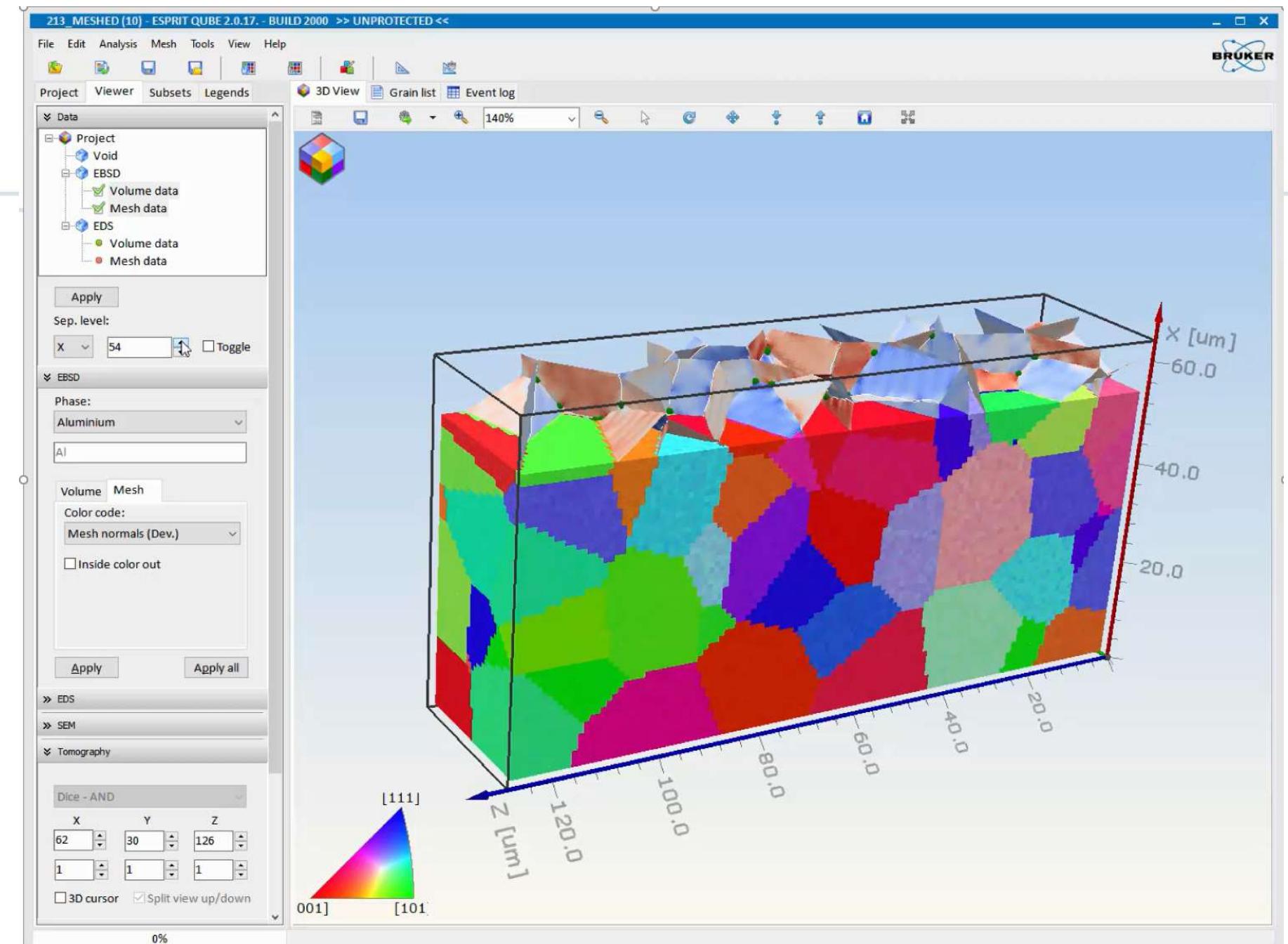
*Simultaneous viewing of data sets / representations:*

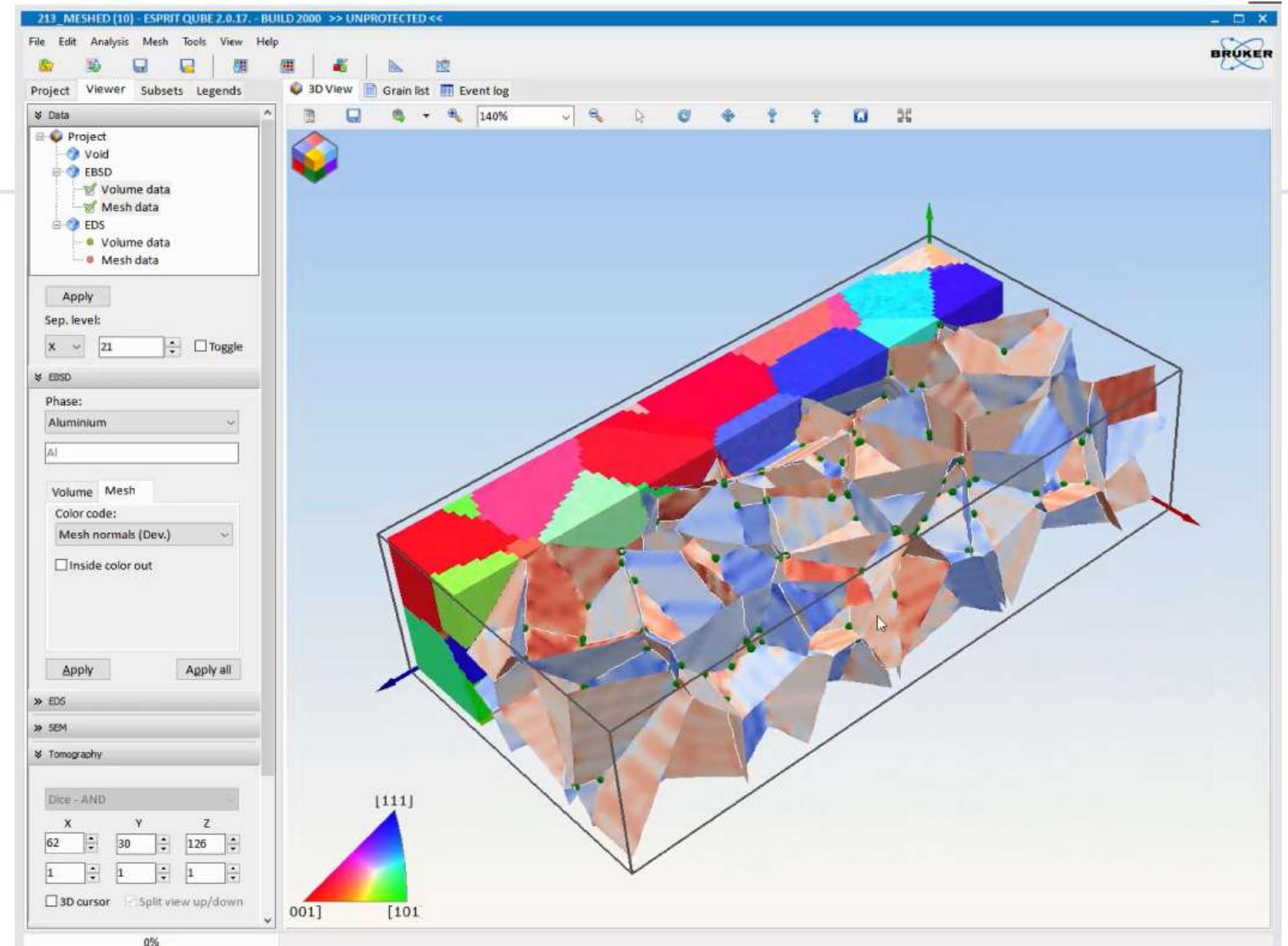
- Color blending: volume - volume
- Separation: volume – mesh

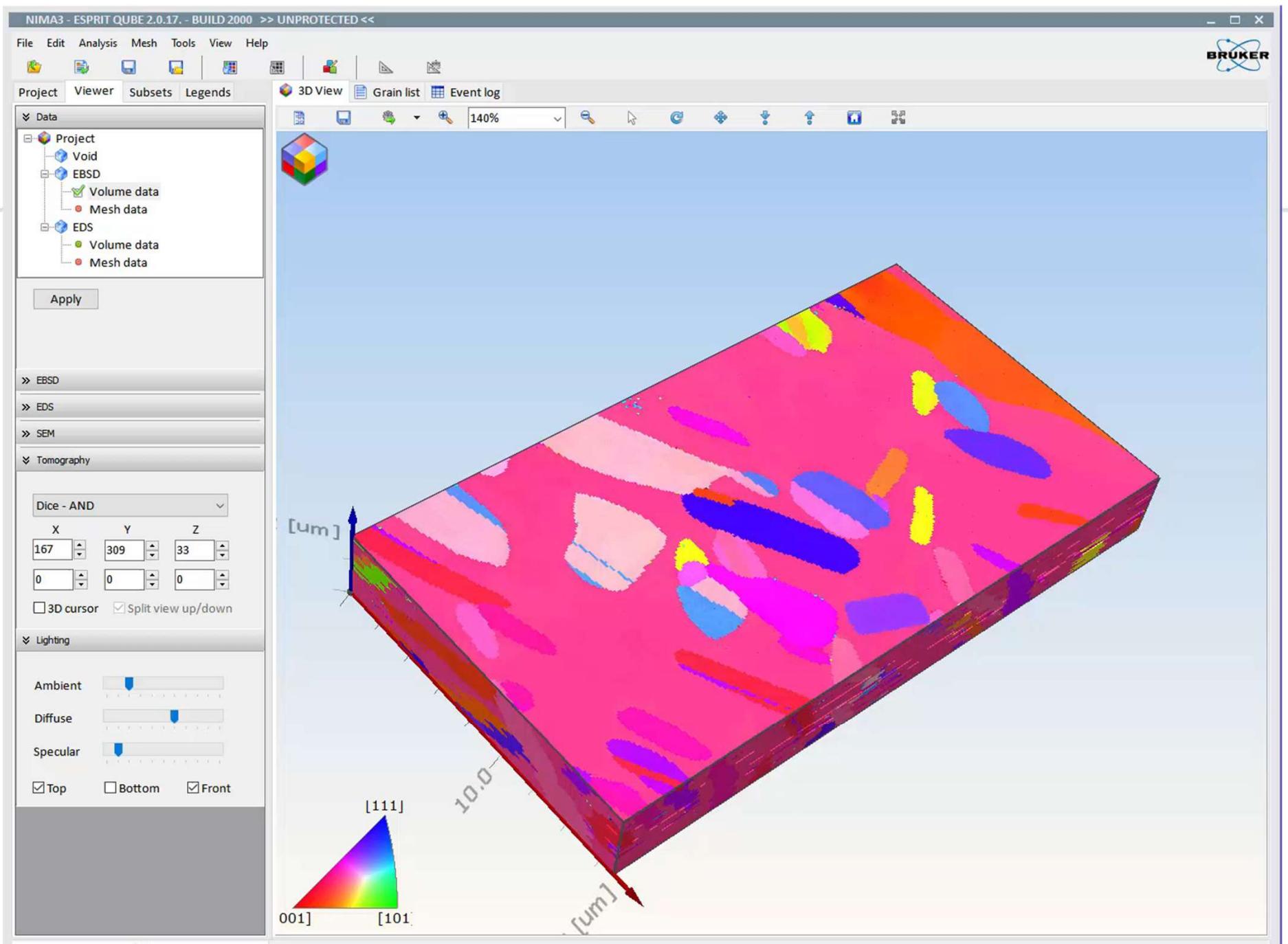


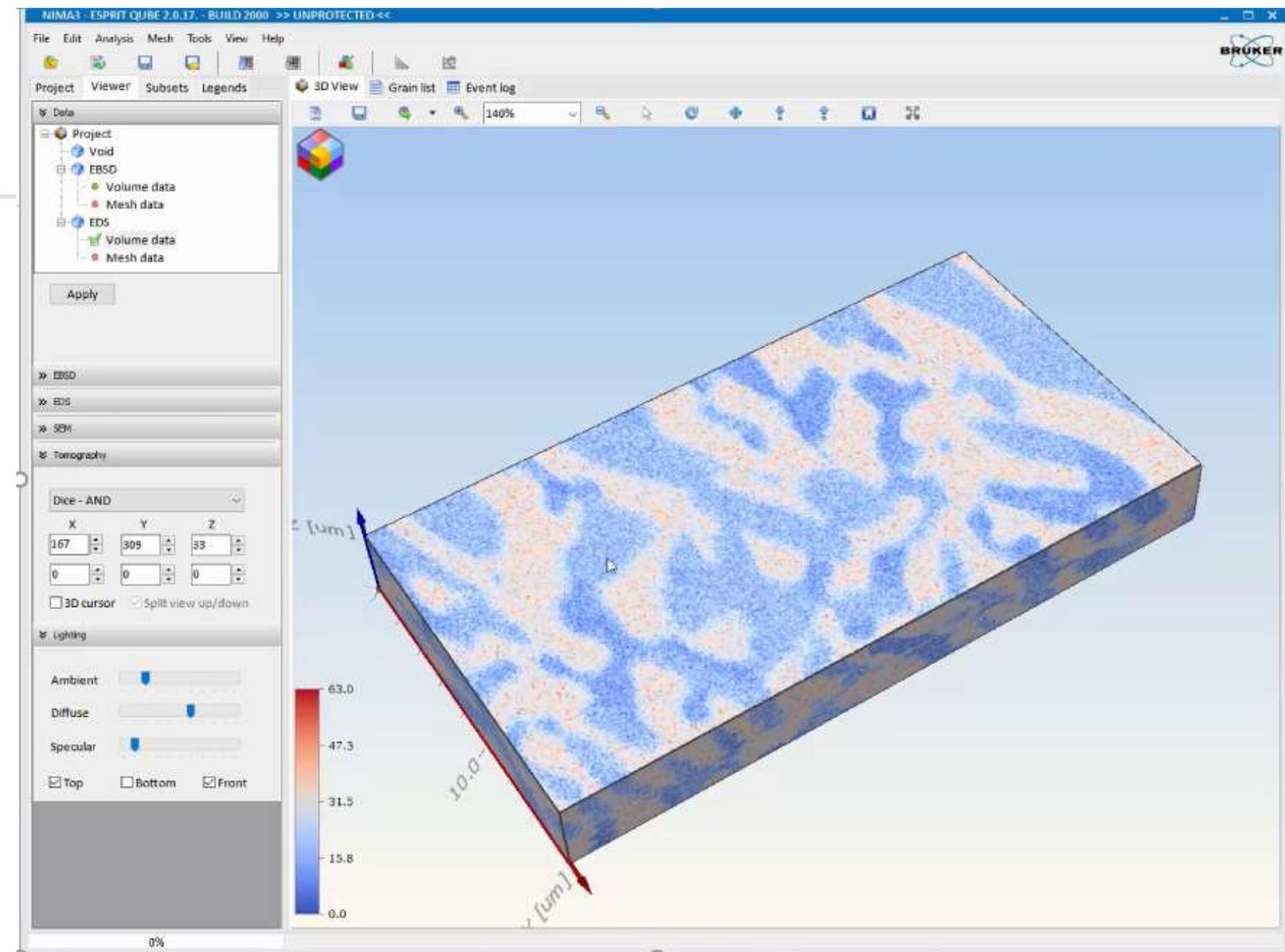


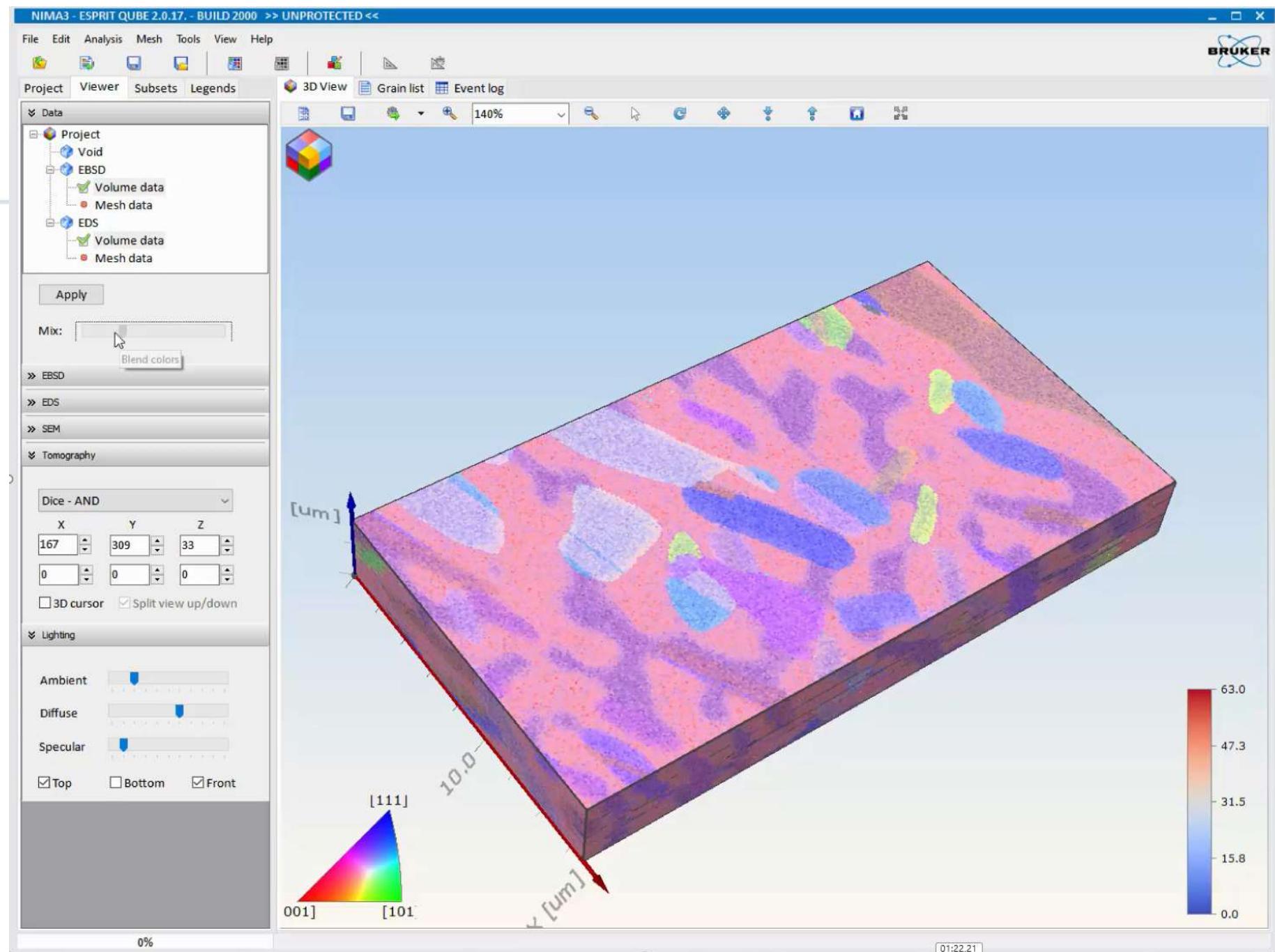












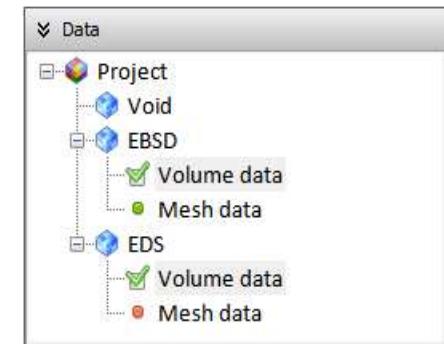
# ESPRIT QUBE

## Data synergy



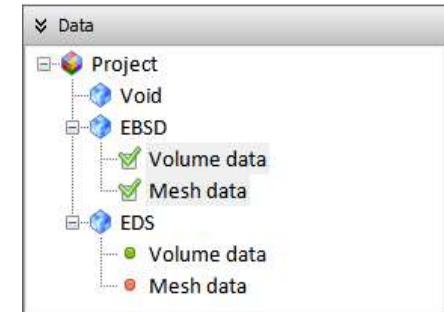
*Simultaneous viewing of data sets / representations:*

- Color blending: volume - volume
- Separation: volume – mesh



*Data set synergy:*

- Operate on multiple data sets simultaneously (limited by the data editing operations)
- Apply subsets across data sets (e.g. apply EBSD subset on EDS data set)



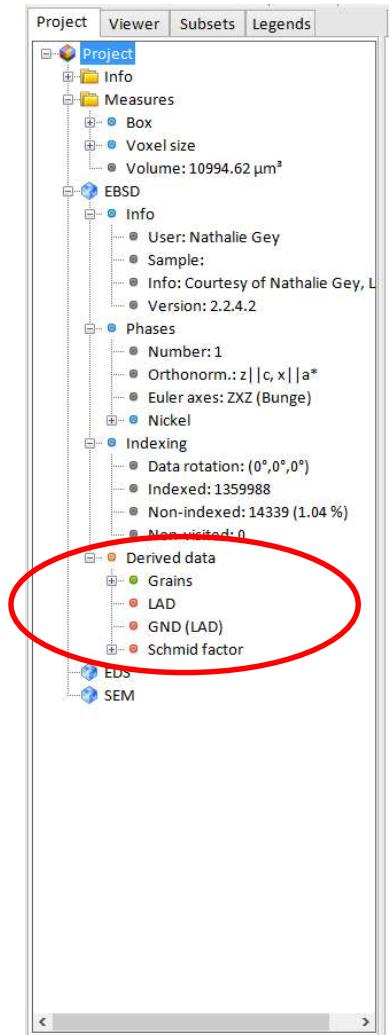
# ESPRIT QUBE

## Data monitoring



*Data compatibility:*

- Signals whether derived child data is still in sync with parent data.



# ESPRIT QUBE

## Data monitoring



### *Data compatibility:*

- Signals whether derived child data is still in sync with parent data

### *History:*

- Data operations are logged sequentially in project file

### *Reversibility:*

- Data changing operations can be undone

3D View	Grain list	Event log
		z = 12: Ni_ken_2nd_Slice0050.ctf
		z = 11: Ni_ken_2nd_Slice0051.ctf
		z = 10: Ni_ken_2nd_Slice0052.ctf
		z = 9: Ni_ken_2nd_Slice0053.ctf
		z = 8: Ni_ken_2nd_Slice0054.ctf
		z = 7: Ni_ken_2nd_Slice0055.ctf
		z = 6: Ni_ken_2nd_Slice0056.ctf
		z = 5: Ni_ken_2nd_Slice0057.ctf
		z = 4: Ni_ken_2nd_Slice0058.ctf
		z = 3: Ni_ken_2nd_Slice0059.ctf
		z = 2: Ni_ken_2nd_Slice0060.ctf
		z = 1: Ni_ken_2nd_Slice0061.ctf
		z = 0: Ni_ken_2nd_Slice0062.ctf
		Finished : 06/06/2016 20:07:23
		Cropping XY dimensions
		Started : 06/06/2016 20:09:17
		New X-size : 418 (@ old X=205)
		New Y-size : 383 (@ old Y=58)
		New/old : 0.51
		Finished : 06/06/2016 20:09:25
		Cropping XY dimensions
		Started : 14/06/2016 16:34:29
		New X-size : 171 (@ old X=130)
		New Y-size : 141 (@ old Y=110)
		New/old : 0.15
		Finished : 14/06/2016 16:34:31
		Median orientation filtering for all phases
		Started : 14/06/2016 16:35:31
		Kernel size : 3
		Thrshld angle : 3 deg
		Conv. angle : 0.1 deg
		Failed voxels : 0
		Finished : 14/06/2016 16:36:35
		Reconstructing grains
		Started : 14/06/2016 18:02:22
		Aborted : 14/06/2016 18:02:55
		Recovery : failed
		Reconstructing grains
		Started : 14/06/2016 18:03:05
		Thrshld angle : 5
		Neighbors : 1st 2nd 3rd
		Clean up : add to similar NB - keep orientations
		Thrshld vol : 3
		Grns removed : 520
		States chngd : 0
		Grns total : 964
		Finished : 14/06/2016 18:03:24



## Summary

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- Tool for post-acquisition analysis of tomographic data sets
- Dedicated for EBSD and EDS data sets
- Wysiwyg
- Extensive subset possibilities
- Convenient data monitoring
- Growing functionality

## Q&A

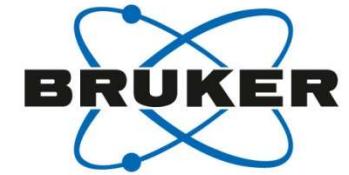
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### Are There Any Questions?

Please type in the questions you might have  
in the Q&A box and press *Send*

## More Information



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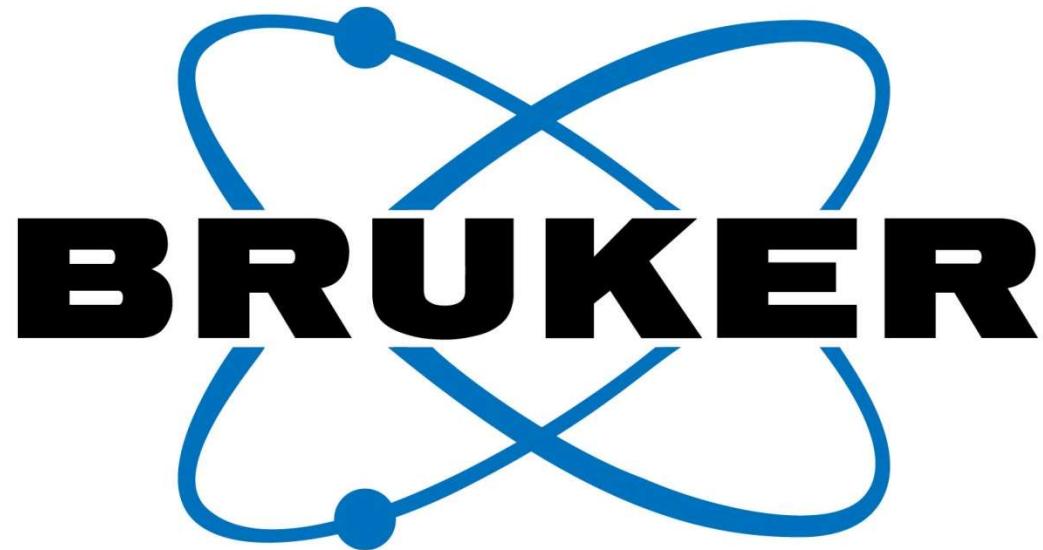
**For more information, please contact us:**

[laurie.palasse@bruker.com](mailto:laurie.palasse@bruker.com)

[peter.konijnenberg@bruker.com](mailto:peter.konijnenberg@bruker.com)

[info.bna@bruker.com](mailto:info.bna@bruker.com)

<https://www.bruker.com/products/x-ray-diffraction-and-elemental-analysis/eds-wds-ebsd-sem-micro-xrf-and-sem-micro-ct/quantax-ebsd/overview.html>



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