The Digital Twin – A comparative study of material simulation on µCT-scanned and modelled microstructures

Constantin Bauer

Math2Market GmbH

GeoDict
The Digital Material Laboratory

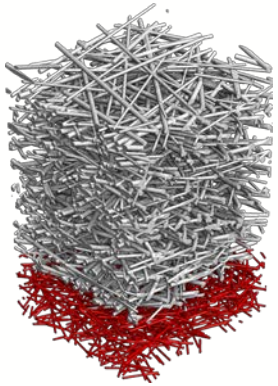
MATH 2 MARKET

What is GeoDict?

Import

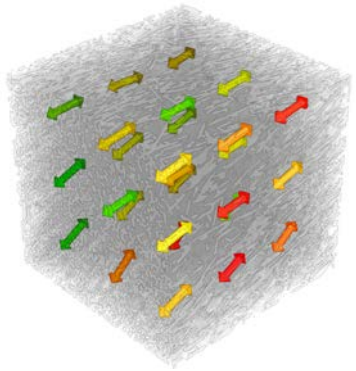
Diverse ways to import materials for modeling

Model



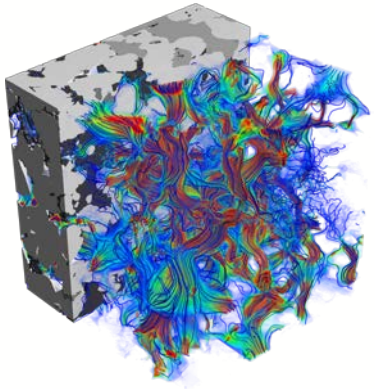
Detailed material models created in 3D

Analyze



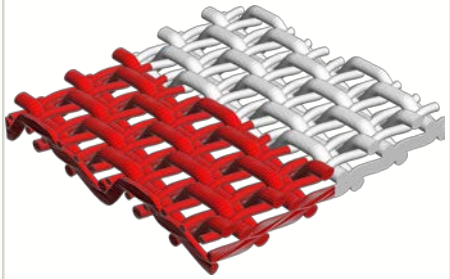
Extensive analysis and evaluation of structural material properties

Predict



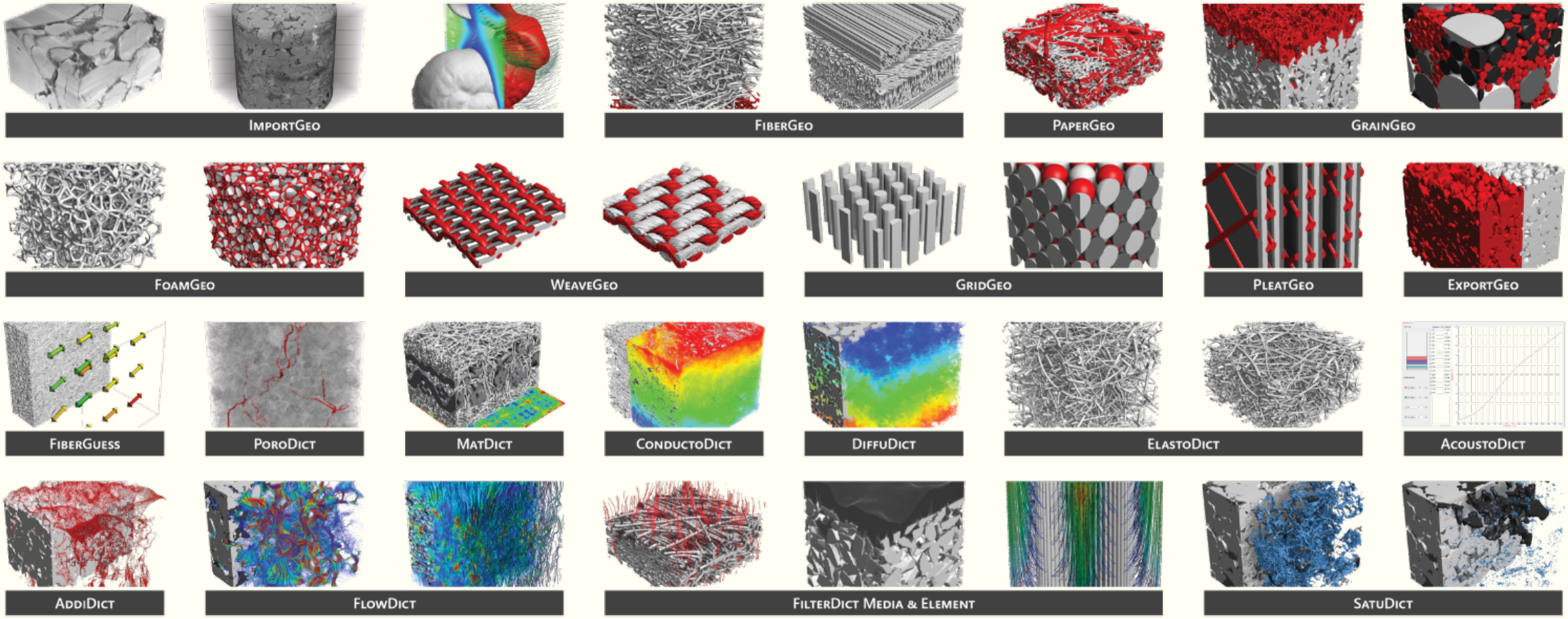
In-depth analysis and prediction of material behavior

Export



GeoDict models made available for standard workflows

GeoDict Module Overview

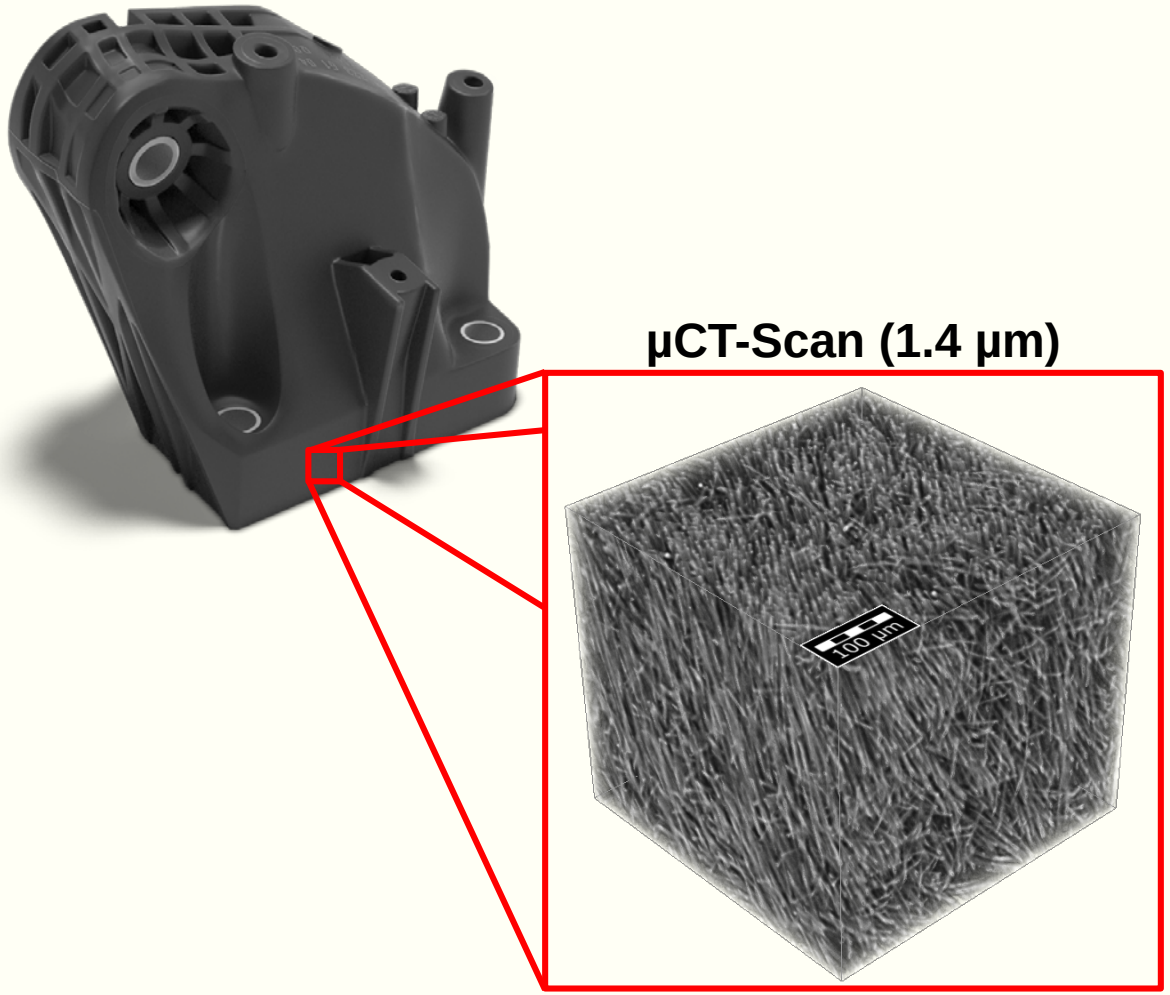


What material are we looking at?

- PA6GF50
  - Polyamide 6 matrix
  - short glass fiber reinforcement
  - 50 % fibers by weight

- produced by injection molding

- used in mass production for structural components (e.g. engine bearer)

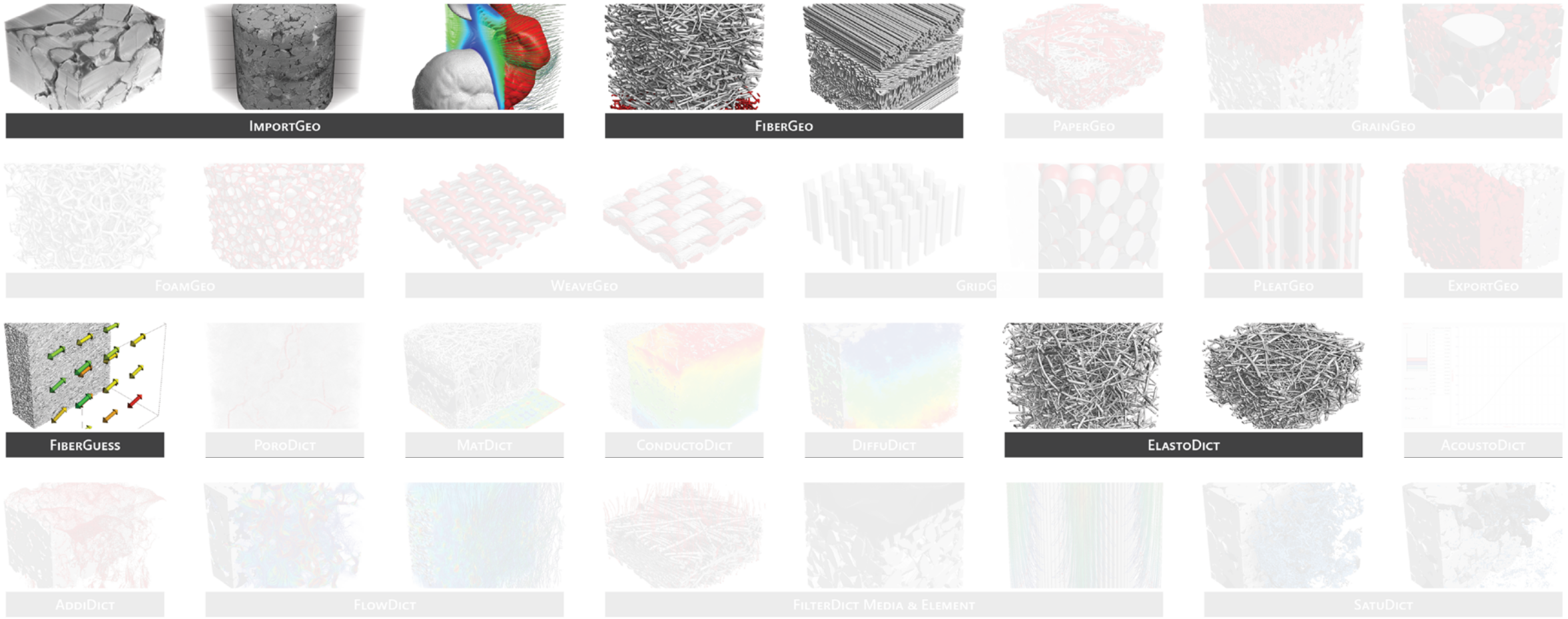


6 Steps to the Digital Twin

1. Import, process and segment the µCT-scan
2. Calculate the mechanical properties directly on the µCT-scan
3. Determine the geometrical properties of the material

   (fiber diameter, fiber orientation, fiber length)
4. Model the digital twin
5. Calculate the mechanical properties of the digital twin
6. Comparison of the results

used GeoDict Modules



Import and Segmentation

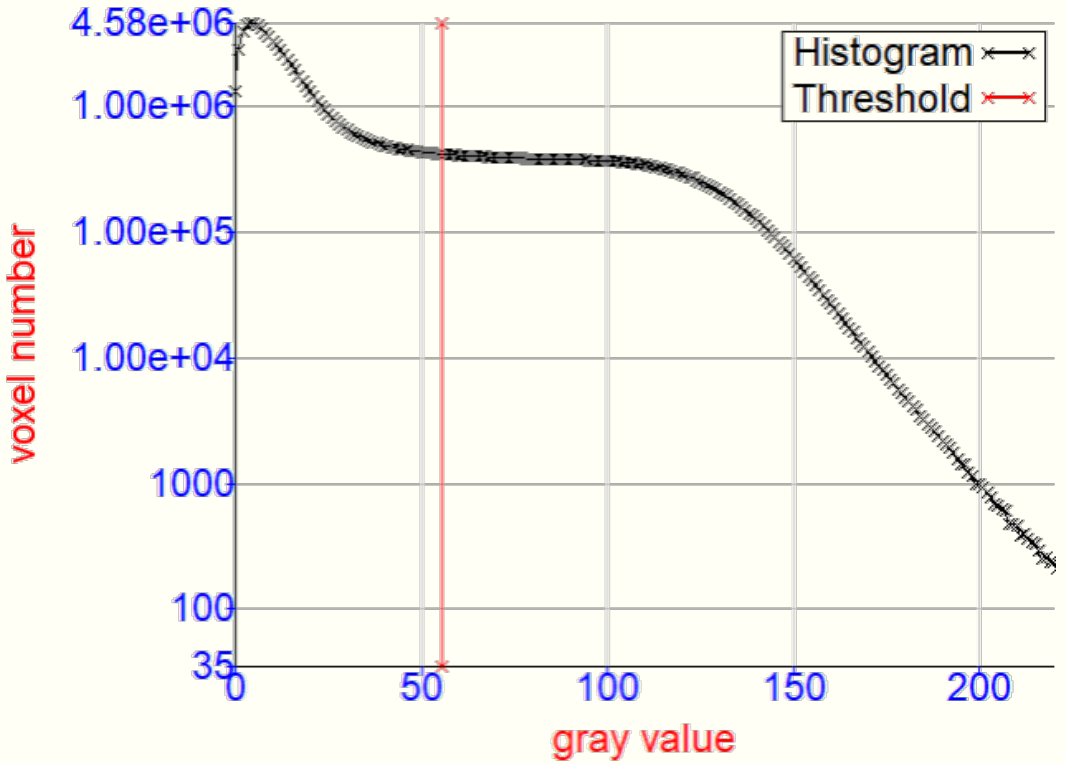
- Import a stack of 2d images
- Image processing to improve quality for segmentation

  (e.g. noise reduction, edge sharpening)

Applying a Non-Local Means Filter for noise reduction

Import and Segmentation

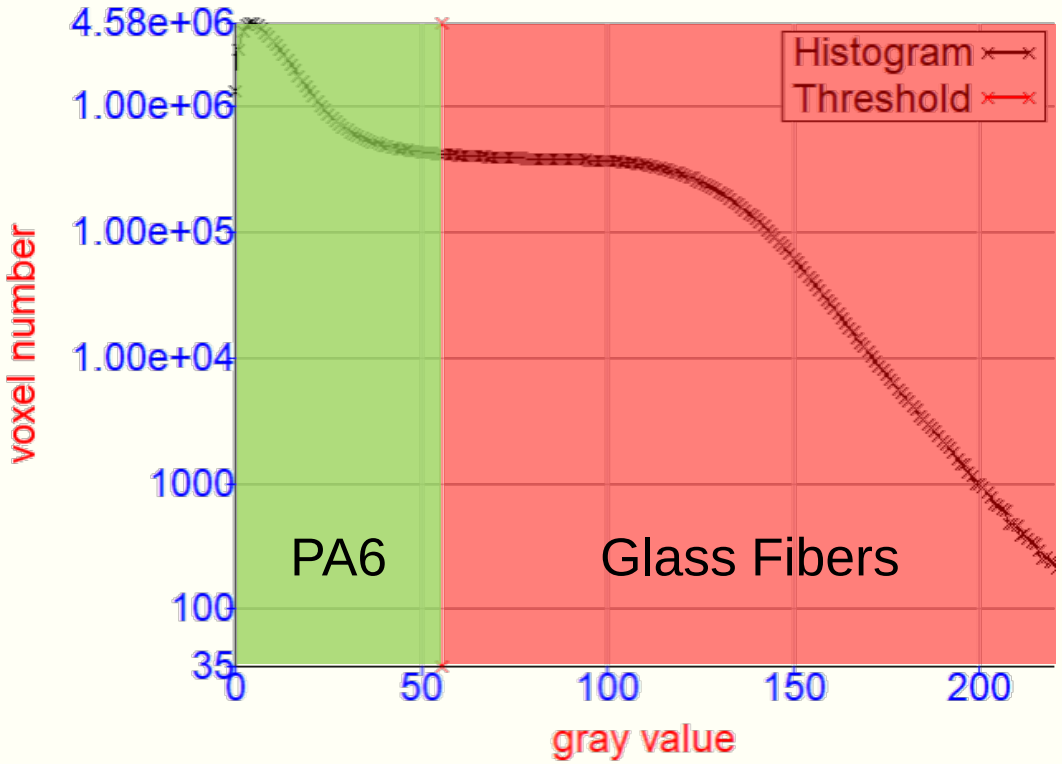
- automated thresholding using OTSU[1] algorithm



[1]Nobuyuki Otsu (1979). "A threshold selection method from gray-level histograms". IEEE Trans. Sys., Man., Cyber. 9 (1): 62–66

Import and Segmentation

- automated thresholding using OTSU[1] algorithm



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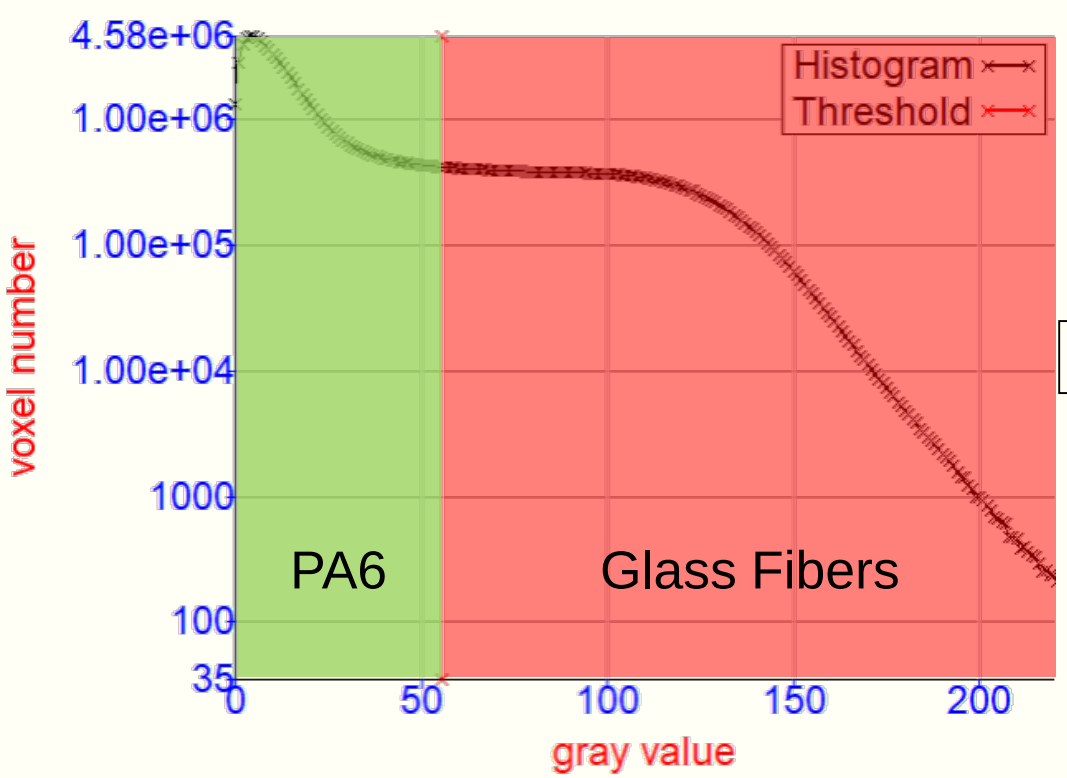
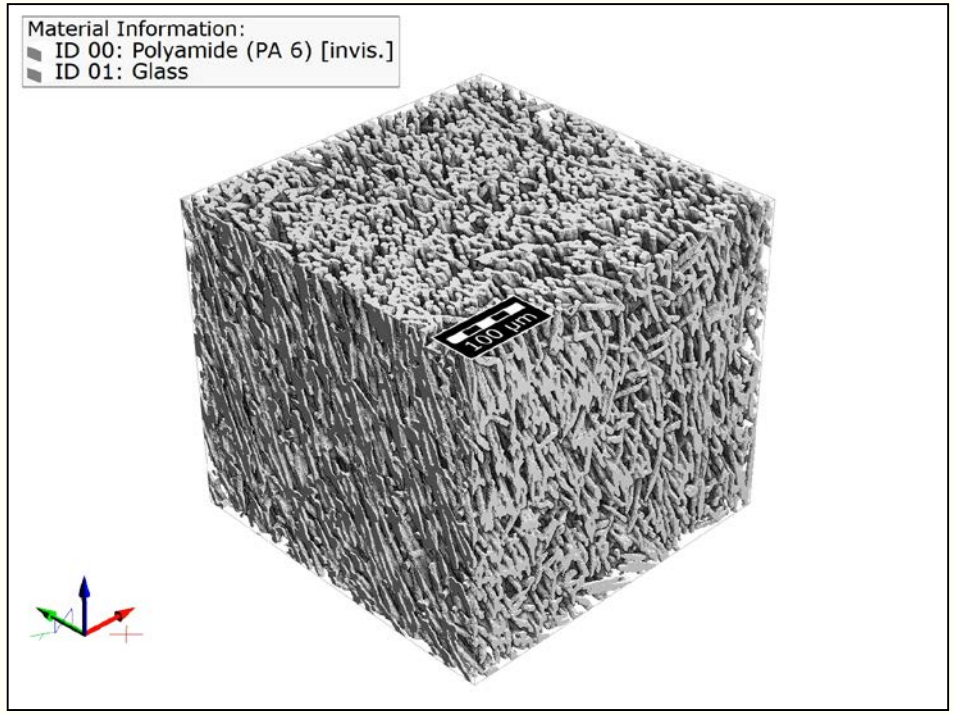


segmentation



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Mechanical Analysis - µCT scan

- linear elastic simulation of 6 different load cases
  - 3 uniaxial experiments
  - 3 shear experiments

$$C_{\alpha\beta} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix}$$

- used material properties
  - PA6: E=2.8 GPa / v=0.39
  - Glass: E=72 GPa / v=0.22

- computation time: 589 s
  - 4 CPUs
  - 0.5 GB memory

Mechanical Analysis - µCT scan

- calculated engineering parameters and stiffness tensor

Orthotropic Approximation

	Strain Equivalence	Energy Equivalence	Mean Value
Young's Modulus E_1 / (GPa)	7.1211	7.1213	7.1212 +- 0.0001
Young's Modulus E_2 / (GPa)	7.9283	7.9285	7.9284 +- 0.0001
Young's Modulus E_3 / (GPa)	11.3851	11.3852	11.3852 +- 0.0000
Poisson Ratio V_{12}	0.3547	0.3547	0.3547 +- 0.0000
Poisson Ratio V_{13}	0.2160	0.2160	0.2160 +- 0.0000
Poisson Ratio V_{23}	0.2517	0.2517	0.2517 +- 0.0000
Poisson Ratio V_{21}	0.3949	0.3949	0.3949 +- 0.0000
Poisson Ratio V_{31}	0.3454	0.3454	0.3454 +- 0.0000
Poisson Ratio V_{32}	0.3614	0.3614	0.3614 +- 0.0000
Shear Modulus G_{12} / (GPa)	2.7558	2.7557	2.7558 +- 0.0001
Shear Modulus G_{13} / (GPa)	3.0113	3.0111	3.0112 +- 0.0001
Shear Modulus G_{23} / (GPa)	3.8636	3.8635	3.8636 +- 0.0001

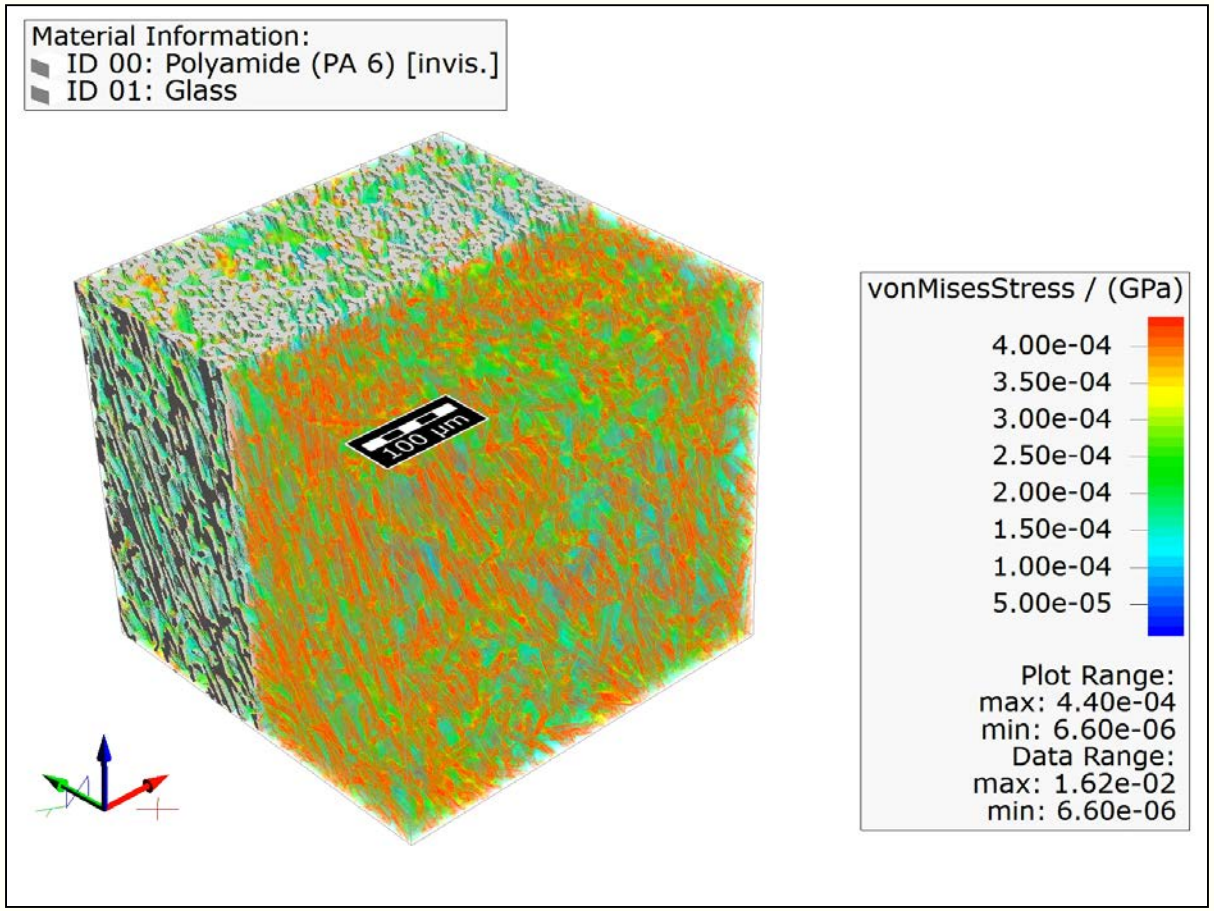
-------- **Anisotropic Elasticity Tensor** --------

Stiffness Formulation for Strain Equivalence / (GPa)

10.232	**5.4243**	**5.4948**	0.025524	-0.010267	0.14141
5.4244	**11.597**	**6.0651**	0.80216	-0.08876	0.12121
5.4949	**6.0652**	**15.475**	1.5932	-0.28255	-0.12848
0.025595	0.80212	1.5932	**3.8636**	-0.24775	-0.17071
-0.010275	-0.088766	-0.28258	-0.24774	**3.0113**	0.091551
0.14133	0.12119	-0.12859	-0.17072	0.091522	**2.7558**

Mechanical Analysis - µCT scan

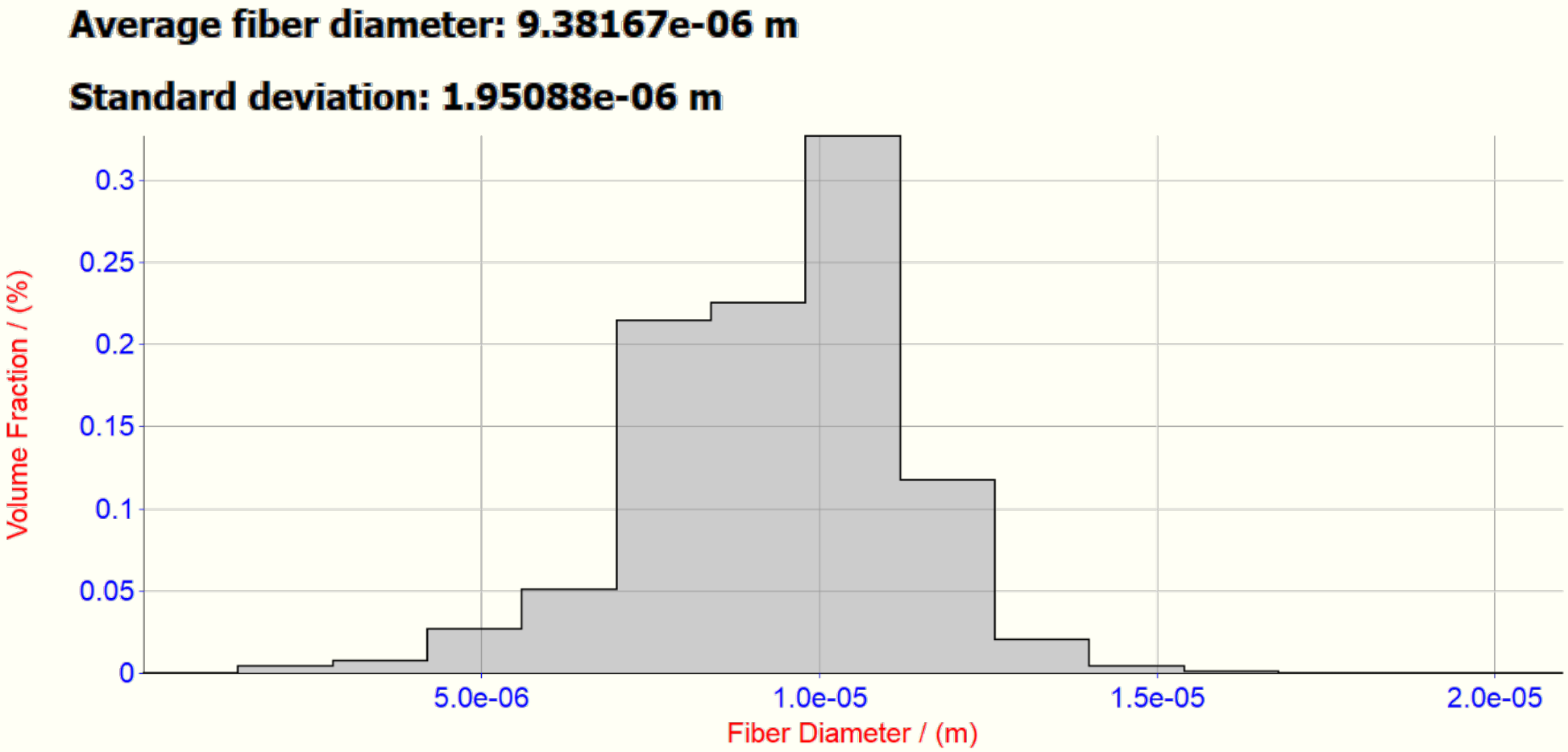
- visualization of the von-Mises stress



Modeling the Digital Twin

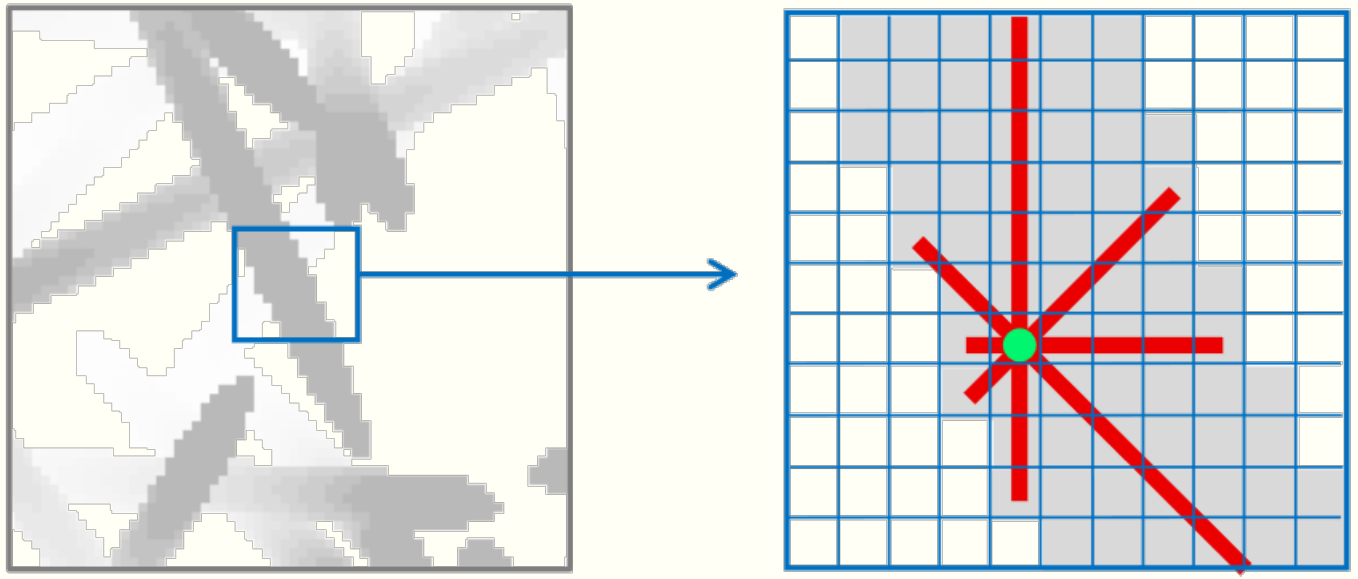
Digital Twin – Geometrical Analysis of µCT-Scan

- fiber diameter distribution



Digital Twin – Geometrical Analysis of µCT-Scan

- fiber orientation analysis
  - using Star Length Distribution Algorithm
  - works on a per-voxel basis
  - analyzes the chord lengths through the voxel for a pre-defined set of directions
  - the relative length of the cords gives the per-voxel orientation tensor
  - tensors are averaged

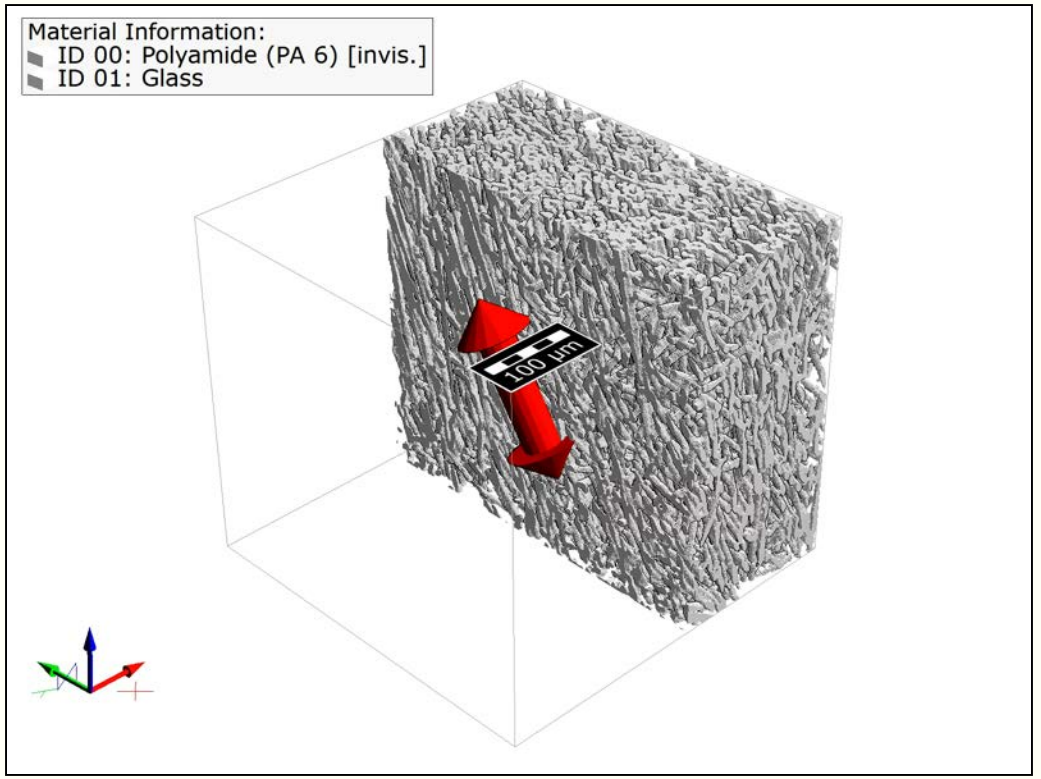


Digital Twin – Geometrical Analysis of µCT-Scan

- fiber orientation analysis
  - homogenized orientation tensor for the entire scan
  - visualization of the main orientation
- calculation of the fiber volume fraction

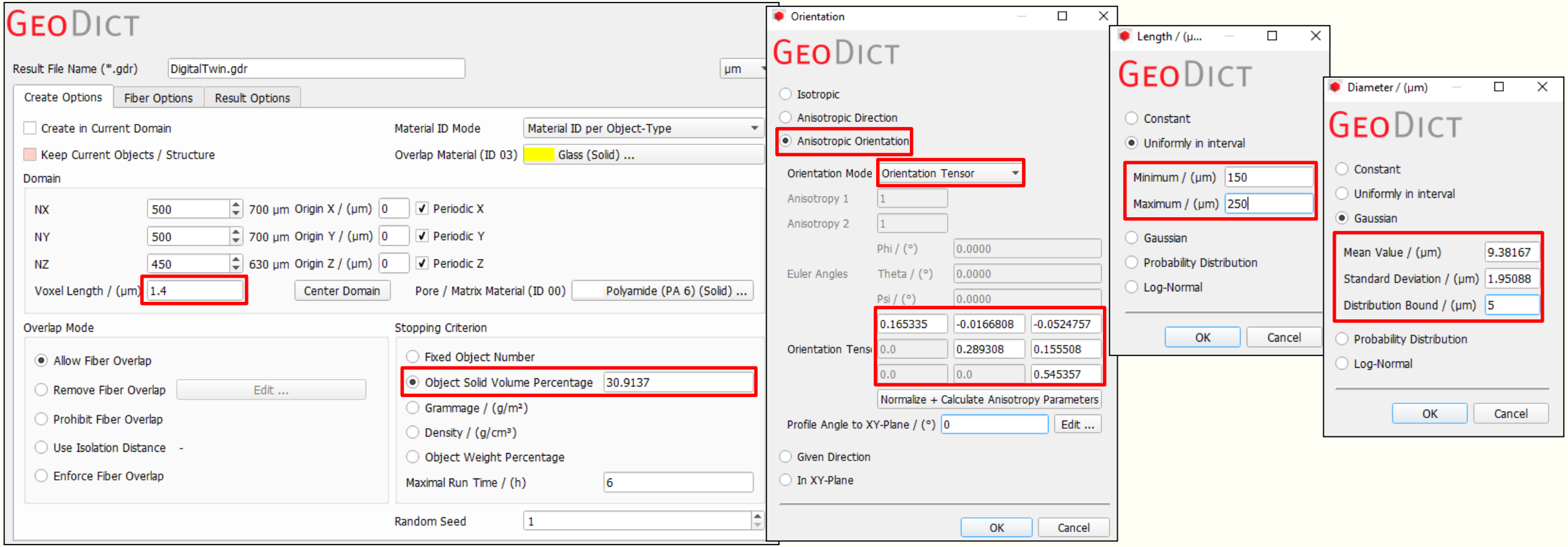
Block 0,0,0: Solid Volume Fraction = 30.9137%

0.165335	-0.0166808	-0.0524757
-	0.289308	0.155508
-	-	0.545357



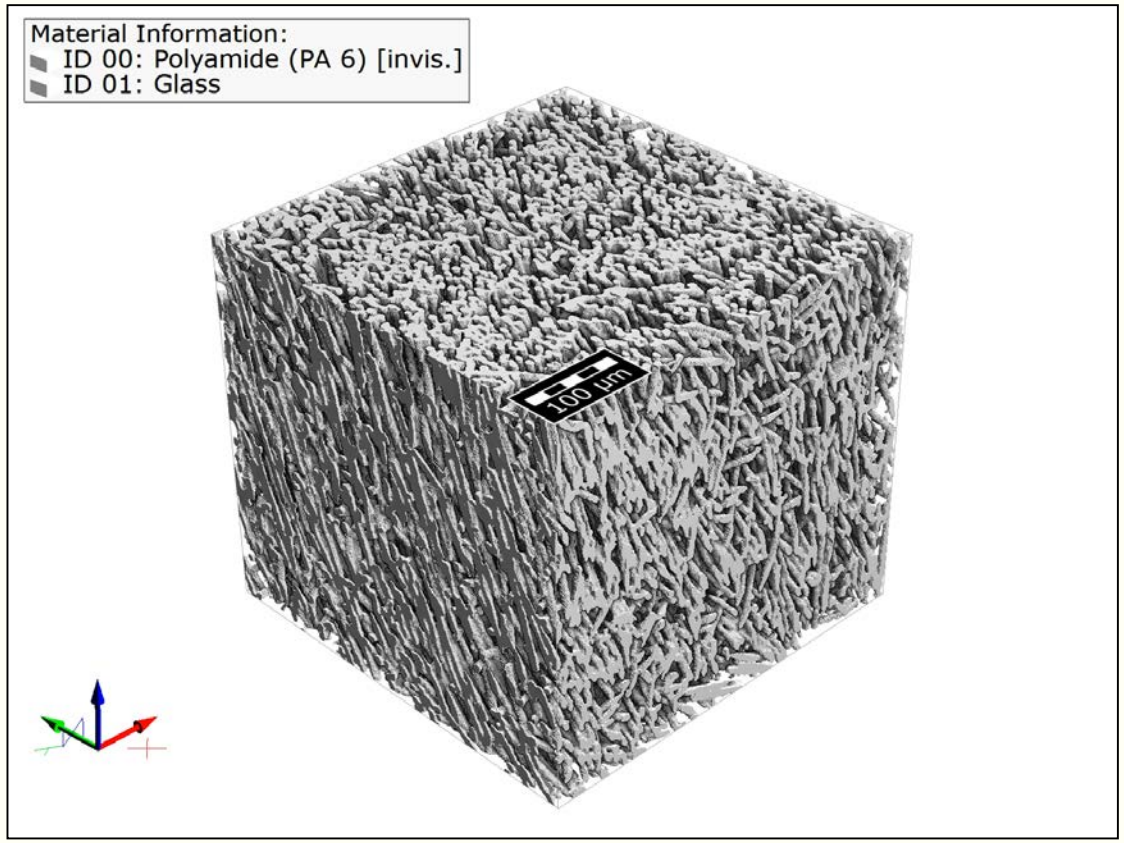
Digital Twin – Modelling

- use all collected geometrical properties of the material for modelling the digital twin in **FiberGeo**

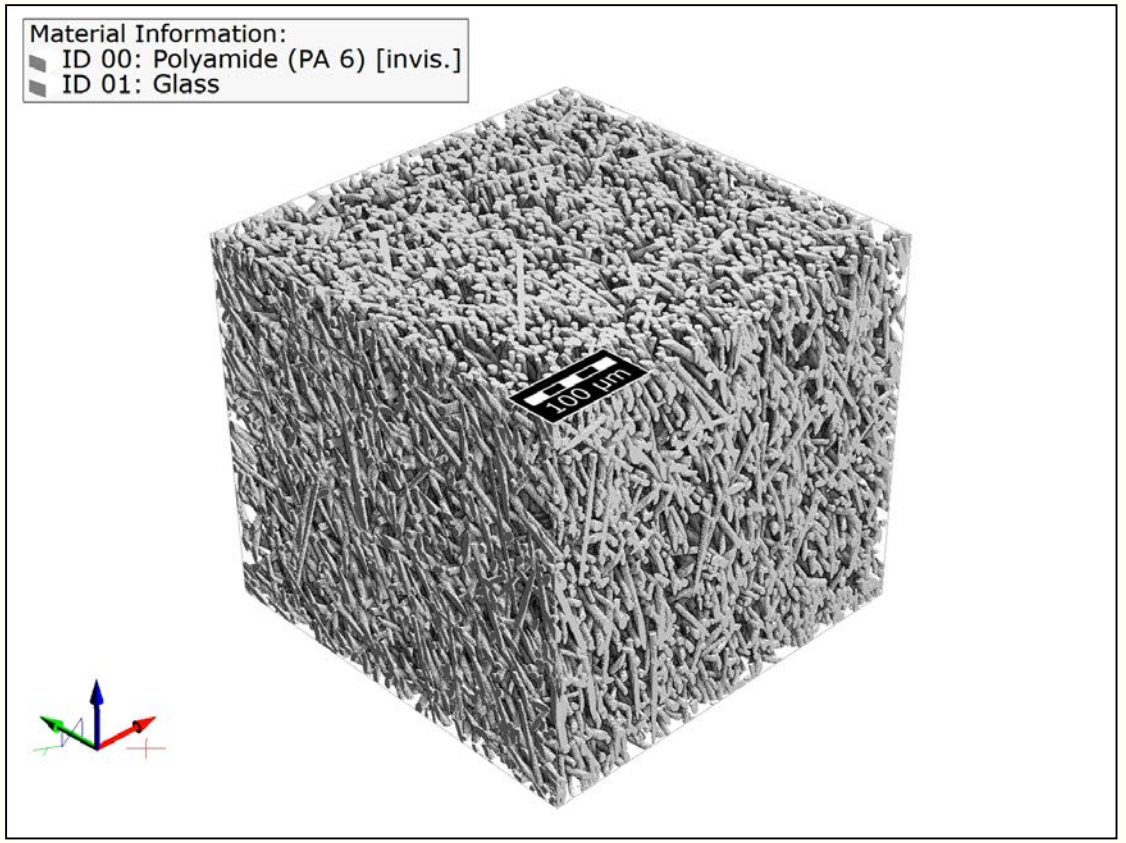


Digital Twin – Modelling

- visual comparison of the twin and the µCT-scan



µCT-Scan



Digital Twin

Digital Twin – Mechanical Analysis

- comparison of the stiffness tensor

-------- Anisotropic Elasticity Tensor --------

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µCT-Scan

-------- Anisotropic Elasticity Tensor --------

Stiffness Formulation for Strain Equivalence / (GPa)

10.757	**5.4859**	**5.5878**	0.053966	0.06989	0.16679
5.4859	**11.688**	**6.0427**	0.78271	-0.070062	0.16912
5.5879	**6.0427**	**14.307**	1.1605	-0.031768	-0.05373
0.054045	0.78275	1.1605	**3.6667**	-0.15612	-0.11499
0.069986	-0.069923	-0.031719	-0.15614	**3.1619**	0.081569
0.16684	0.16916	-0.053757	-0.11499	0.081581	**2.9358**

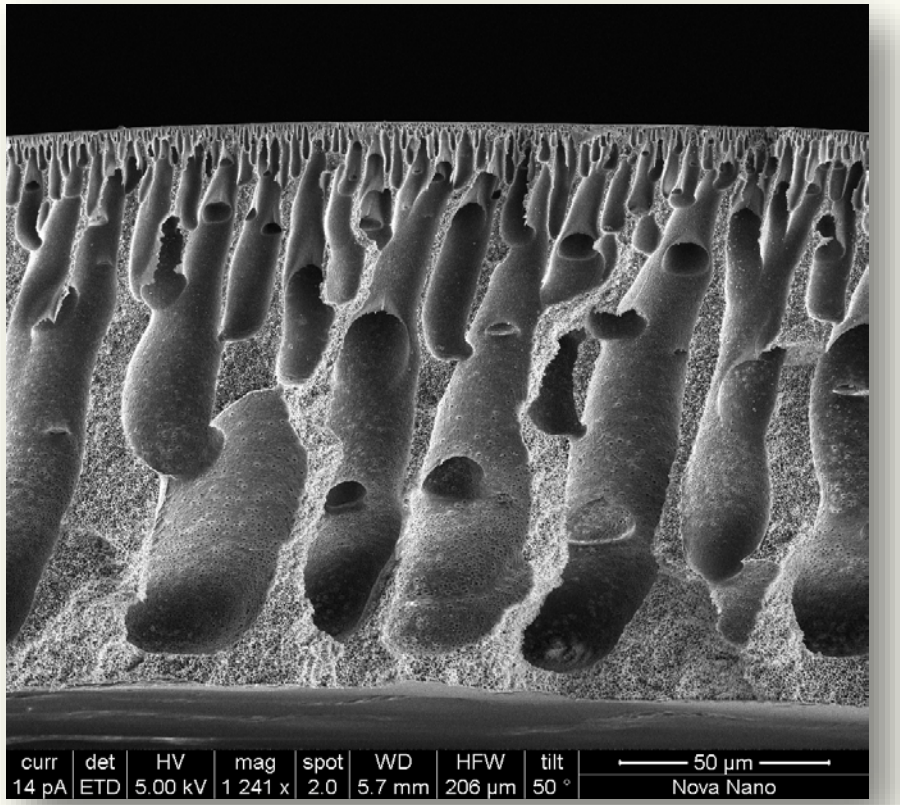
Digital Twin

⇨ **very good agreement between µCT-scan and digital twin**

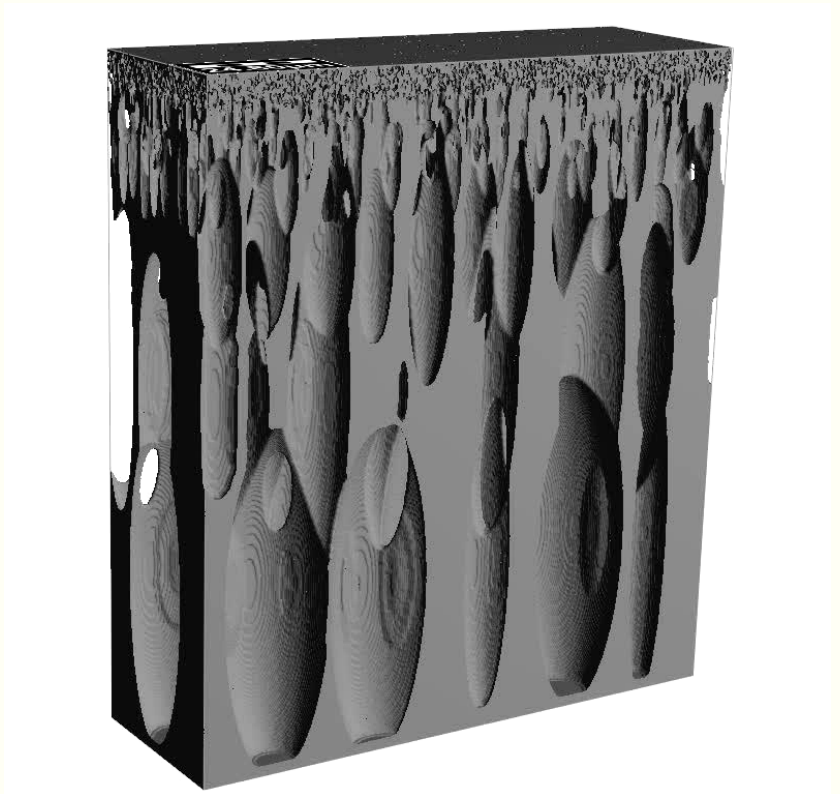
Digital Twin – Some Examples

Digital Twin – Polysulfone micromembrane

- used for seawater desalination



SEM image

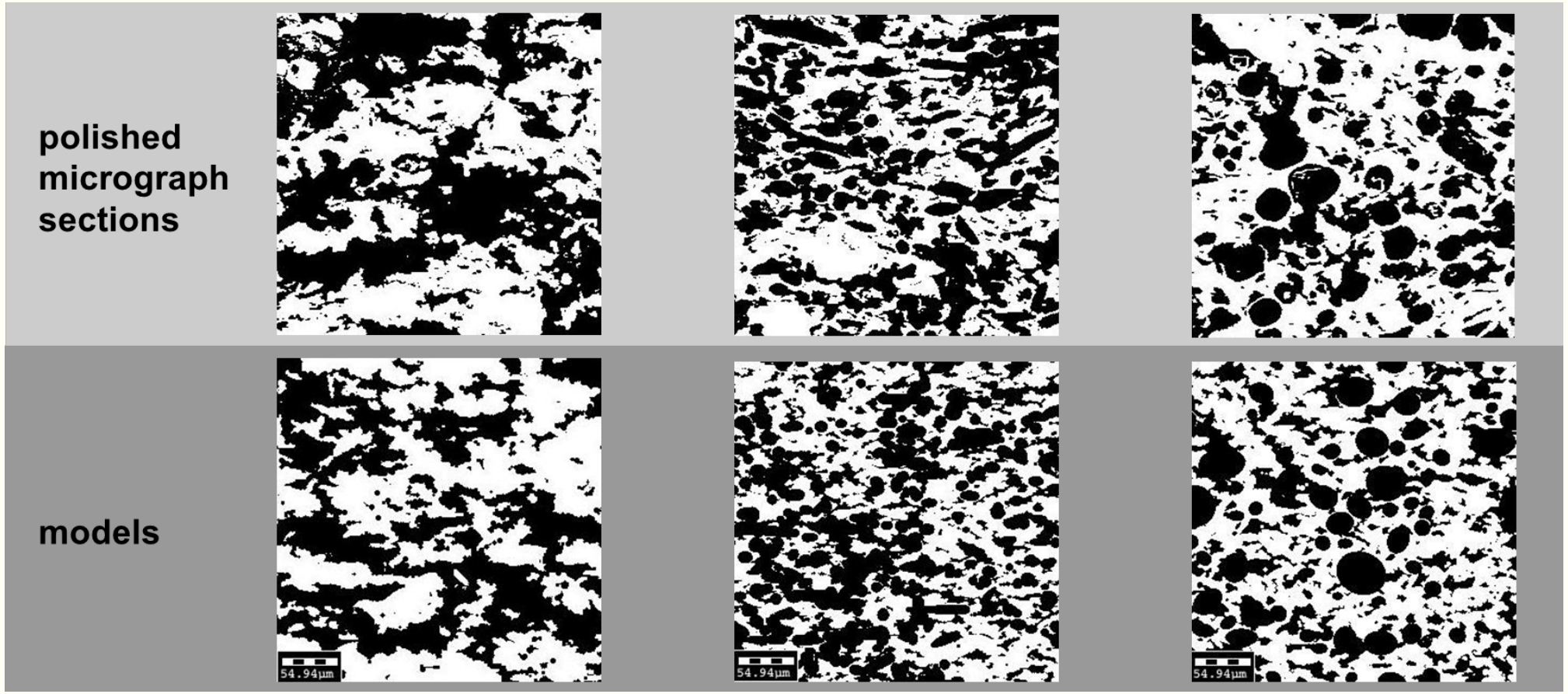


Digital Twin

[Shi et al., Water flow prediction for Membranes using 3D simulations with detailed morphology, 2015, Journal of Membrane Science]

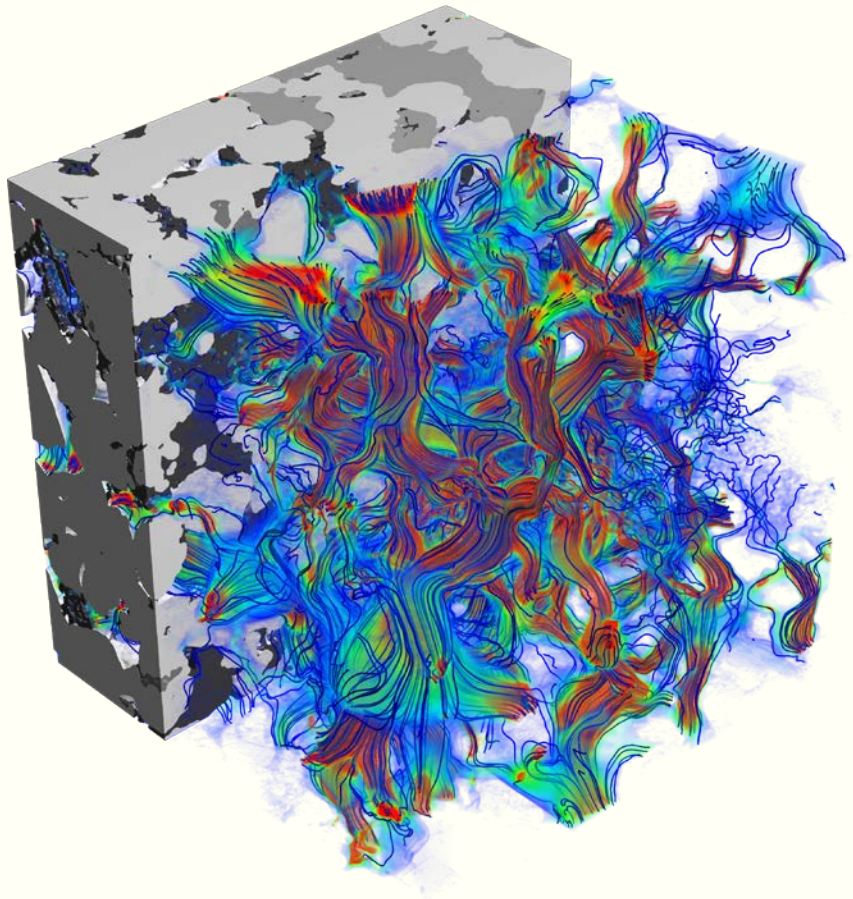
Digital Twin – Sintered Ceramic

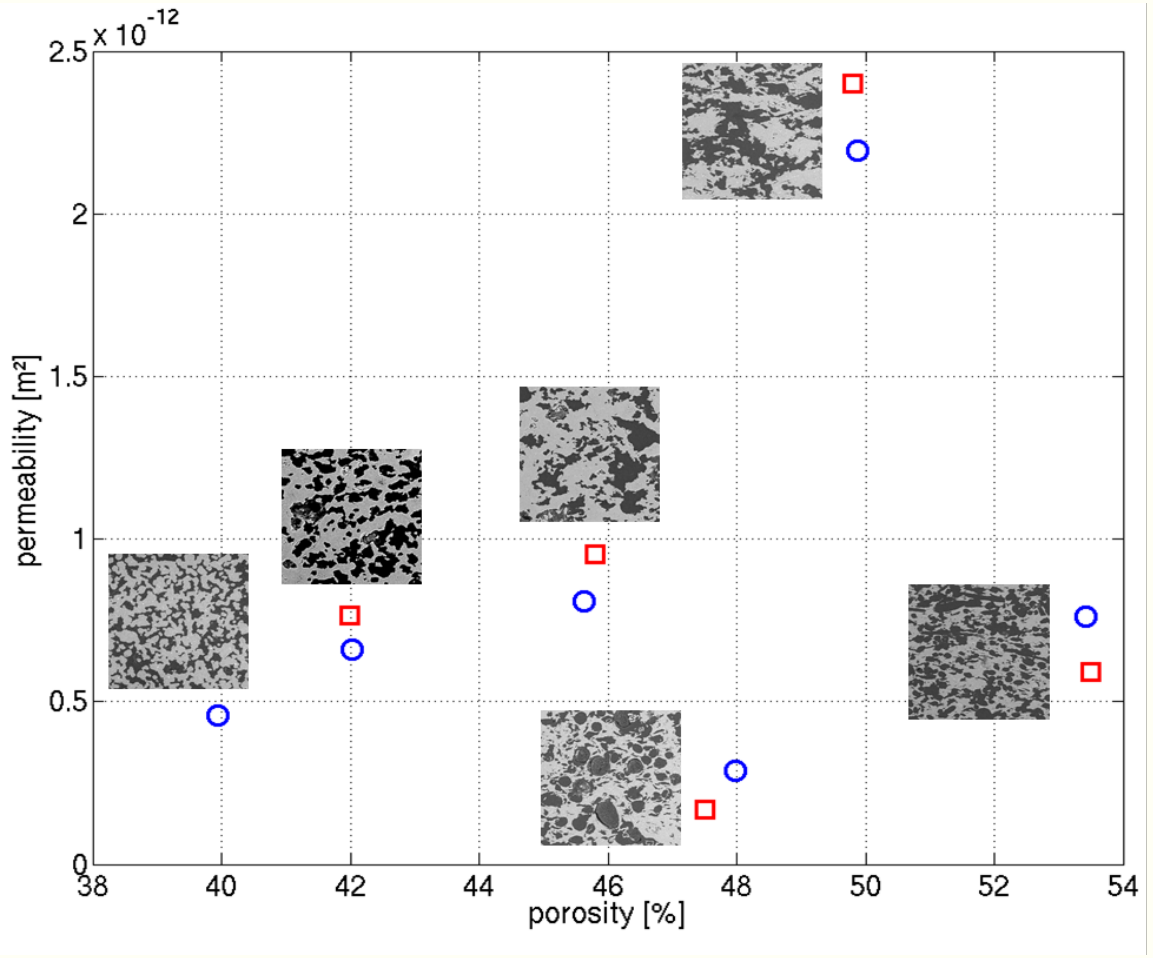
- used for soot particle filters



[Schmidt and Becker, Generating Validated 3D Models of Microporous Ceramics, 2013, Advanced Engineering Materials]

Digital Twin – Sintered Ceramic





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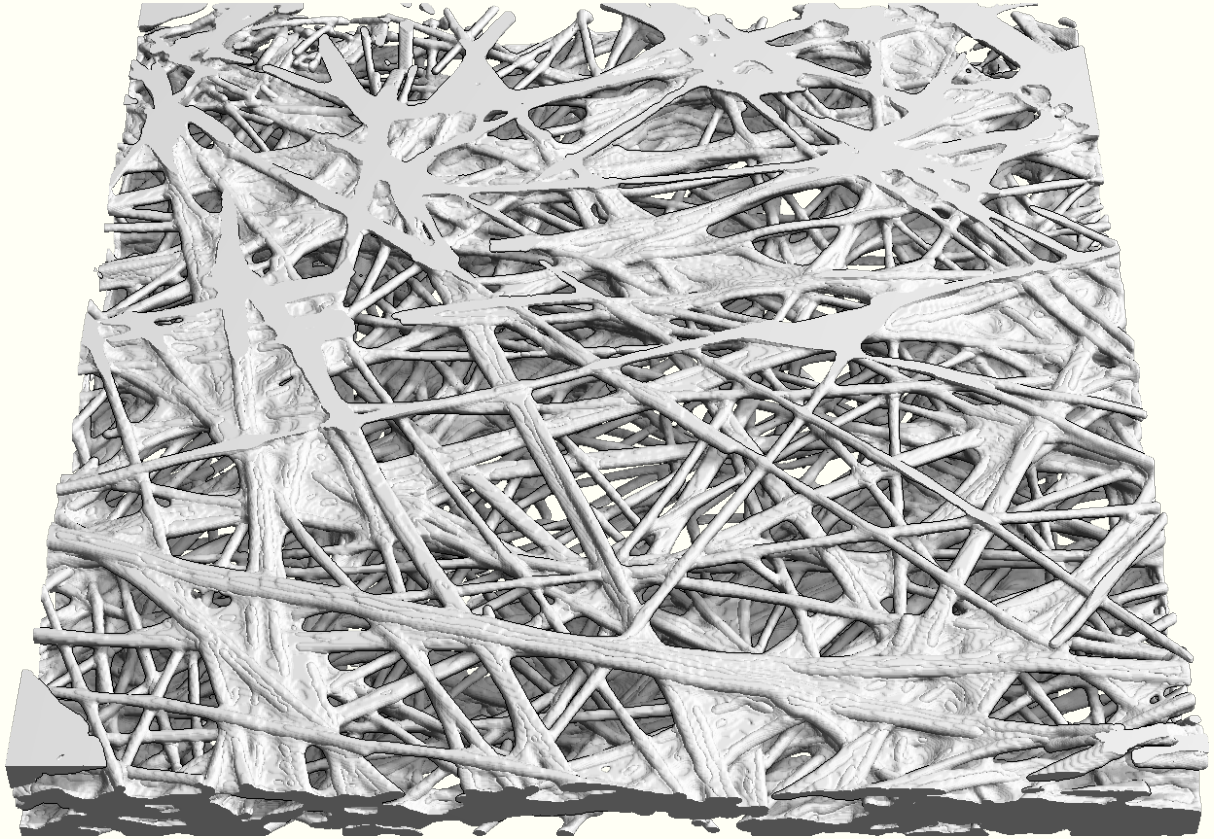
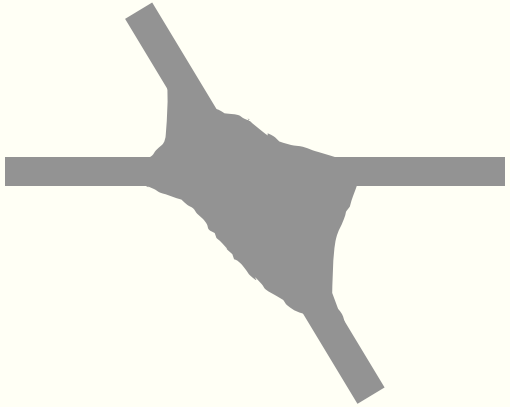
Digital Twin – Gas Diffusion Layer

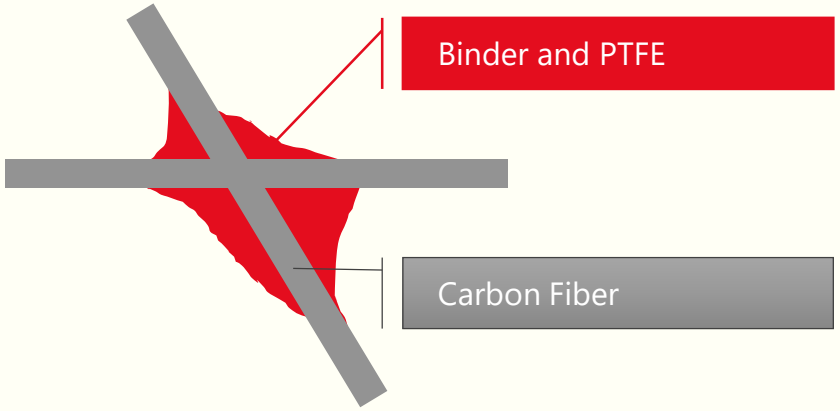
- used in fuel cells



µCT-Scan

Digital Twin – Gas Diffusion Layer

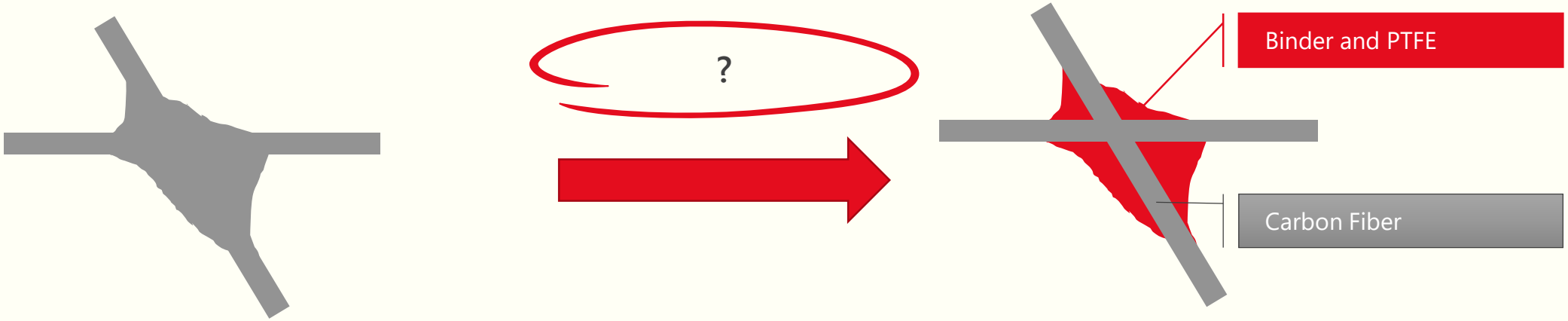




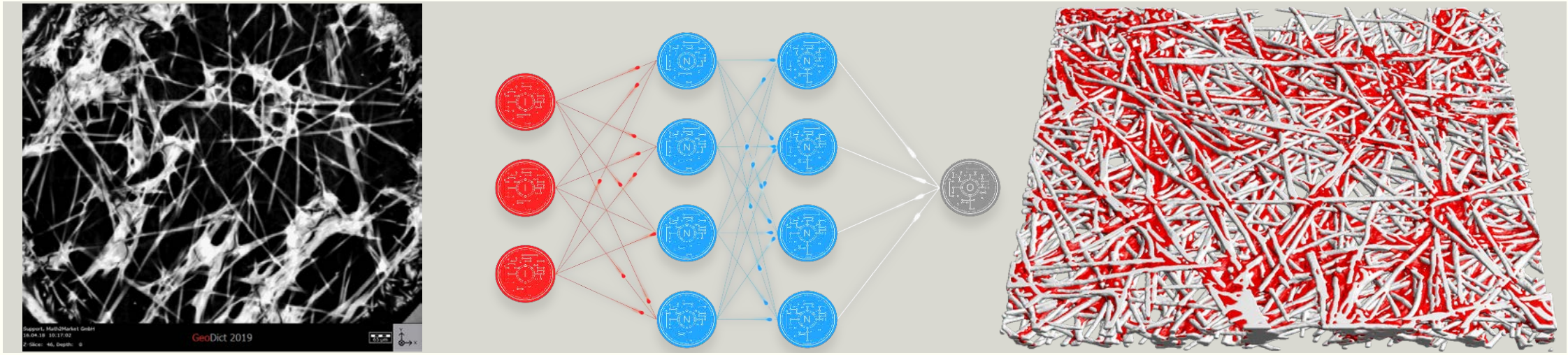
In the original CT Scan binder and fiber can not be separated

It is necessary to differentiate fibers from binder based on the shape

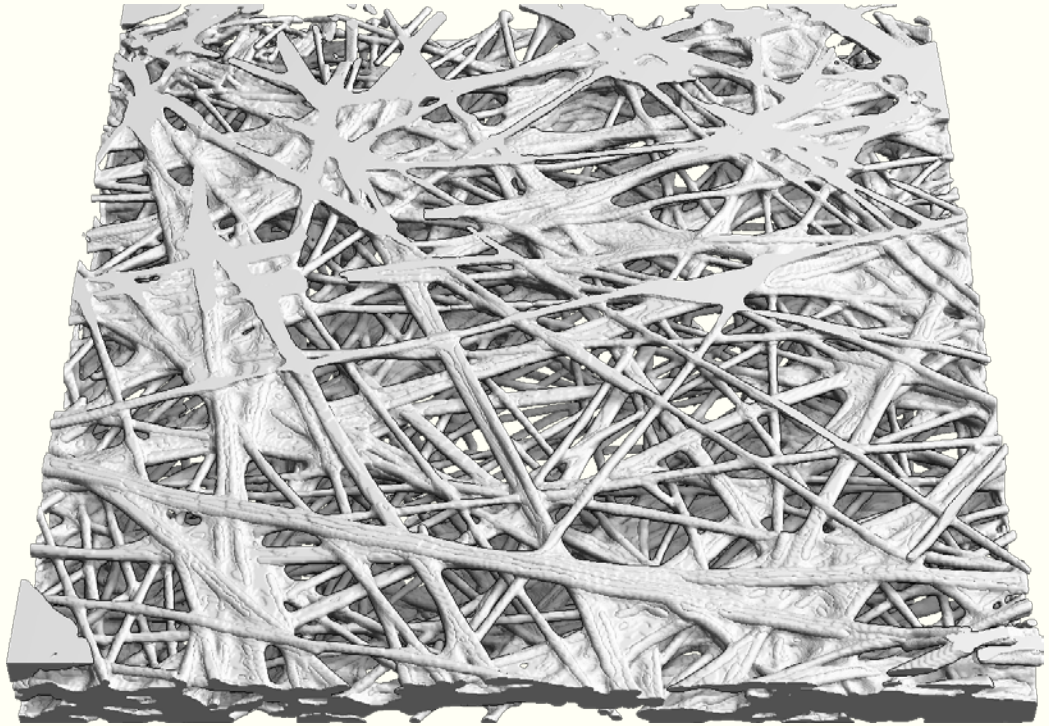
Digital Twin – Gas Diffusion Layer



Identifying binder with Machine Learning



Digital Twin – Gas Diffusion Layer



Fibers: 16.2%
Binder: 13.2%

µCT-Scan

segmented image

Thank You!

Dr.-Ing. Constantin Bauer
Math2Market GmbH
+49 631 205 605 – 28
constantin.bauer@math2market.de
www.geodict.com

GeoDict
The Digital Material Laboratory

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