Analysis of thermal and electrical conductivity of materials with ConductoDict

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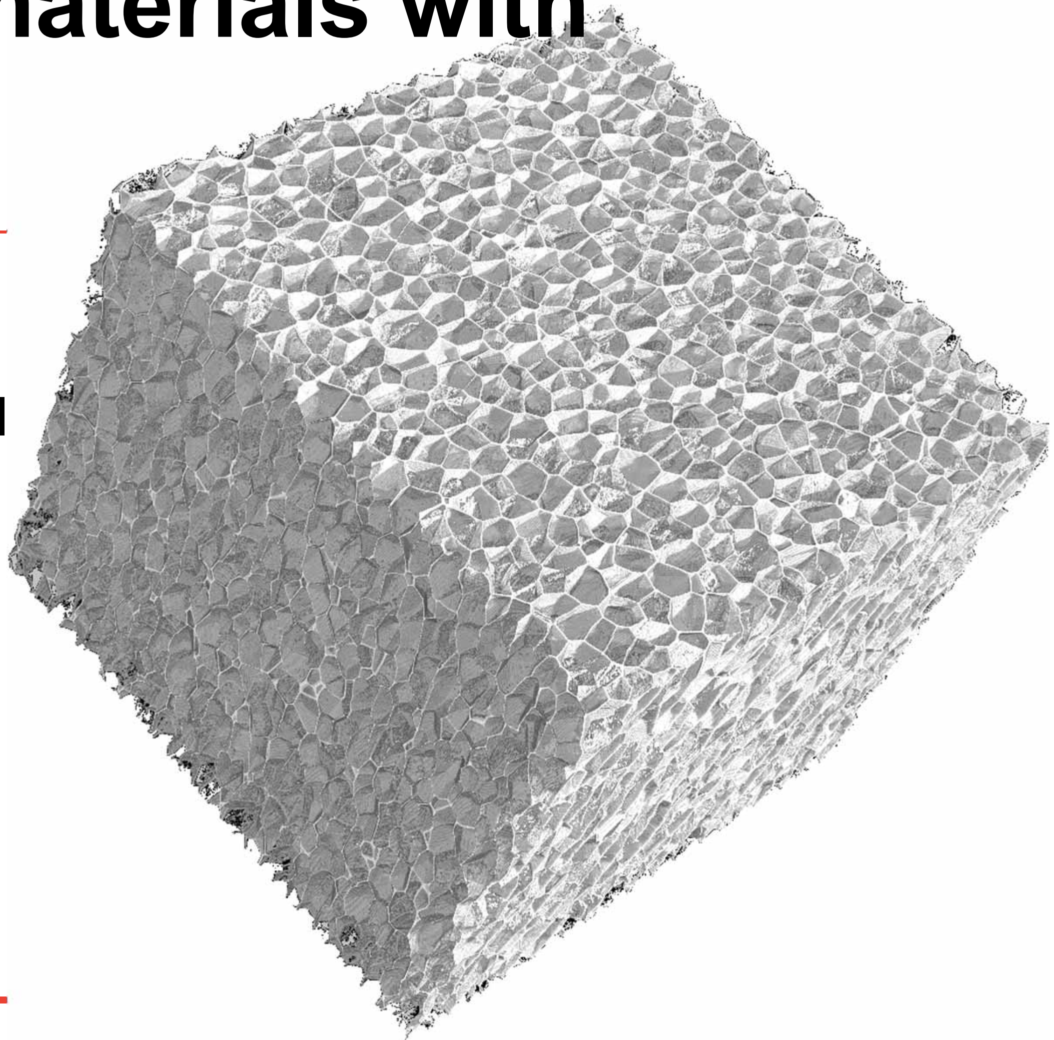

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ConductoDict: compute the effective thermal conductivity (ThermoDict) and electric conductivity (ElectroDict)

Solve the steady diffusion equation

$$\begin{aligned} \nabla\left(\beta(\nabla u + \mathbf{f})\right) &= 0 \in \Omega, \\ u(x + il_x, y + jl_y, z + kl_z) &= u(x, y, z) \text{ for } i, j, k \in \mathbb{Z} \end{aligned}$$

- for temperature u or electric potential u
- with constituent material conductivity β
- for direction of interest f
- And using periodic boundary conditions

to get effective conductivity β^* of the closest possible homogeneous medium

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What is <u>not</u> modelled…

ConductoDict does not treat advective transport.

ConductoDict does not treat radiative transport.

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Computation of the λ-value of foams based on diffusive thermal transport

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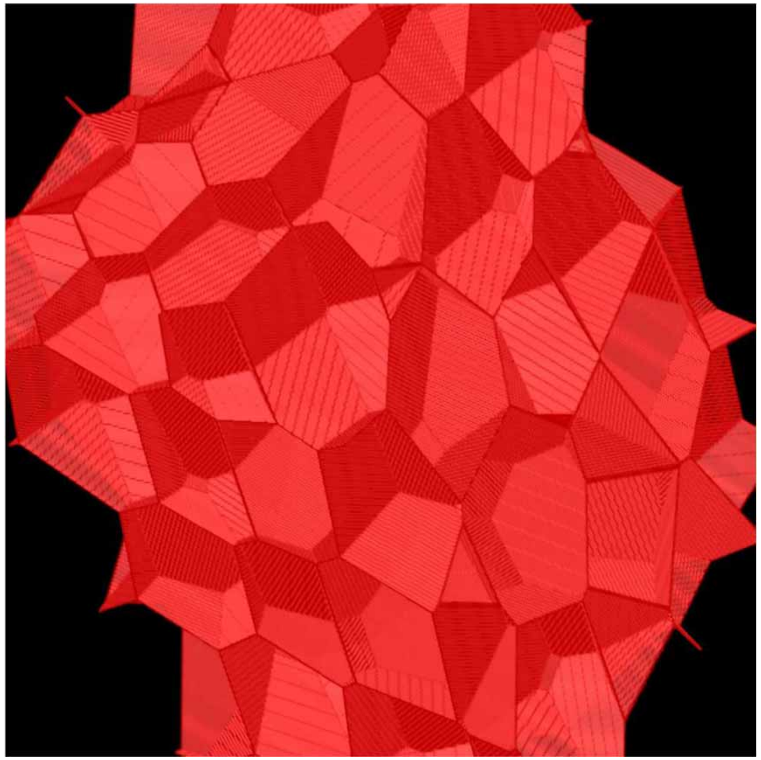
Computation of the λ-value of foams based on diffusive thermal transport



Foam consists of closed cells, offers high surface roughness and high stiffness and low thermal conductivity

Computation of thermal conductivity of foams

- Determination of REVs
- foam models
- Comparison with measurements
- Variation of pore sizes & wall thicknesses

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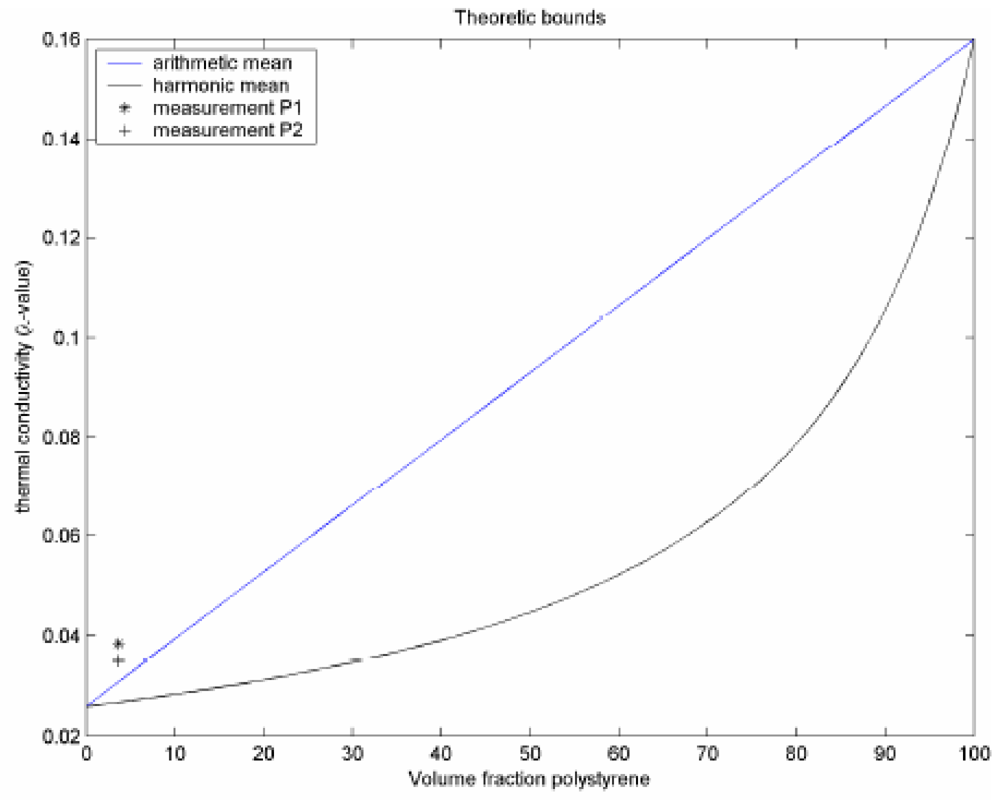
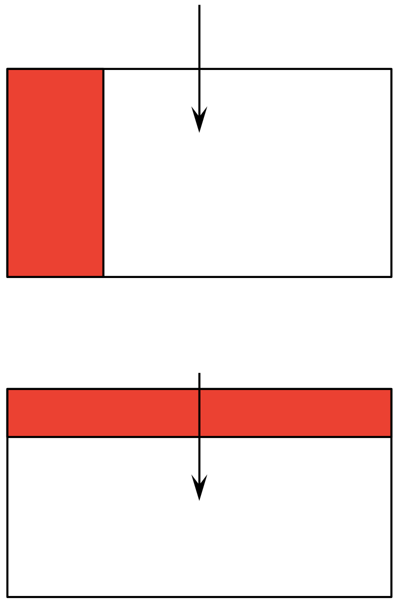
Some useful theory





β_air = 0.026
β_s = 0.16

Theoretial bounds on the λ-value, as a function of solid volume fraction. The arithmetic mean bound (Reuss bound) and the harmonic mean bound (Voigt bound) together form the so-called Wiener box of geometrically independent bounds for the λ-value.

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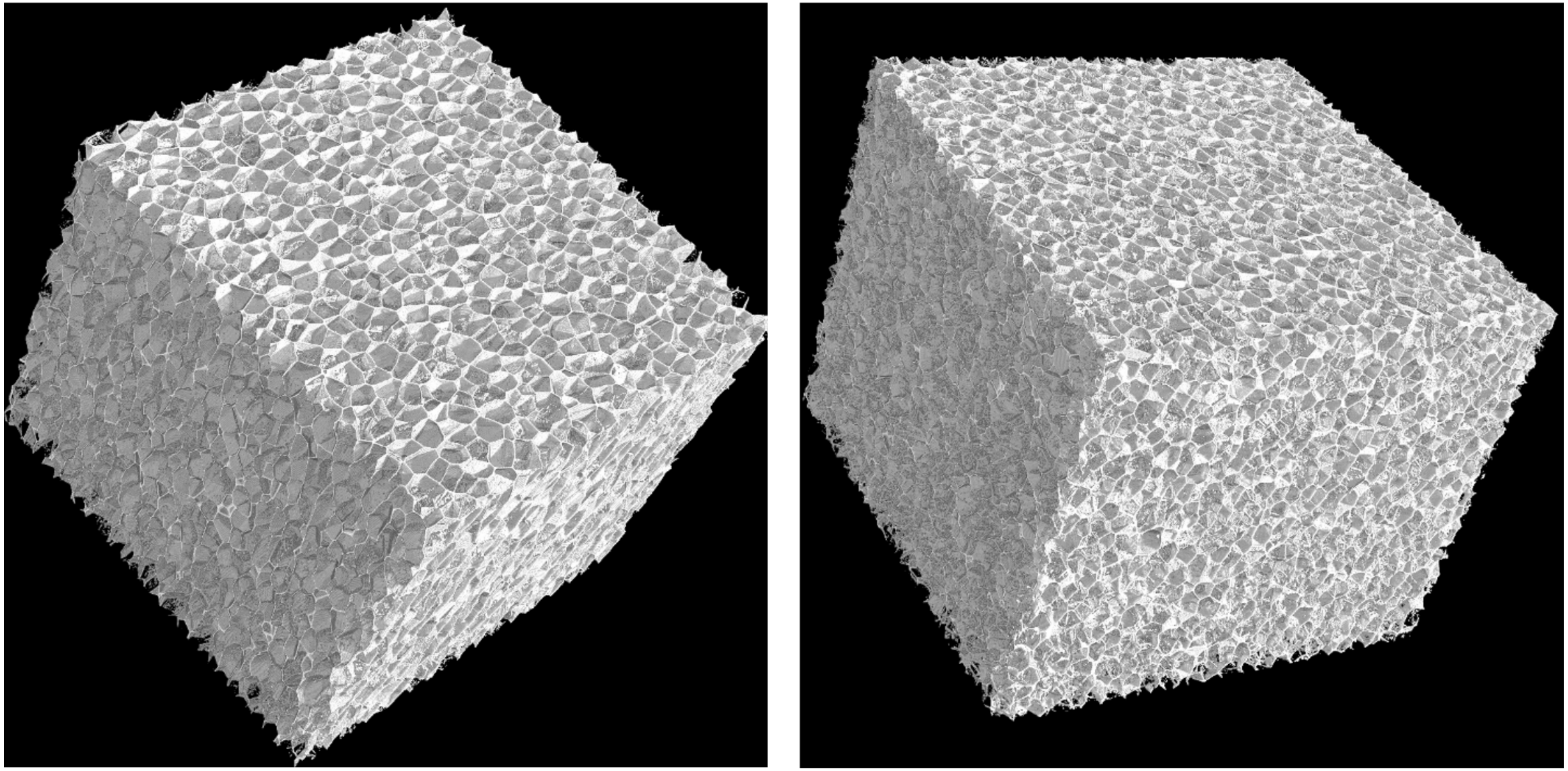
Synchrotron data



3d-synchrotron images of sample 1 2 with gray values between 0 and 255
at 1024 x 1024 x 2000 points, with resolution 5µm

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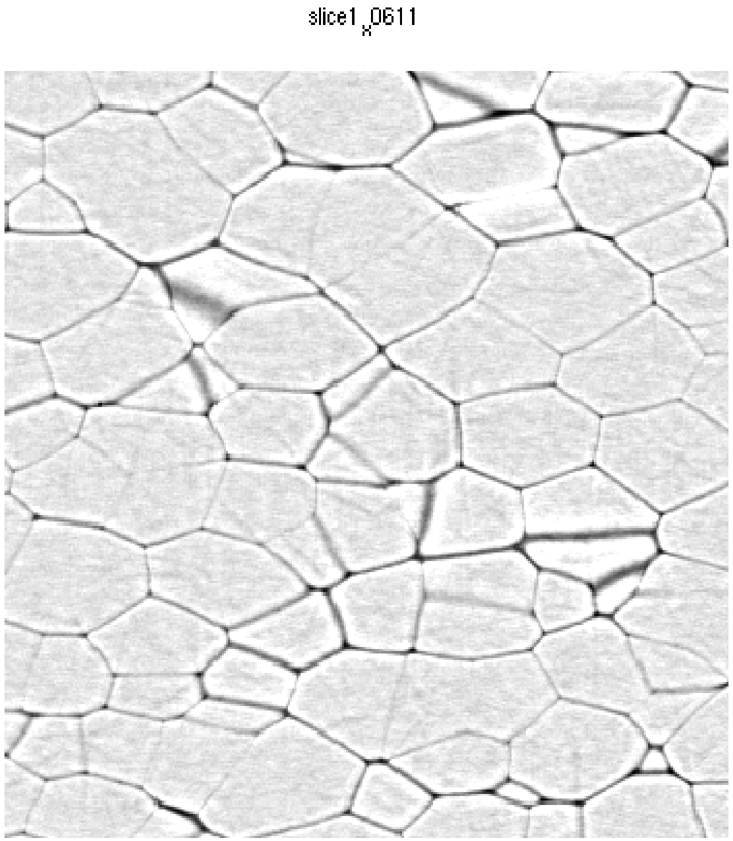
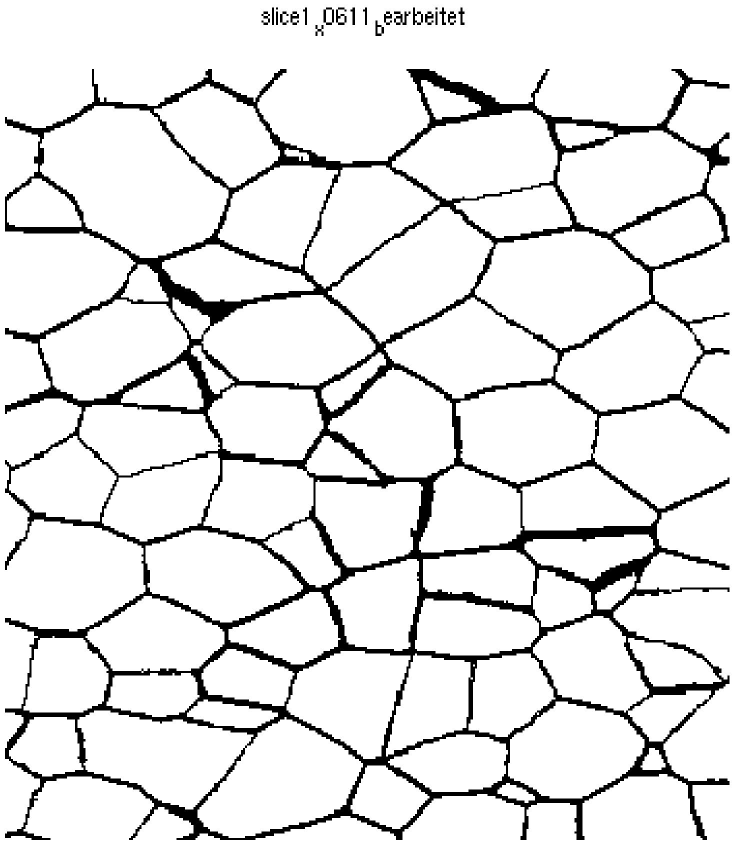
Manual binarization 300x300 cutout





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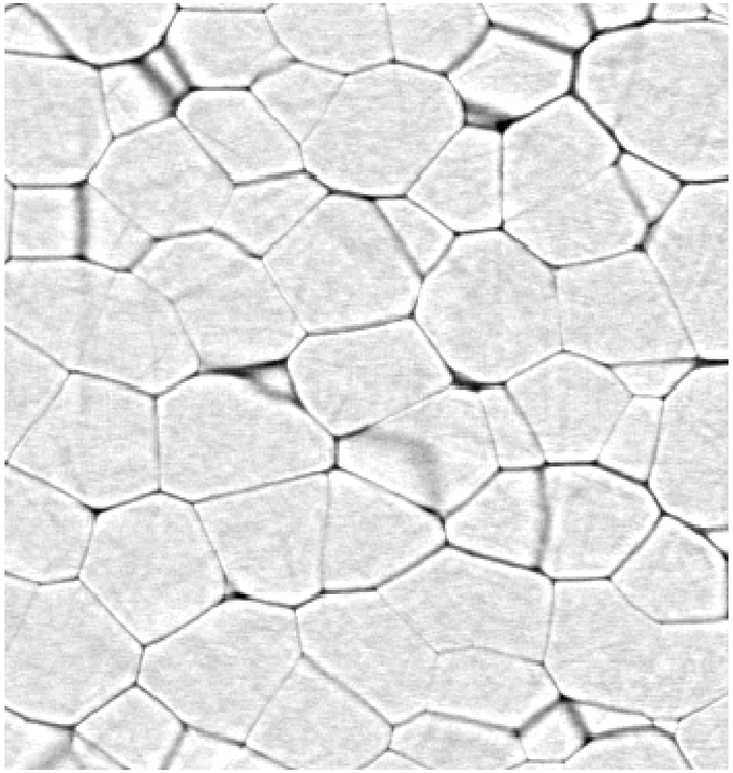
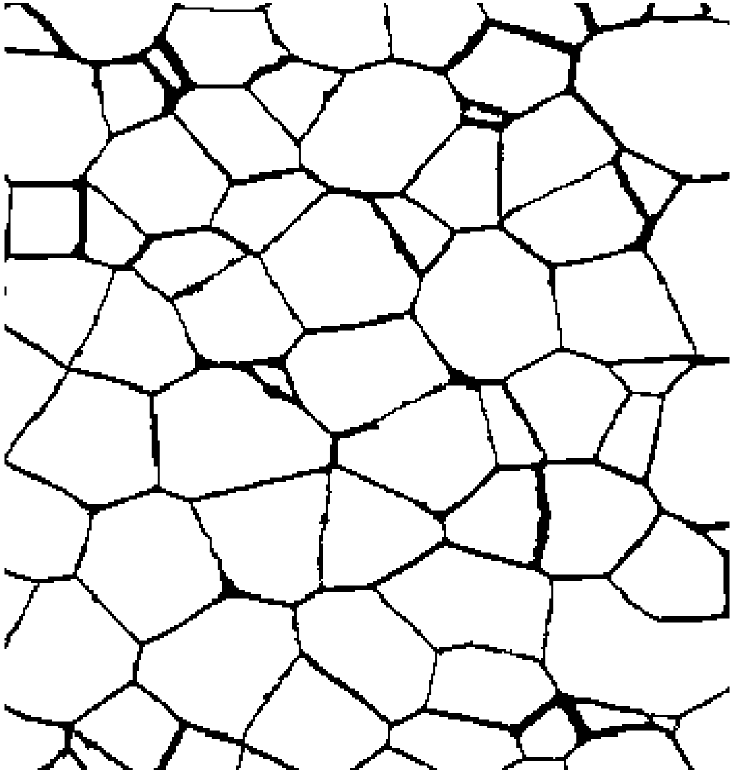
Manual binarization 300x300 cutout

slice1_0611



slice1_0611_bearbeitet



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Why model the foams?

- Synchrotron image 5 μm resolution not capable to resolve 2 μm cell walls.
- Images have 3 times more mass than reality, even for 1 voxel walls.
- Also, a question is if it is really necessary to work on the full images.
- Models can be made fully periodic, avoiding artefacts on boundaries

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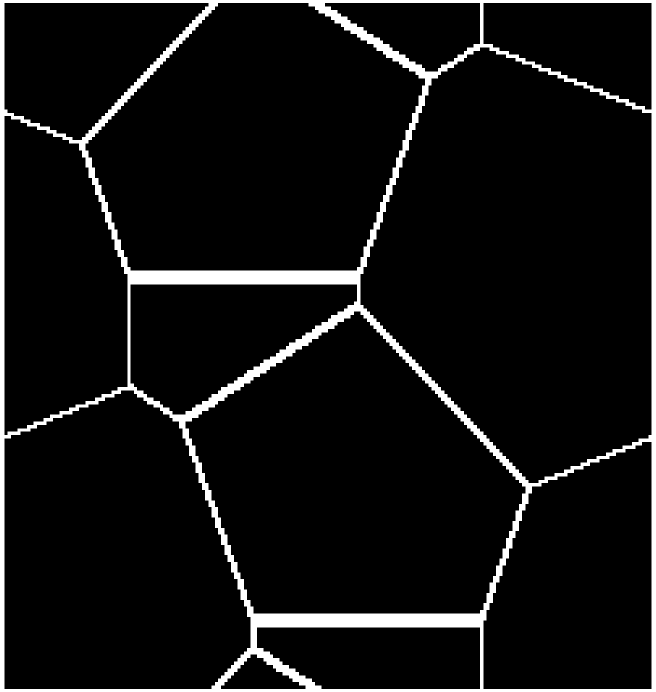
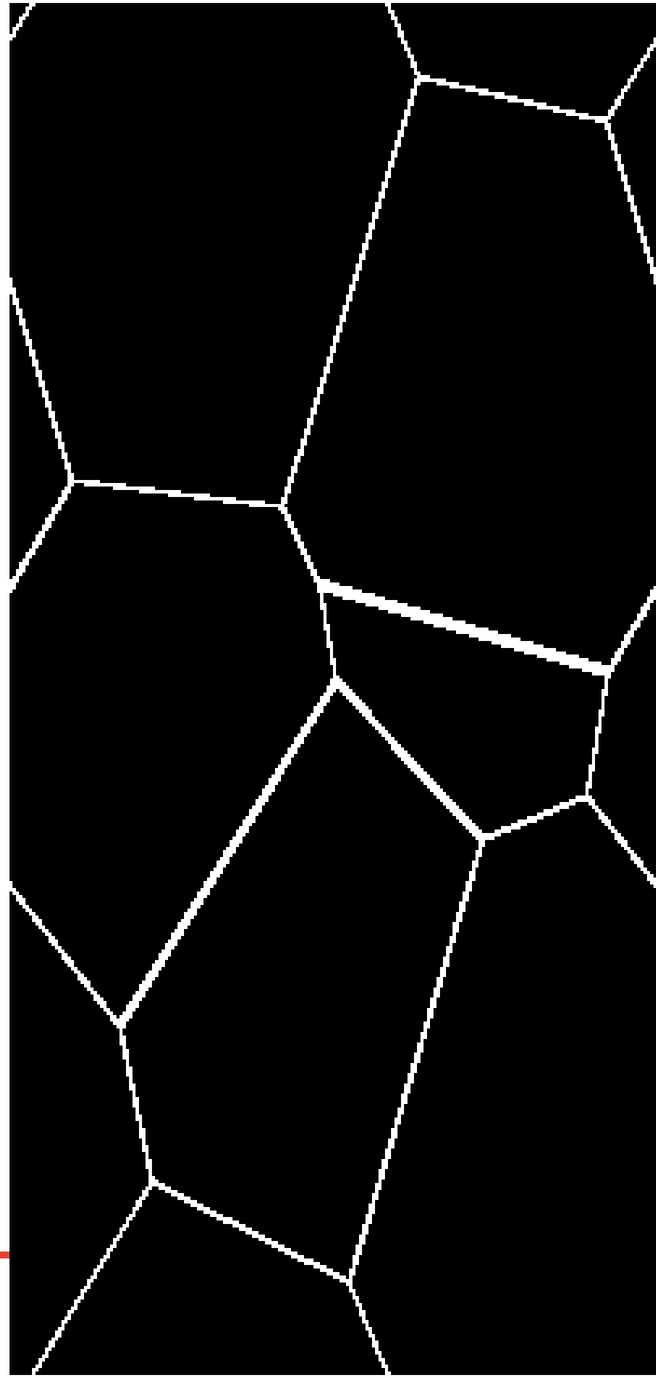
Is a smaller REV possible?



- Laguerre tessellation of space
- Anisotropic foam from ellipsoids
- Mass control by wall thickness



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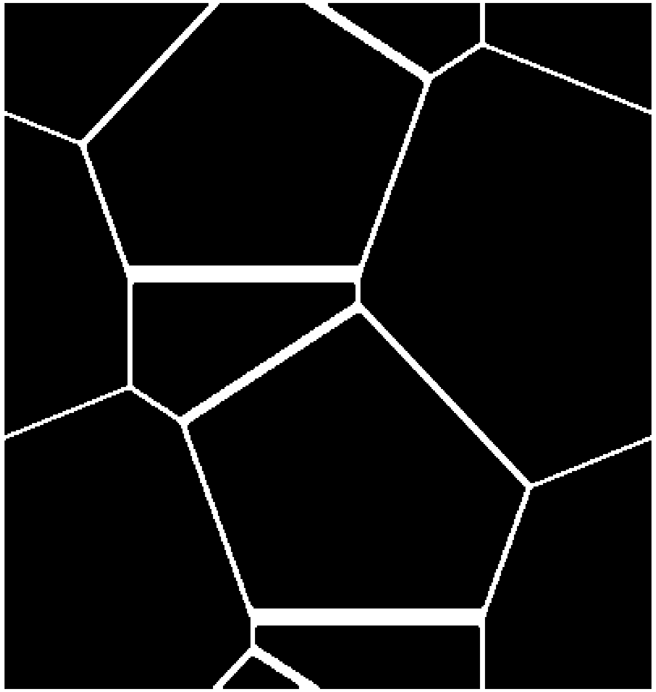
Is a smaller REV possible?



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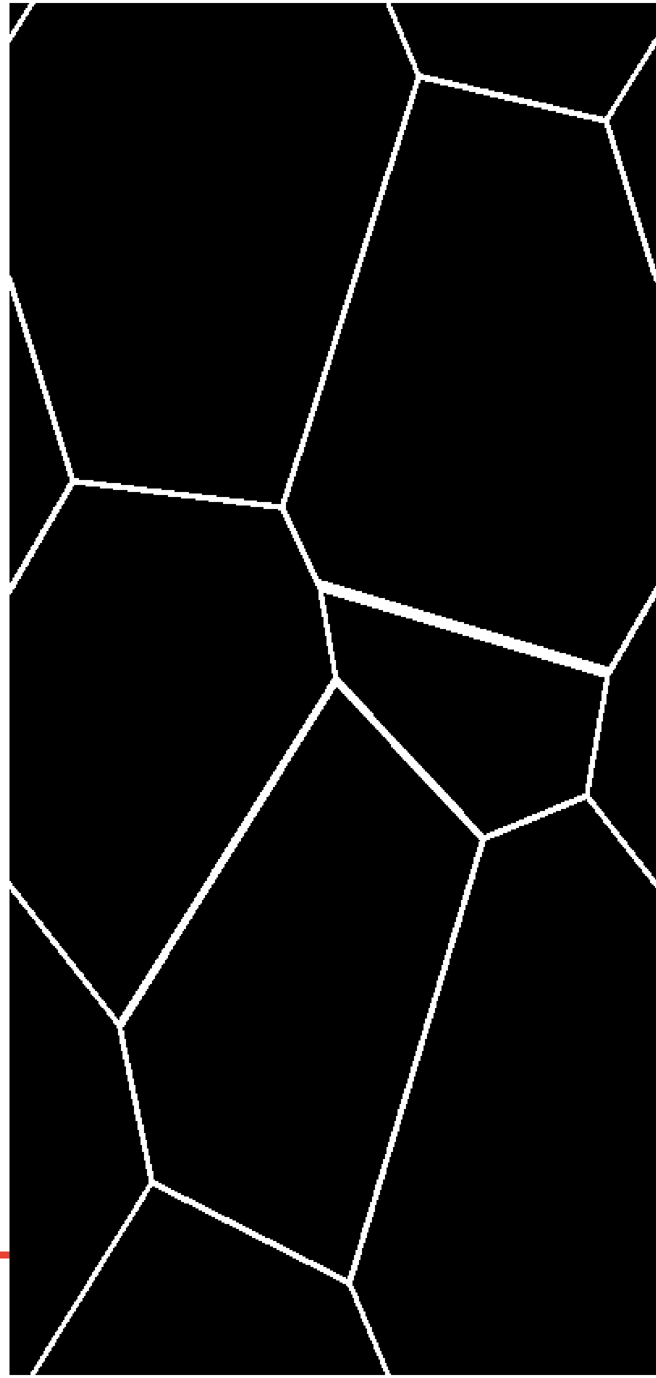
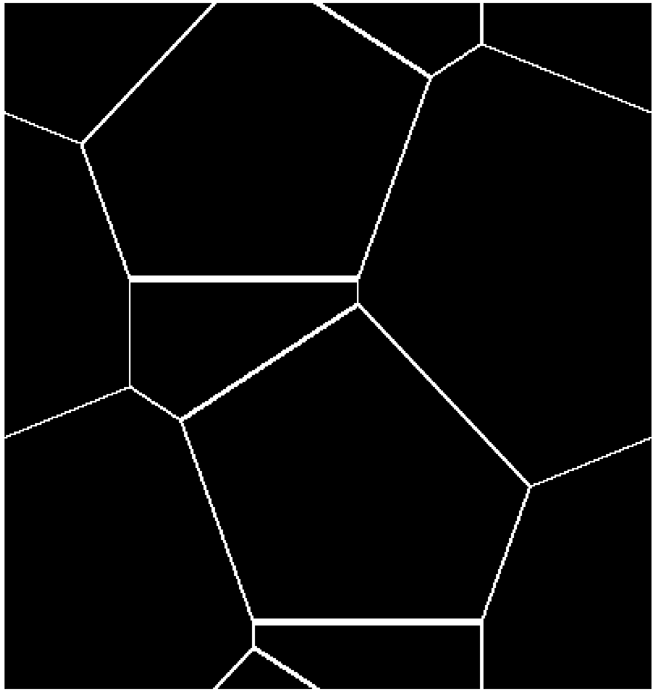
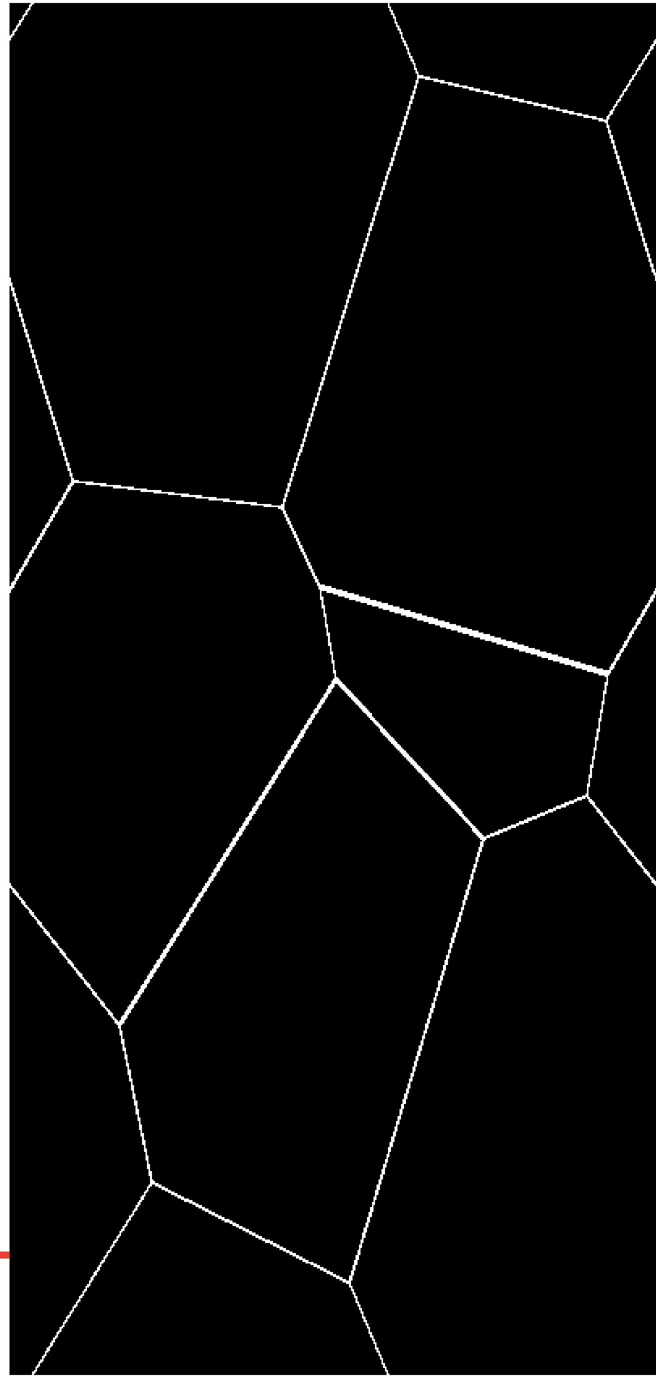


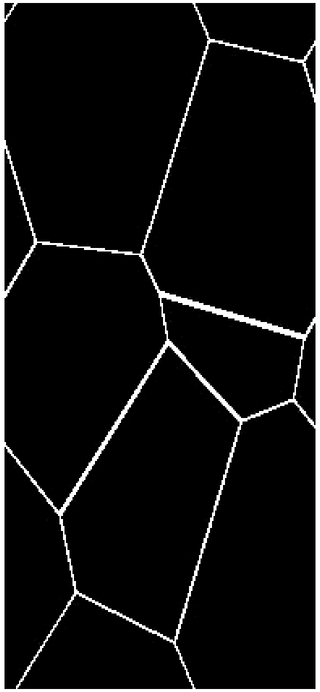
Is a smaller REV possible?

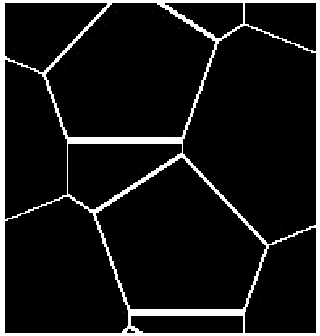




- Laguerre tessellation of space
- Anisotropic foam from ellipsoids
- Mass control by wall thickness

Cross section animations through the generated foams





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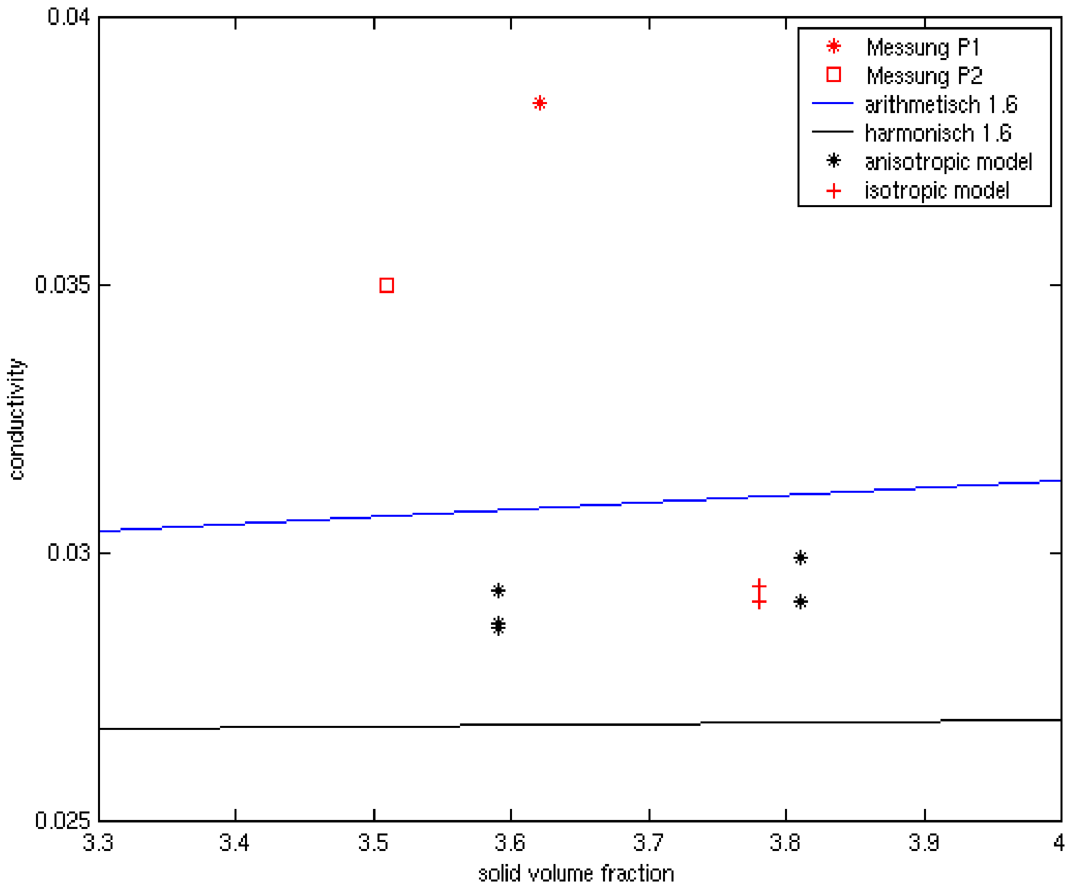
IV. Relation with measurements



Lines are theoretical bounds

Anisotropy and resolution have significant influence and can be reason for differences between samples, but cannot explain the big discrepancy with measurements.

Conclusion from diffusion simulations:

Look for radiation effects.

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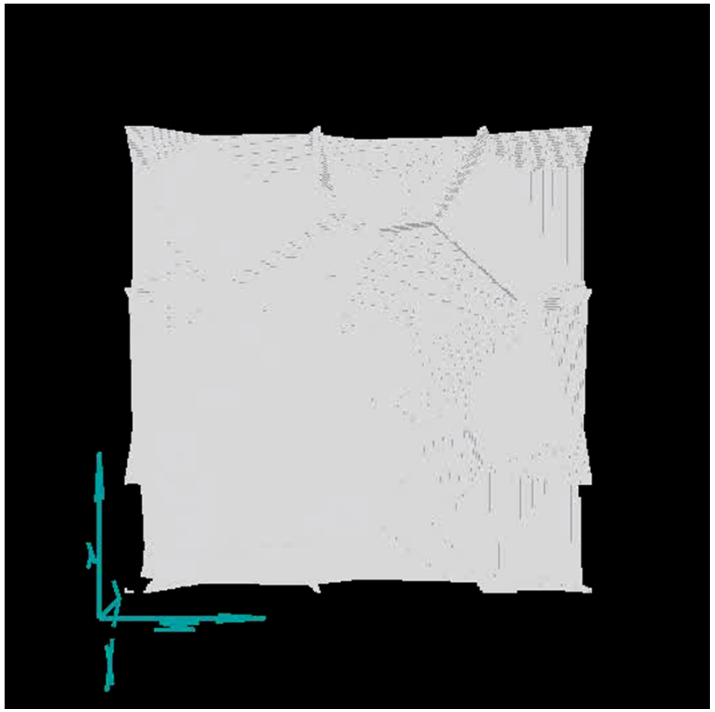
V. Summary



Computed thermal conductivity of foams

- CT image must have enough resolution
- Models for foam structures are available
- Anisotropy of cells can play a role
- Purely diffusive transport model could not reproduce measurements, other effects should be taken into account.

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3D Simulation of Macroscopic heat transfer properties from the microstructure of wood fiber network

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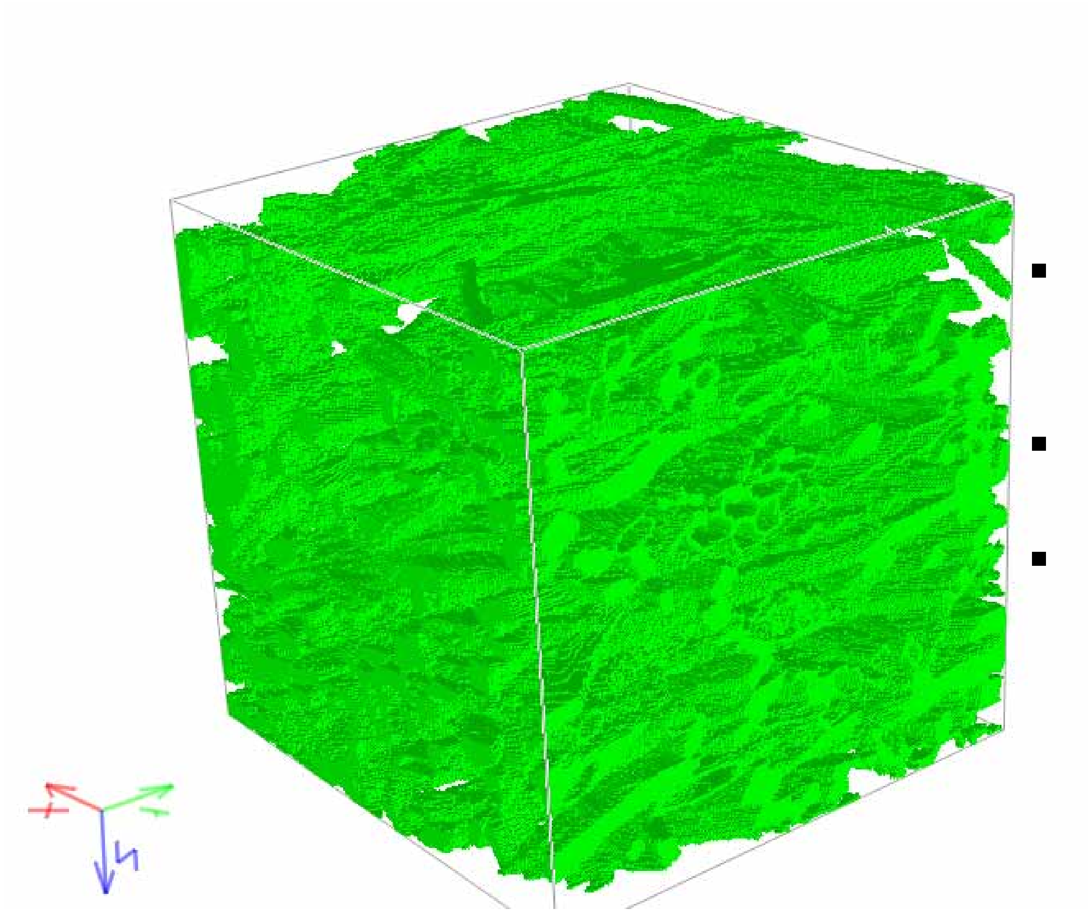
3D Simulation of thermal transport properties from the microstructure of wood fiber network



- Heat and mass transfer properties of natrual fiber-based materials
- Structure generated from X-ray micro-tompography
- Comparison with measurements

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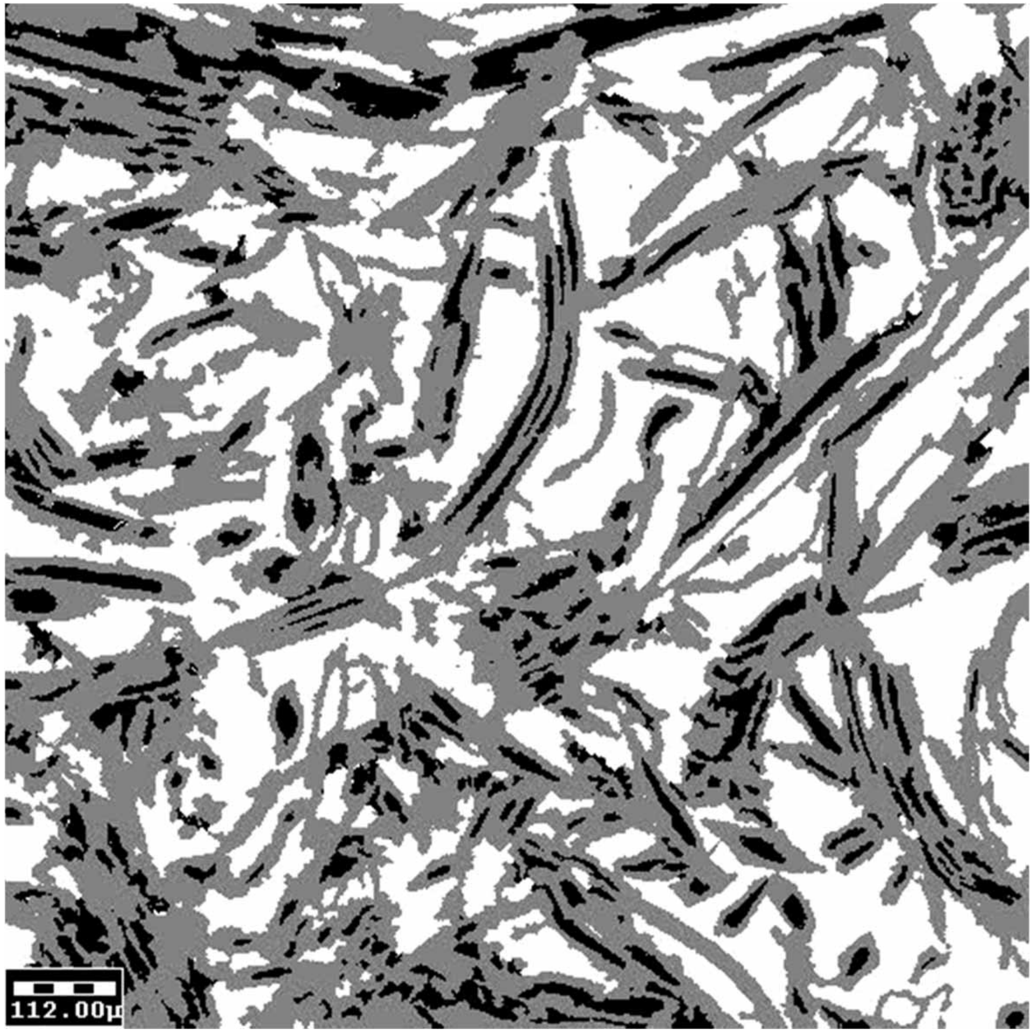
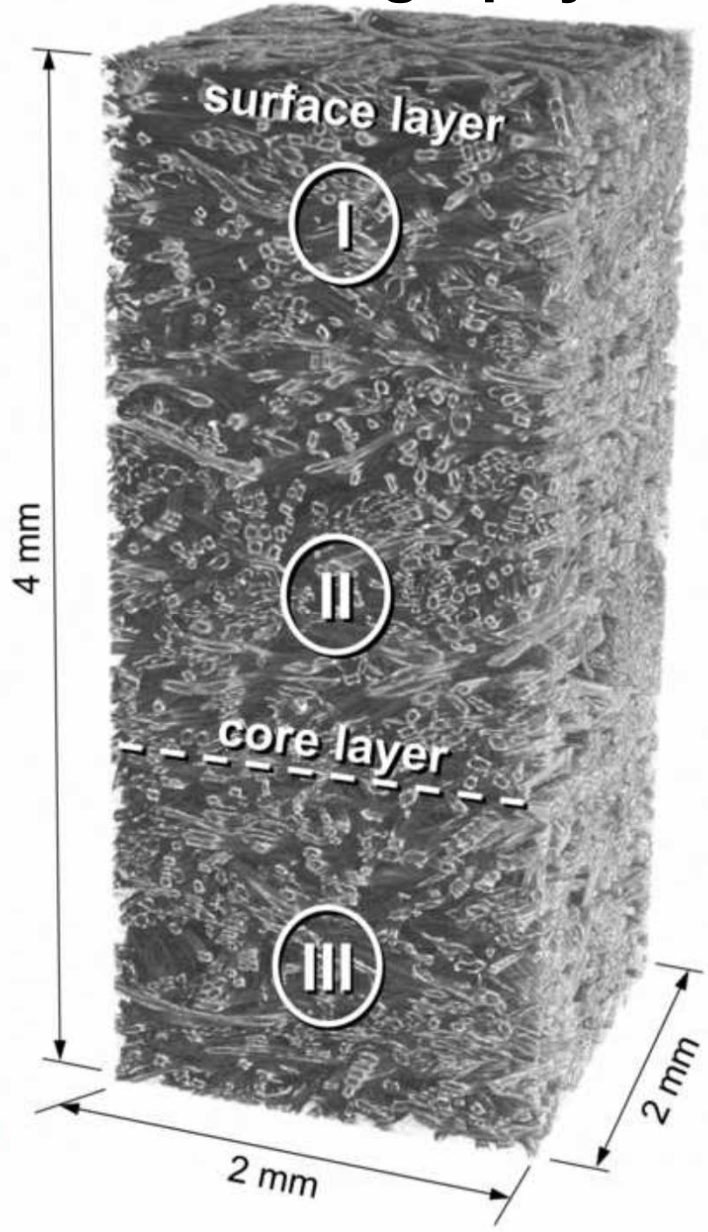
I. Synchrotron radiation based X-ray micro-tomography





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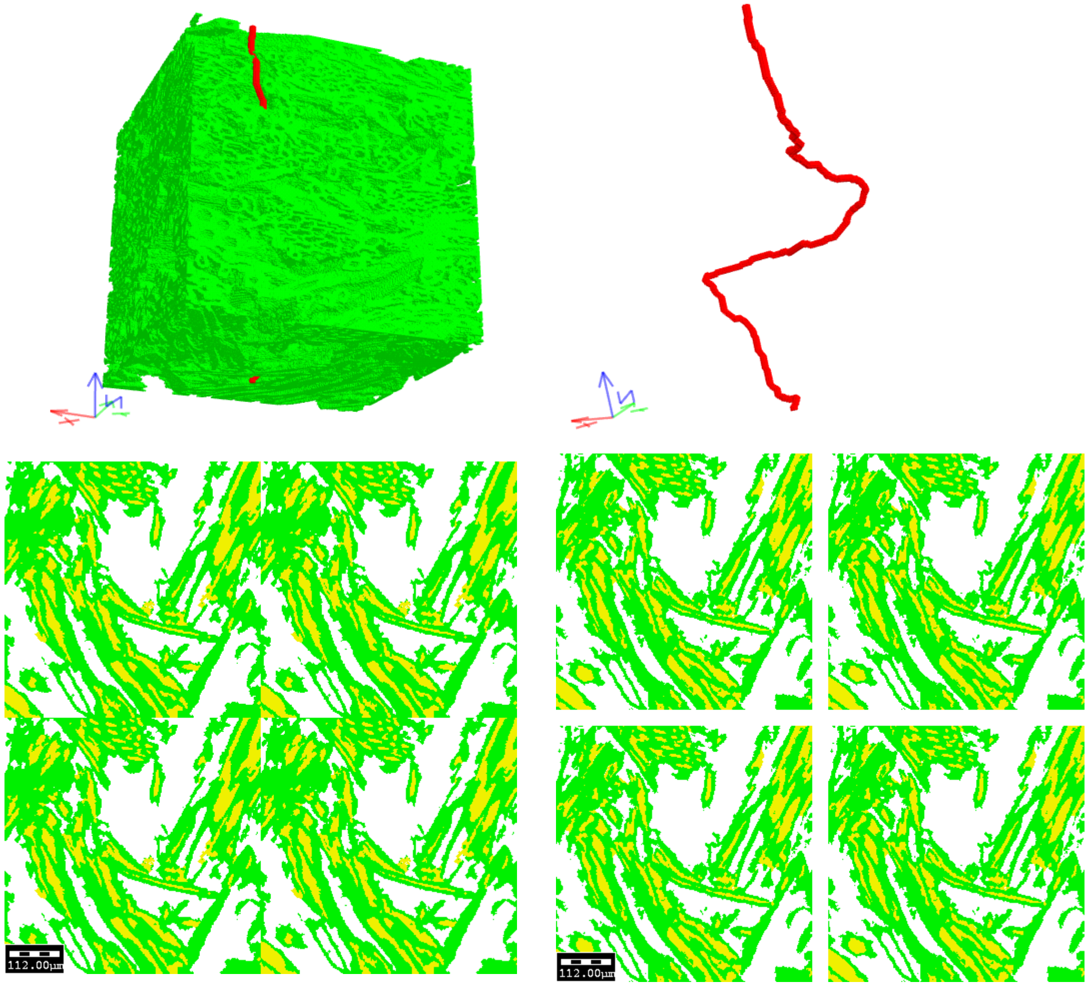
II. Validation of generated structure by percolation path and connected periodicity



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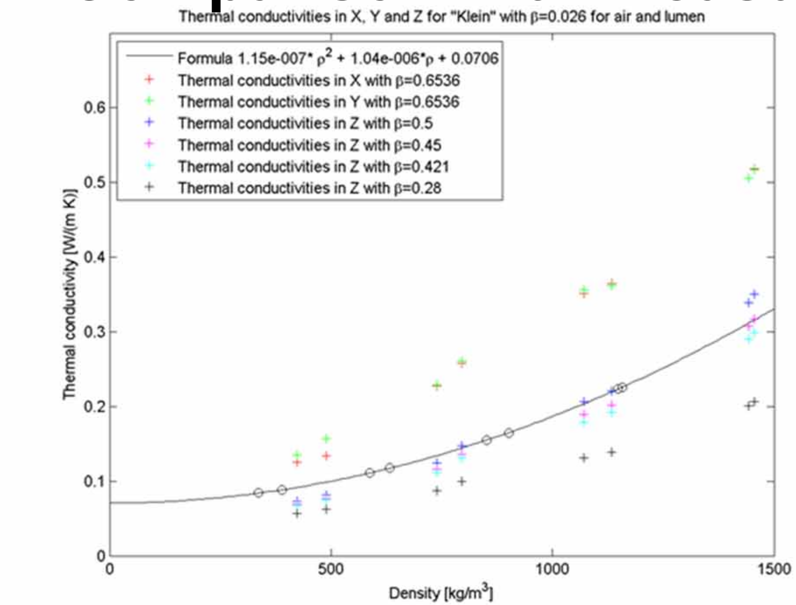
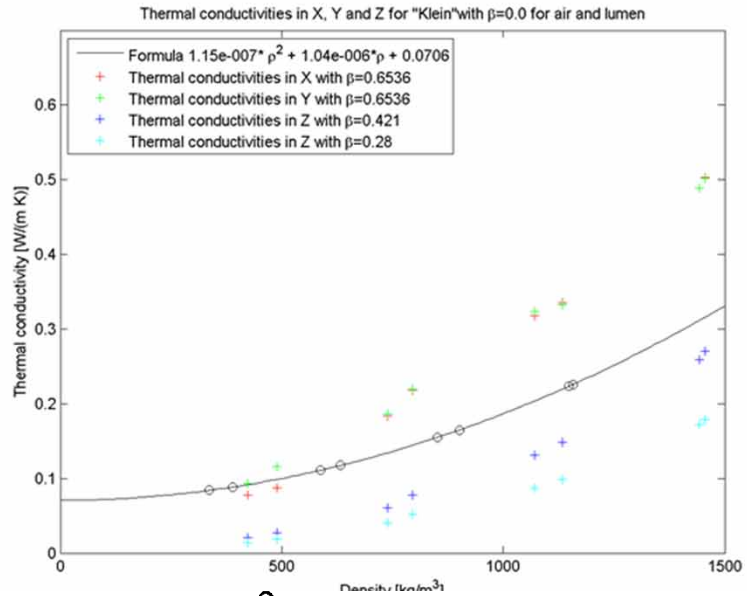
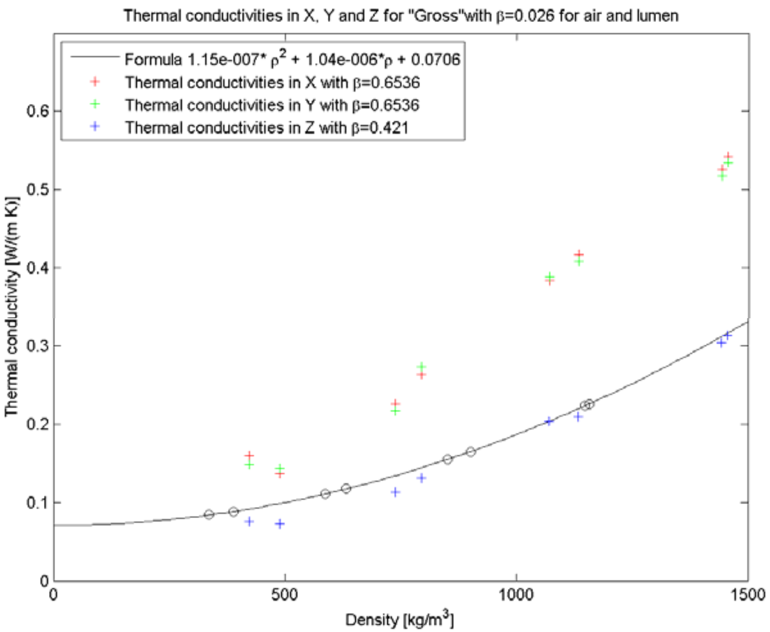
III. Comparison with measurements





$$\lambda = 1.15\text{E-}07\rho^2 + 1.04\text{E-}06\rho + 7.06\text{E-}02 \quad *$$



$\lambda_{w,||} = 0.6536 \text{ W m}^{-1} \text{ k}^{-1}$ **

$\lambda_{w,\perp} = 0.4210 \text{W m}^{-1} \text{ k}^{-1}$

$\lambda_{air} = 0.026 \text{ W m}^{-1} \text{ k}^{-1}$

*Measurement fitting equation by H. Thoemen, Universtiy of Hamburg

** Maku T., Studies on the heat conduction in wood. Wood Res. Bulletin, Kyoto Univ.m Japan 1954; 13:1-80.

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Modeling and prediction of percolation and conductivity properties of CNT-polymer compounds

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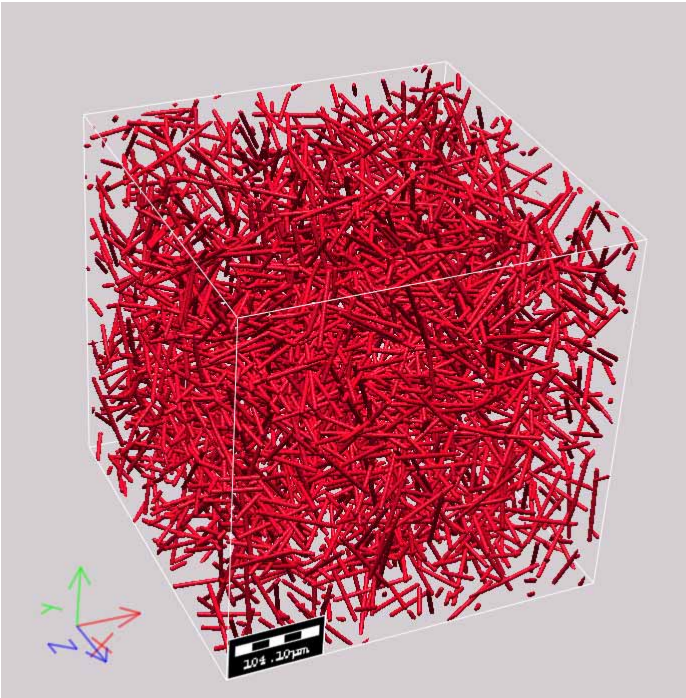
Modeling and prediction of percolation and conductivity properties of CNT-polymer compounds

What, how and why?



- Carbon nano tubes (CNT) can be added to polymers to create conducting plastics
- The specific electrical conductivity of CNT can be up to 20 orders of magnitude (we consider here 1e8) larger than that of the matrix material.
- The specific thermal conductivity of CNT can be 4 orders of magnitude (we consider here 1e4) larger than that of the matrix material.
- A relatively low CNT concentration can dramatically change the polymer's electrical conductivity by orders of magnitude, from an insulator to a conductor.
- CNT are expensive: Want to use as few CNT as possible, yet create conductors.
- Enhanced conductivity requires a connected path of CNT through the part.

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Method

➢Transverse Isotrope Fiber Orientation Probability and Nonwoven Material Density

- Transverse isotrope fiber orientation probability: compression in theta-direction, isotrope for β=1, compressed for β>1.

$$p(\vartheta,\varphi)=\frac{1}{4\pi}\frac{\beta\sin\vartheta}{(1+(\beta^2-1)\cos^2\vartheta)^{3/2}} \quad , \qquad \vartheta\in[0,\pi),\varphi\in[0,2\pi)$$

- For two fiber types with probability $0 \leq p \leq 1$ and 1-p, generate random number n between 0 and 1 and select first type if $n \leq p$ and second type if $n>p$.

- Generate fibers until the desired solid volume fraction f_V is reached based on comparing the voxels occupied by the generated fibers with the total amount of voxels in the volume.

- Can select overlapping and nonoverlapping fibers, the latter with limits on the desired solid volume fraction.

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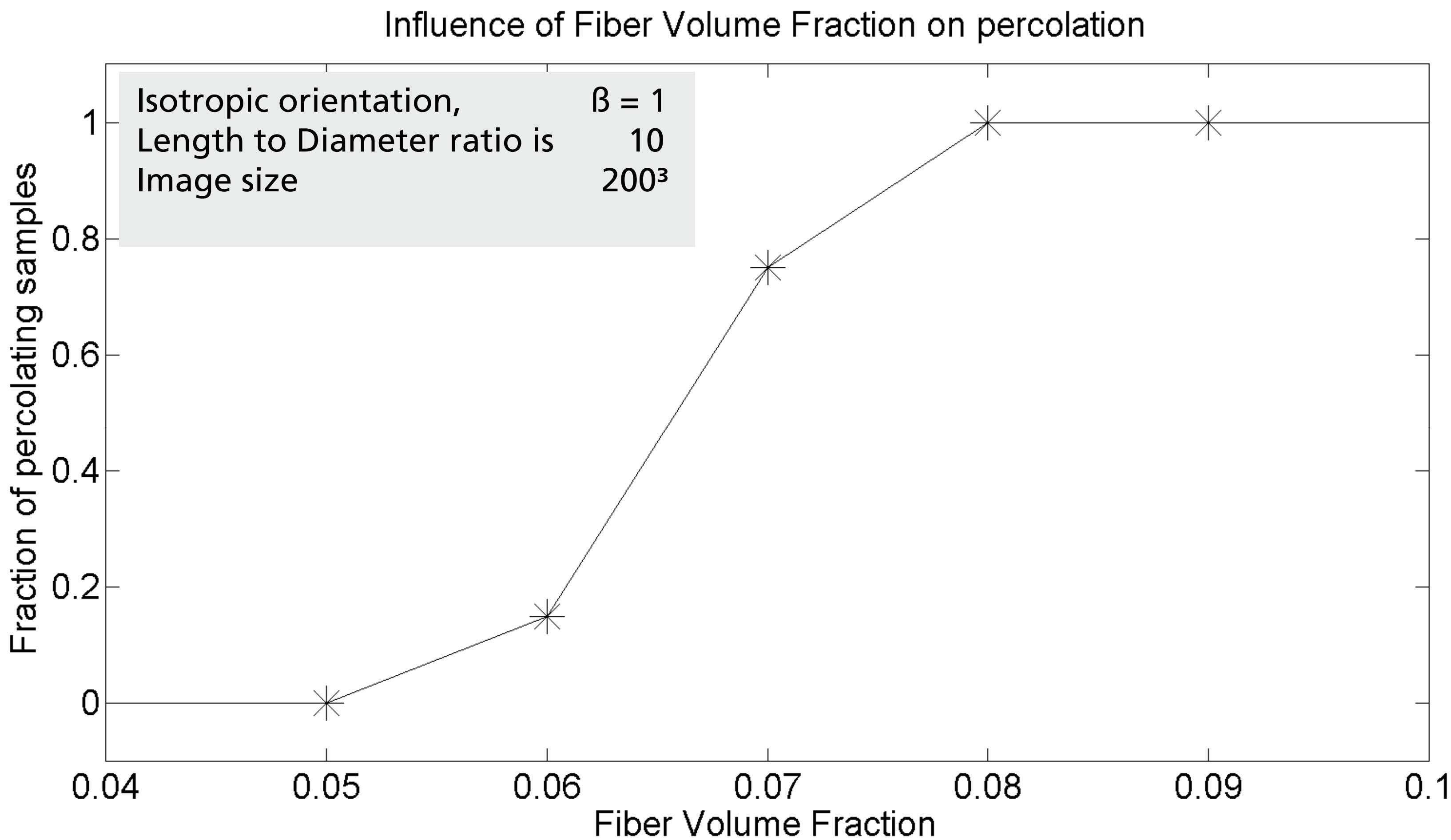
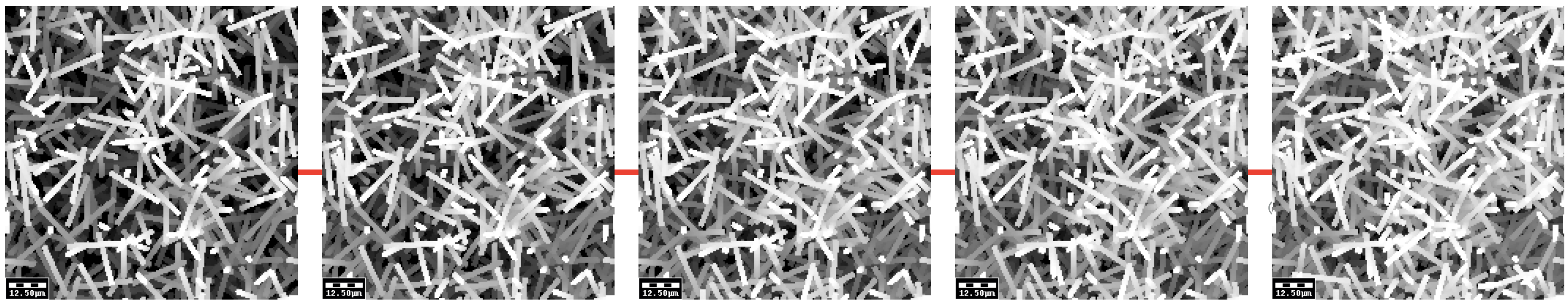
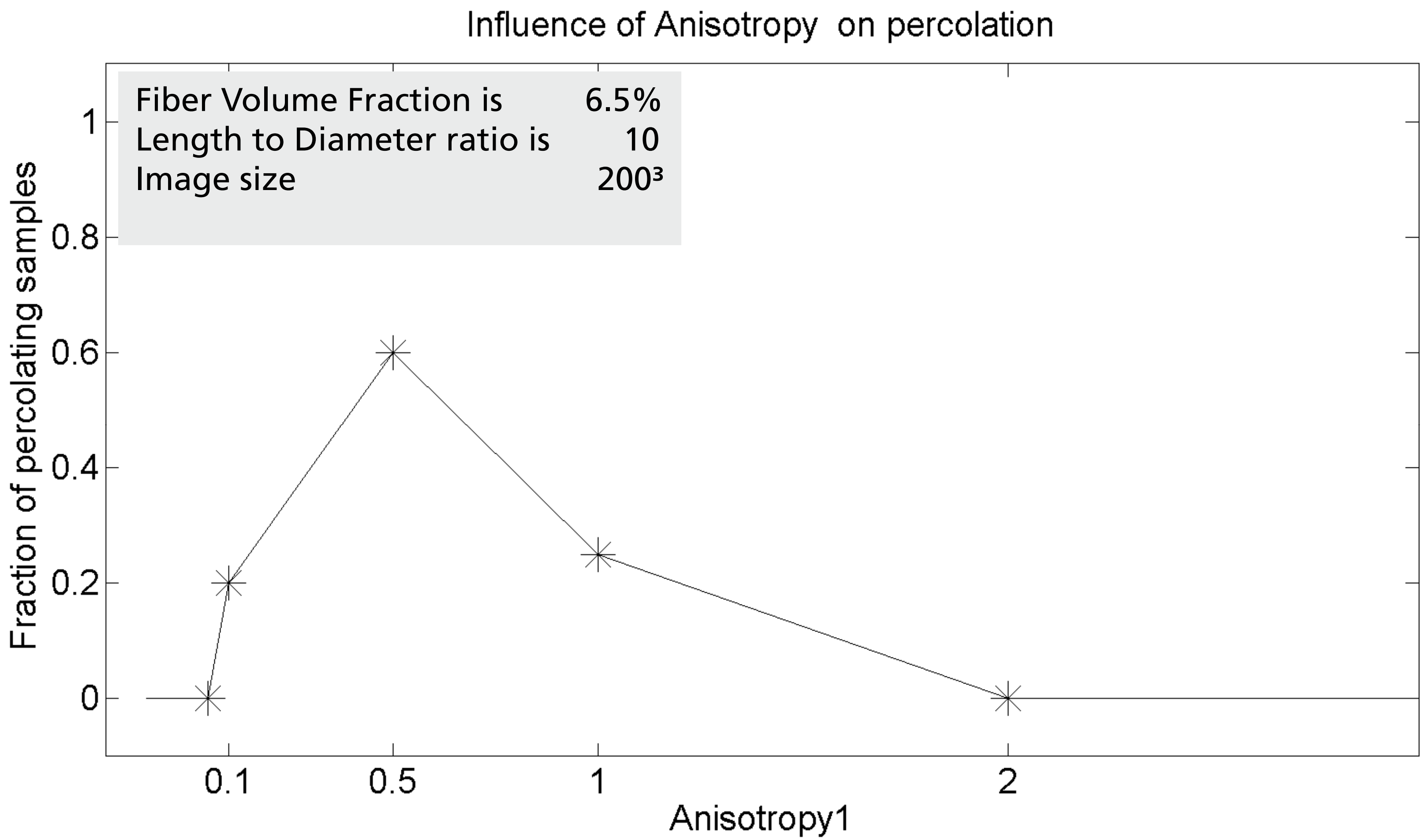
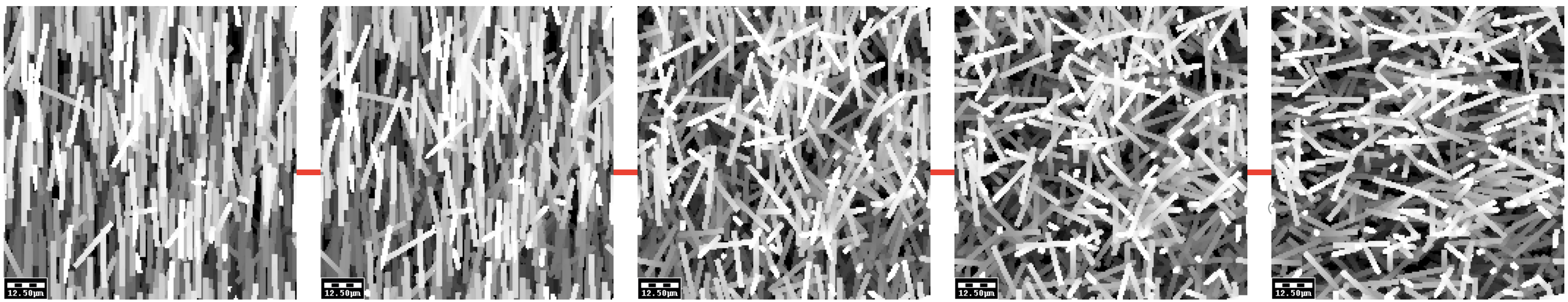
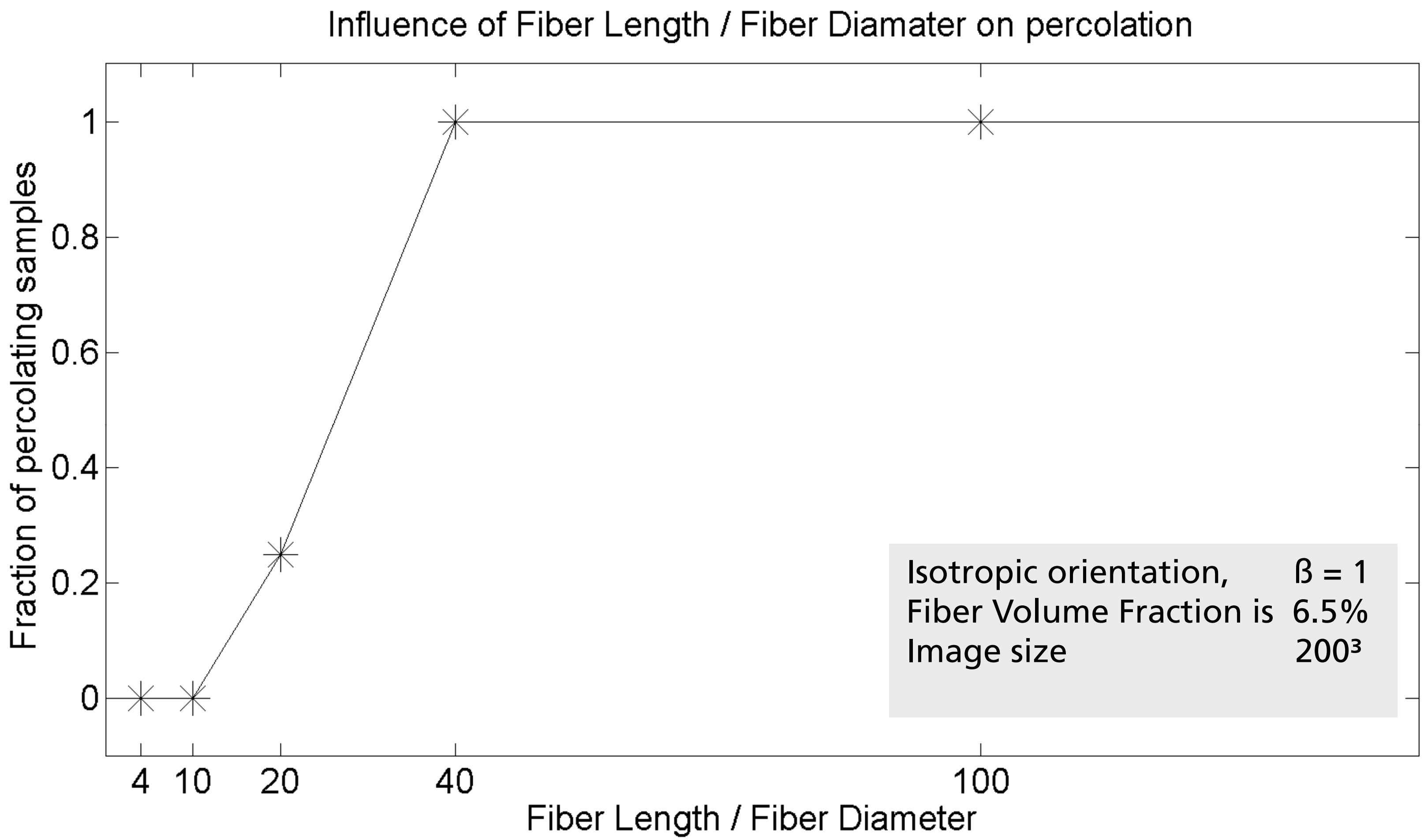
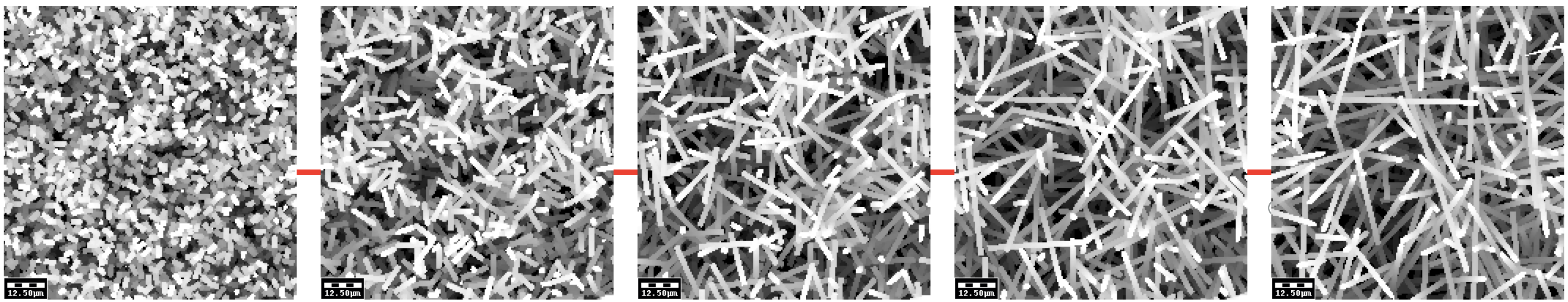

Influence of Fiber Volume Fraction on percolation
Isotropic orientation, ß = 1
Length to Diameter ratio is 10
Image size 200³
Fraction of percolating samples
0
0.2
0.4
0.6
0.8
1
0.04
0.05
0.06
0.07
0.08
0.09
0.1
Fiber Volume Fraction

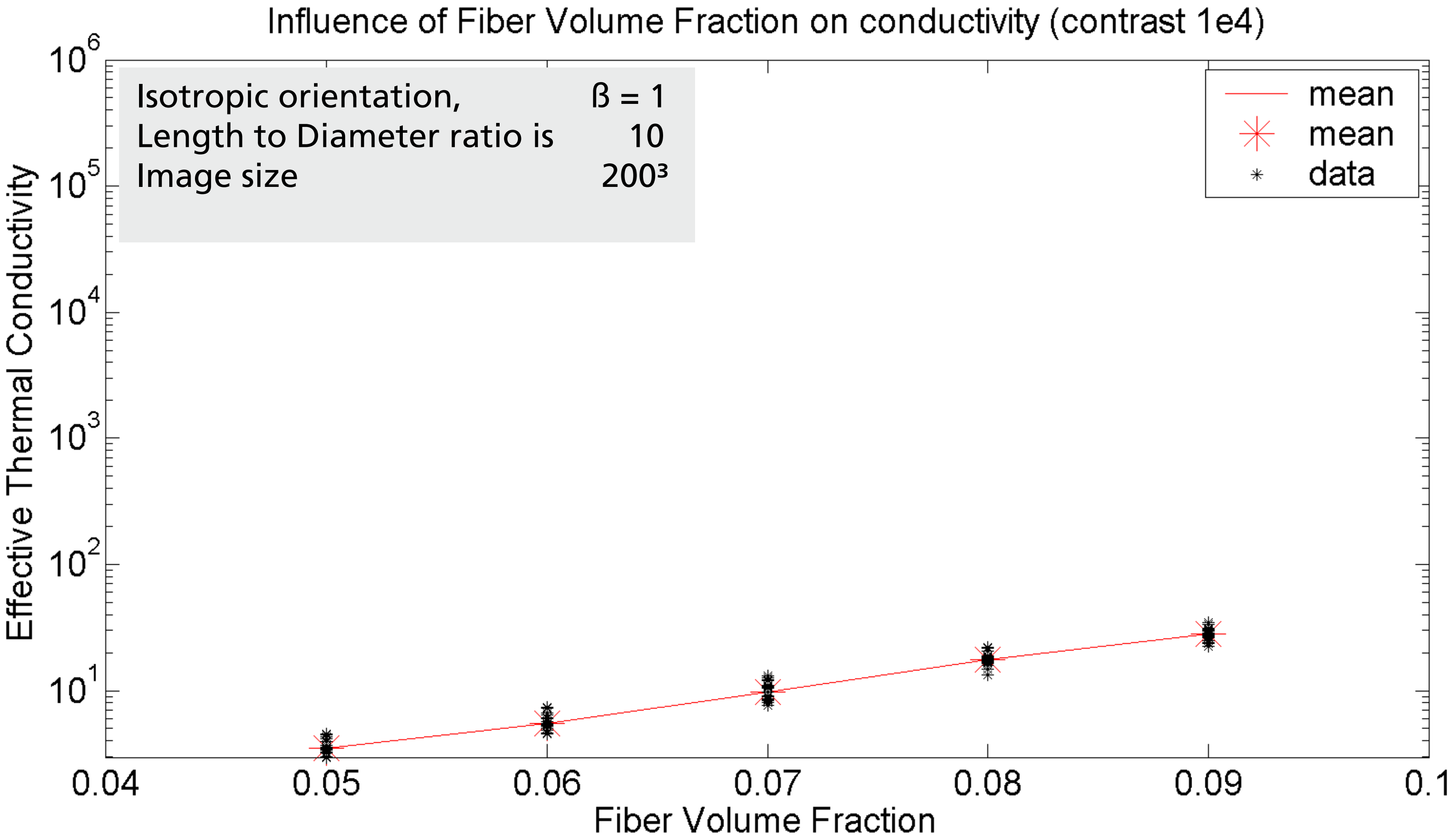


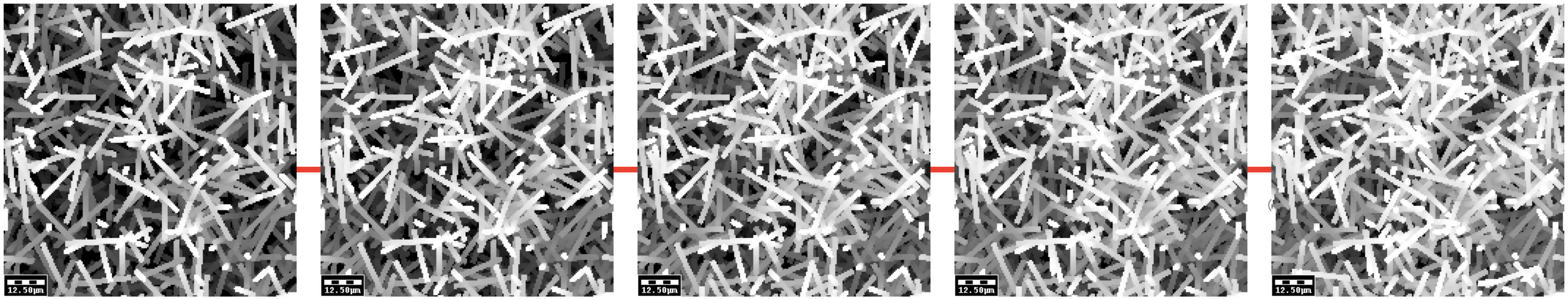

Influence of Anisotropy on percolation
Fiber Volume Fraction is 6.5%
Length to Diameter ratio is 10
Image size 200³
Fraction of percolating samples
0
0.2
0.4
0.6
0.8
1
0.1
0.5
1
2
Anisotropy1

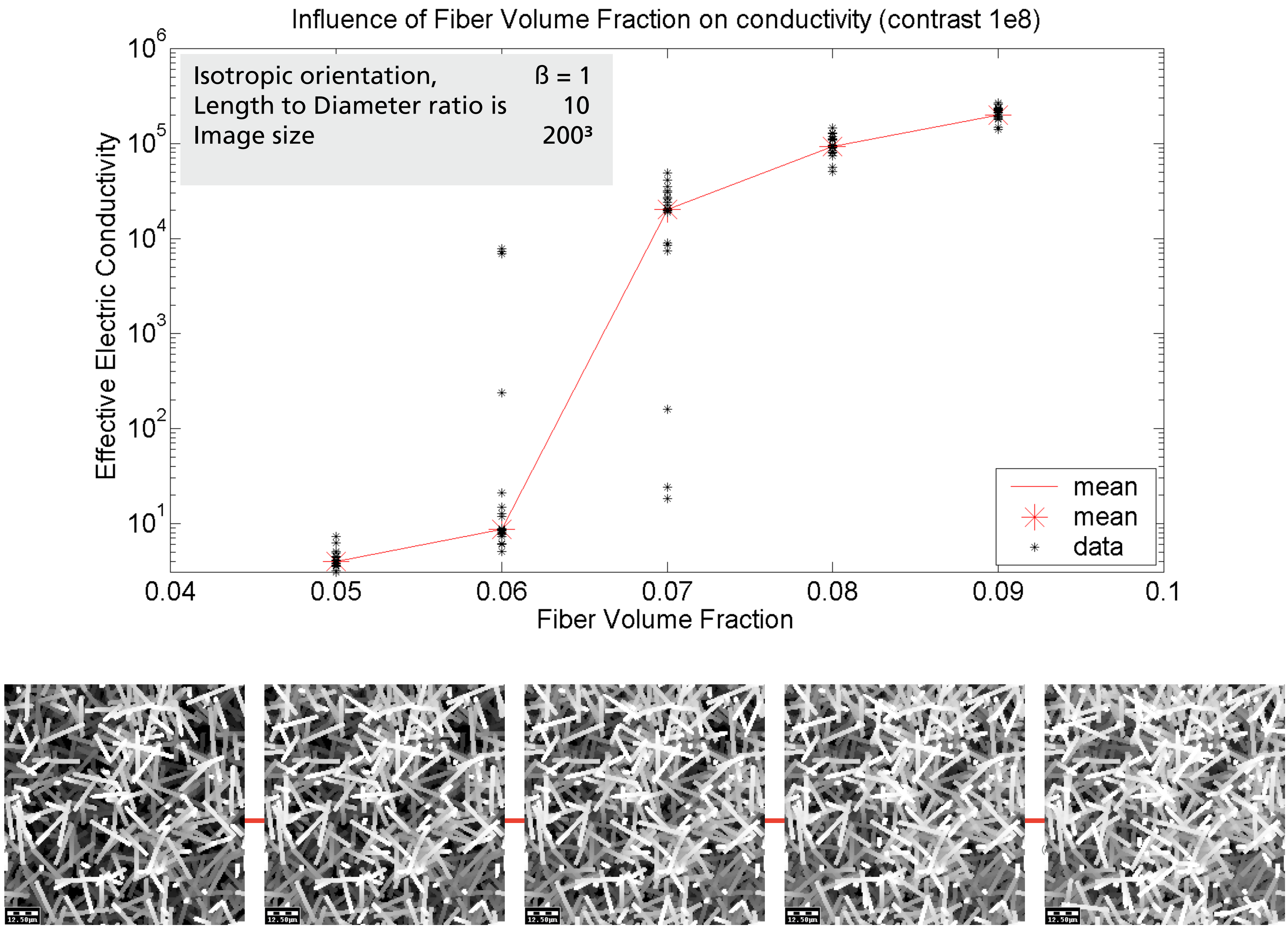

12.50µm
12.50µm
12.50µm
12.50µm
12.50µm


Influence of Fiber Length / Fiber Diamater on percolation
Fraction of percolating samples
0
0.2
0.4
0.6
0.8
1
4
10
20
40
100
Fiber Length / Fiber Diameter
Isotropic orientation, ß = 1
Fiber Volume Fraction is 6.5%
Image size 200³




Influence of Fiber Volume Fraction on conductivity (contrast 1e4)
Isotropic orientation, ß = 1
Length to Diameter ratio is 10
Image size 200³
mean
mean
data
Effective Thermal Conductivity
10^{6}
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
0.04
0.05
0.06
0.07
0.08
0.09
0.1
Fiber Volume Fraction




Influence of Fiber Volume Fraction on conductivity (contrast 1e8)
Isotropic orientation, ß = 1
Length to Diameter ratio is 10
Image size 200³
Effective Electric Conductivity
Fiber Volume Fraction
10^6
10^5
10^4
10^3
10^2
10^1
0.04
0.05
0.06
0.07
0.08
0.09
0.1
mean
mean
data
12.50μm
12.50μm
12.50μm
12.50μm
12.50μm

GeoDict

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