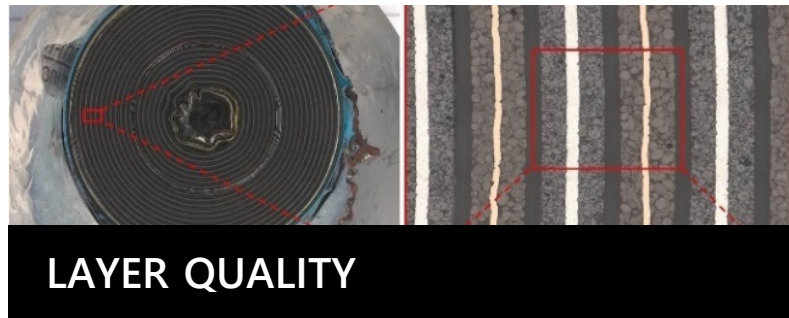


OPTIMUM REGION-SIZE FOR BATTERY CHARGING SIMULATIONS ON THE MICROSCALE

Dr. Ilona Glatt, Aaron Widera, Andreas Wiegmann PhD
(Math2Market)

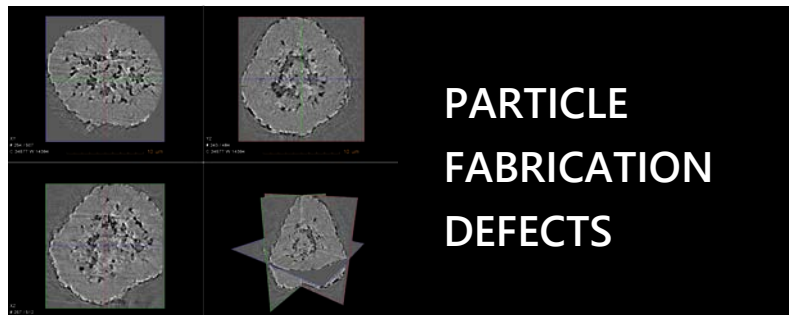
Li-Ion Batteries: A Complex, Multi-Scale Problem



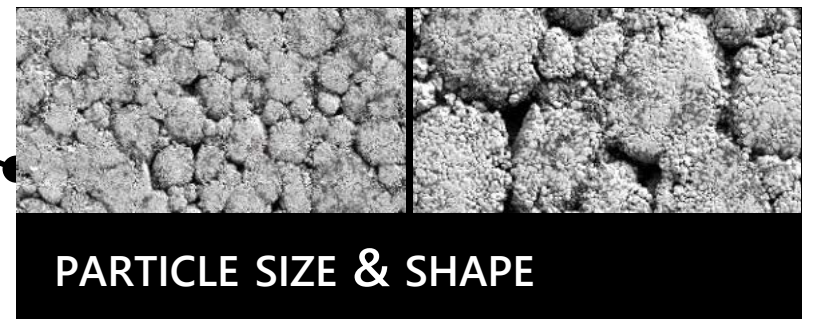
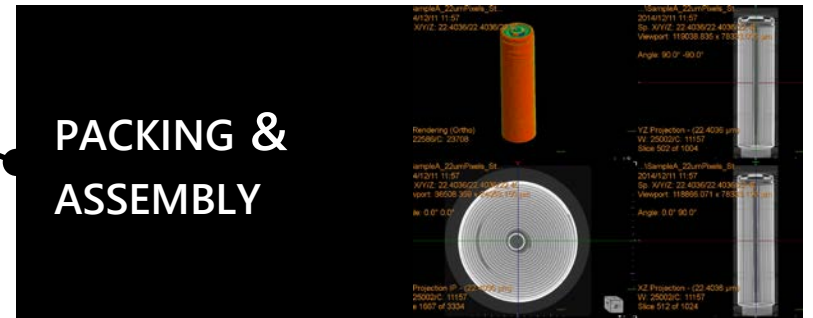
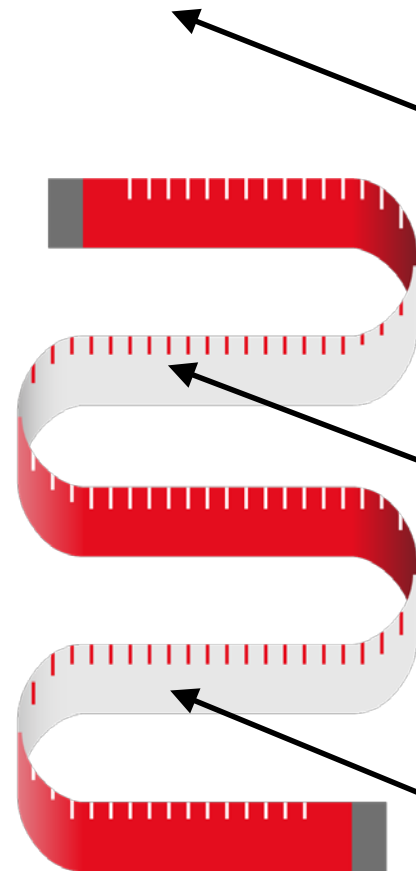
mm



μm



nm



What is GeoDict?

GEO-DICT® IS

DATA-DRIVEN DIGITAL MATERIAL DESIGN

IN AN EASY-TO-USE SOFTWARE SOLUTION

The innovative and easy-to-use material simulator GeoDict® is the most complete solution for multi-scale 3D image processing, modeling of materials, visualization, material property characterization, simulation-based material development, and optimization of processes.



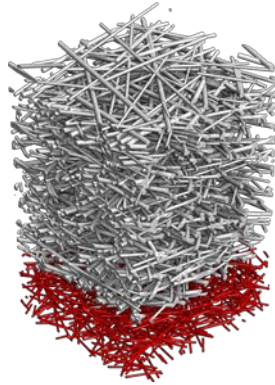
The GeoDict workflow

IMPORT



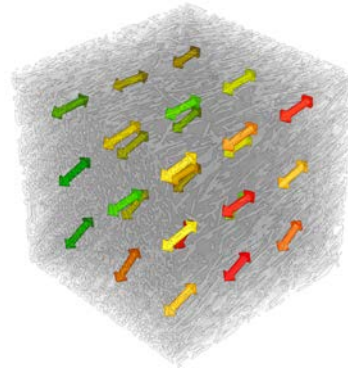
Diverse ways to import materials for modeling

MODEL



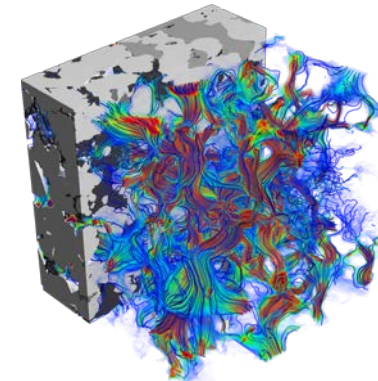
Detailed material models created in 3D

ANALYZE



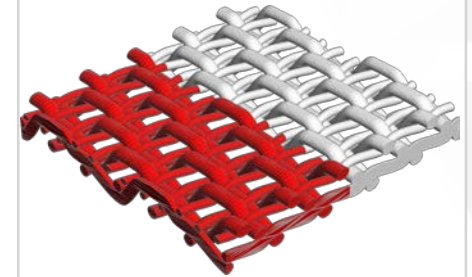
Extensive analysis and evaluation of structural material properties

PREDICT



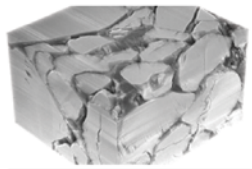
In-depth analysis and prediction of material behavior

EXPORT

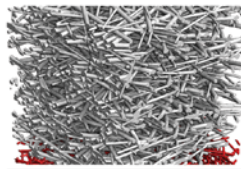
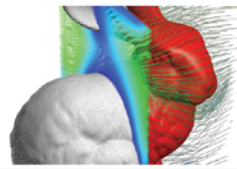
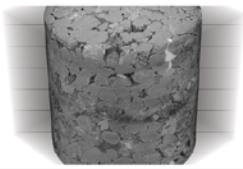


GeoDict models made available for standard workflows

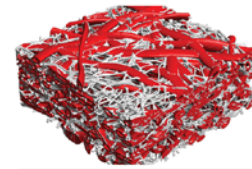
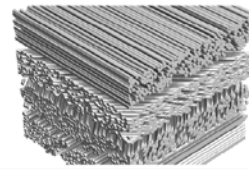
Overview of GeoDict modules and versatility



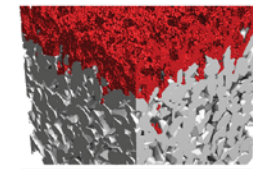
IMPORTGEO



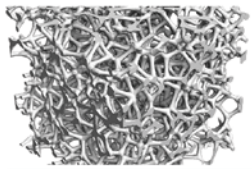
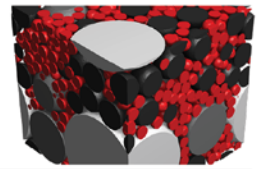
FIBERGEO



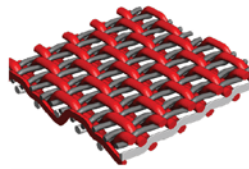
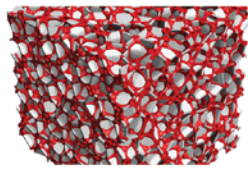
PAPERGEO



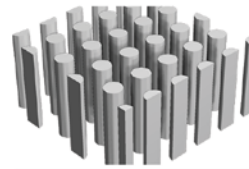
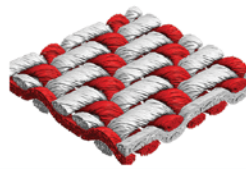
GRAINGEO



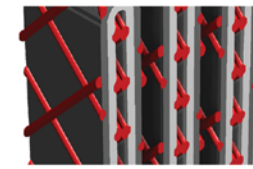
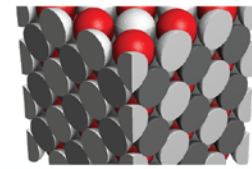
FOAMGEO



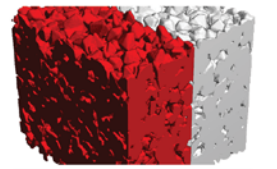
WEAVEGEO



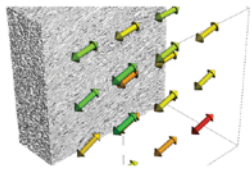
GRIDGEO



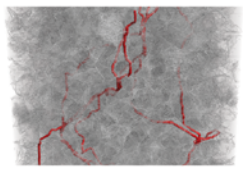
PLEATGEO



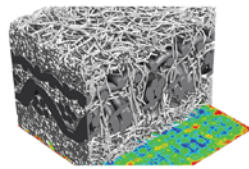
EXPORTGEO



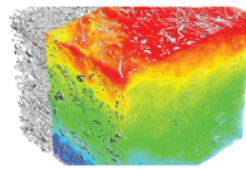
FIBERGEO



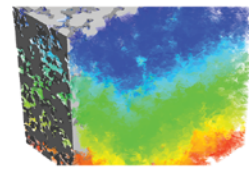
PORODICT



MATDICT



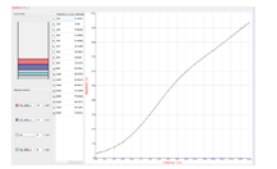
CONDUCTODICT



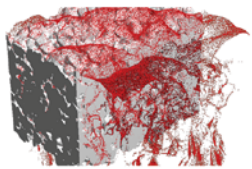
DIFFUDICT



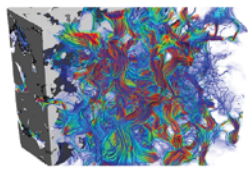
ELASTODICT



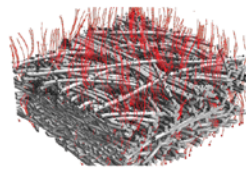
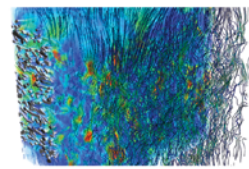
ACOUSTODICT



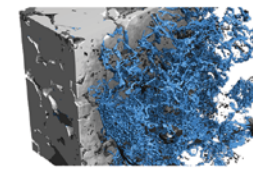
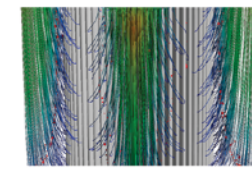
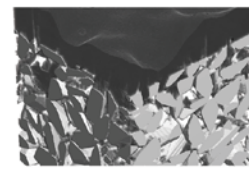
ADDIDICT



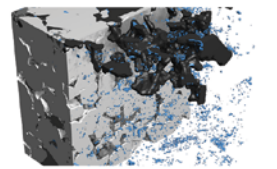
FLOWDICT



FILTERDICT MEDIA & ELEMENT

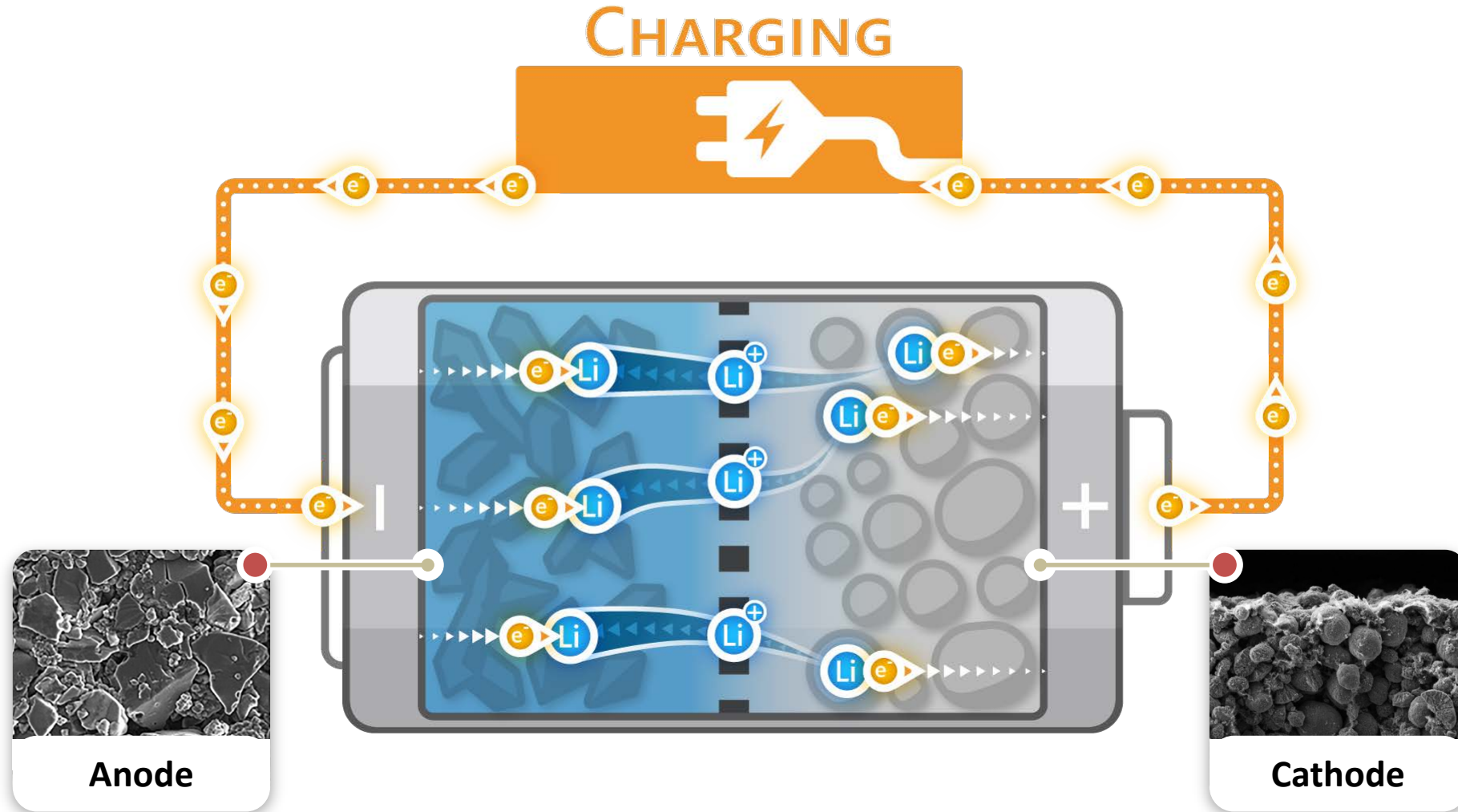


SATUDICT

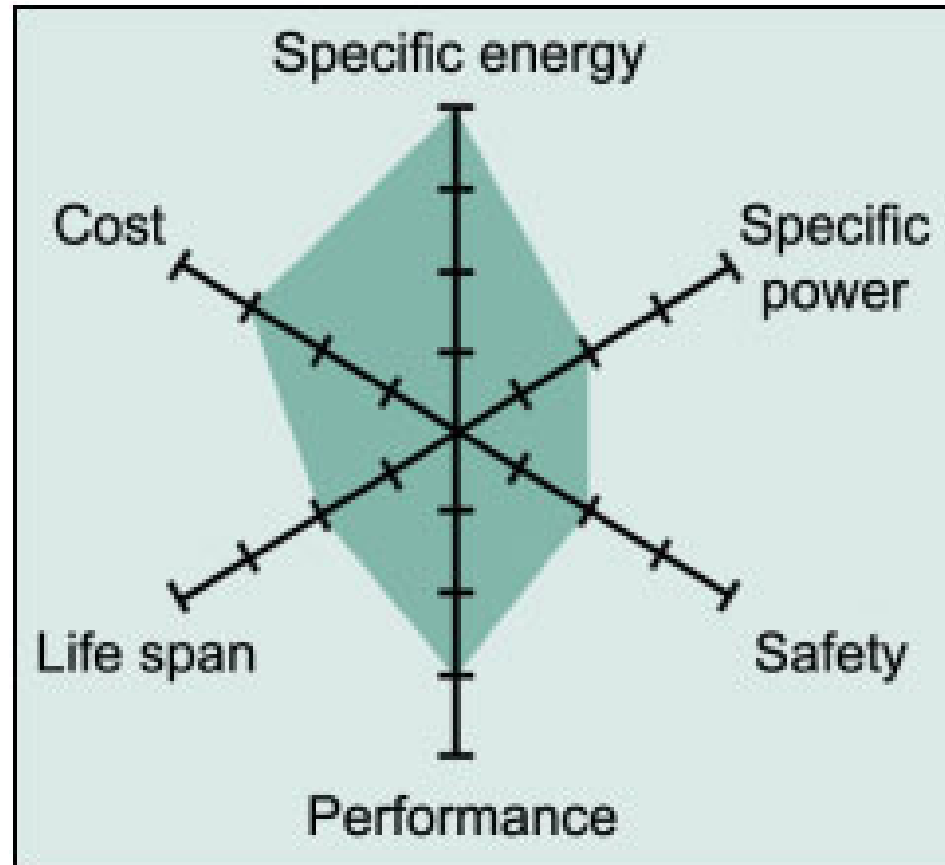


Introduction

Schematic of a Li-Ion battery



Interplaying properties in a Li-ion cell



Source: http://batteryuniversity.com/learn/article/types_of_lithium_ion

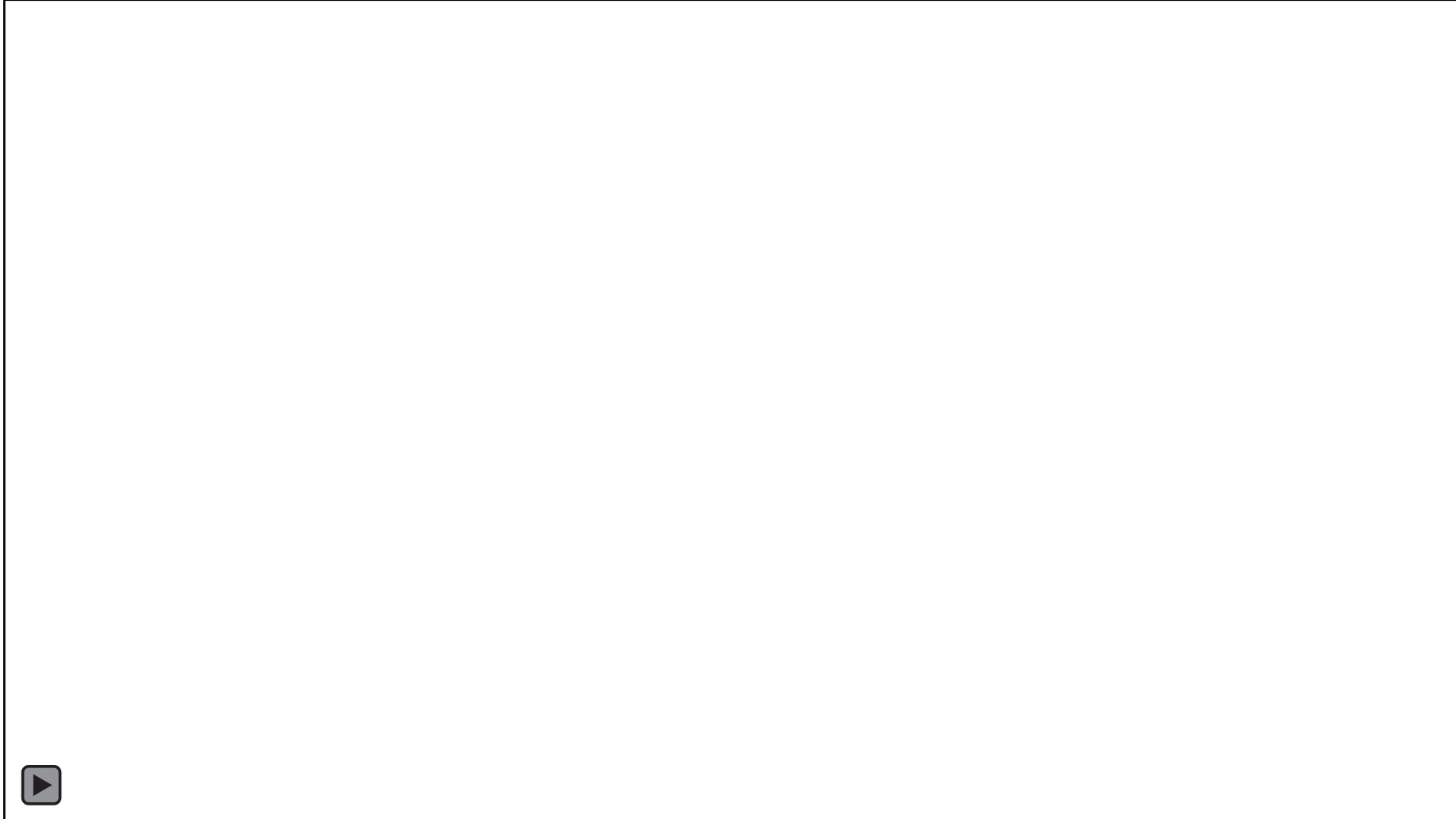
Transportation is crucial



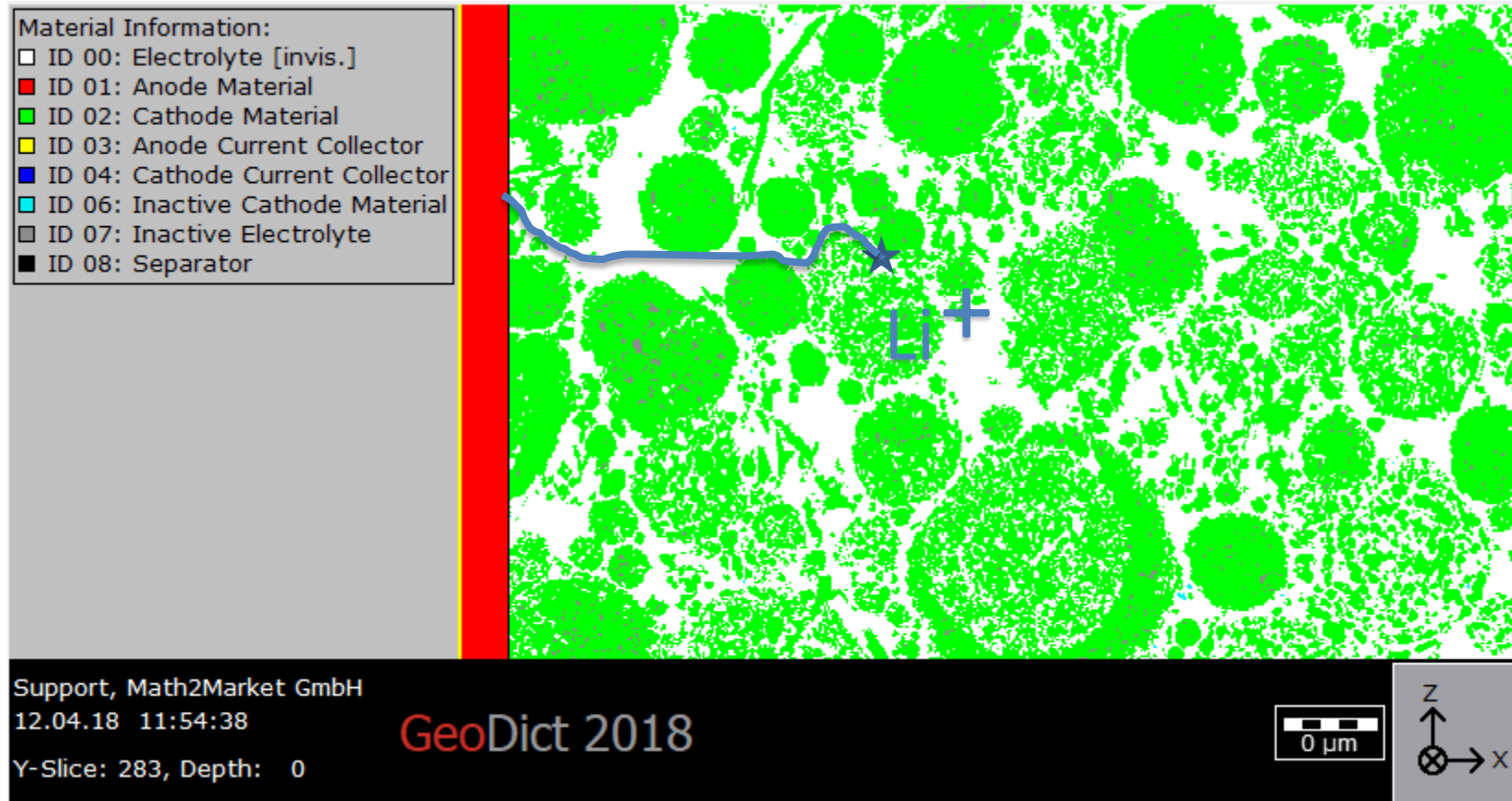
Traffic routes in Ludwigshafen, Germany
Source: <https://www.stuttgarter-zeitung.de>

LiFePO₄ – cathode

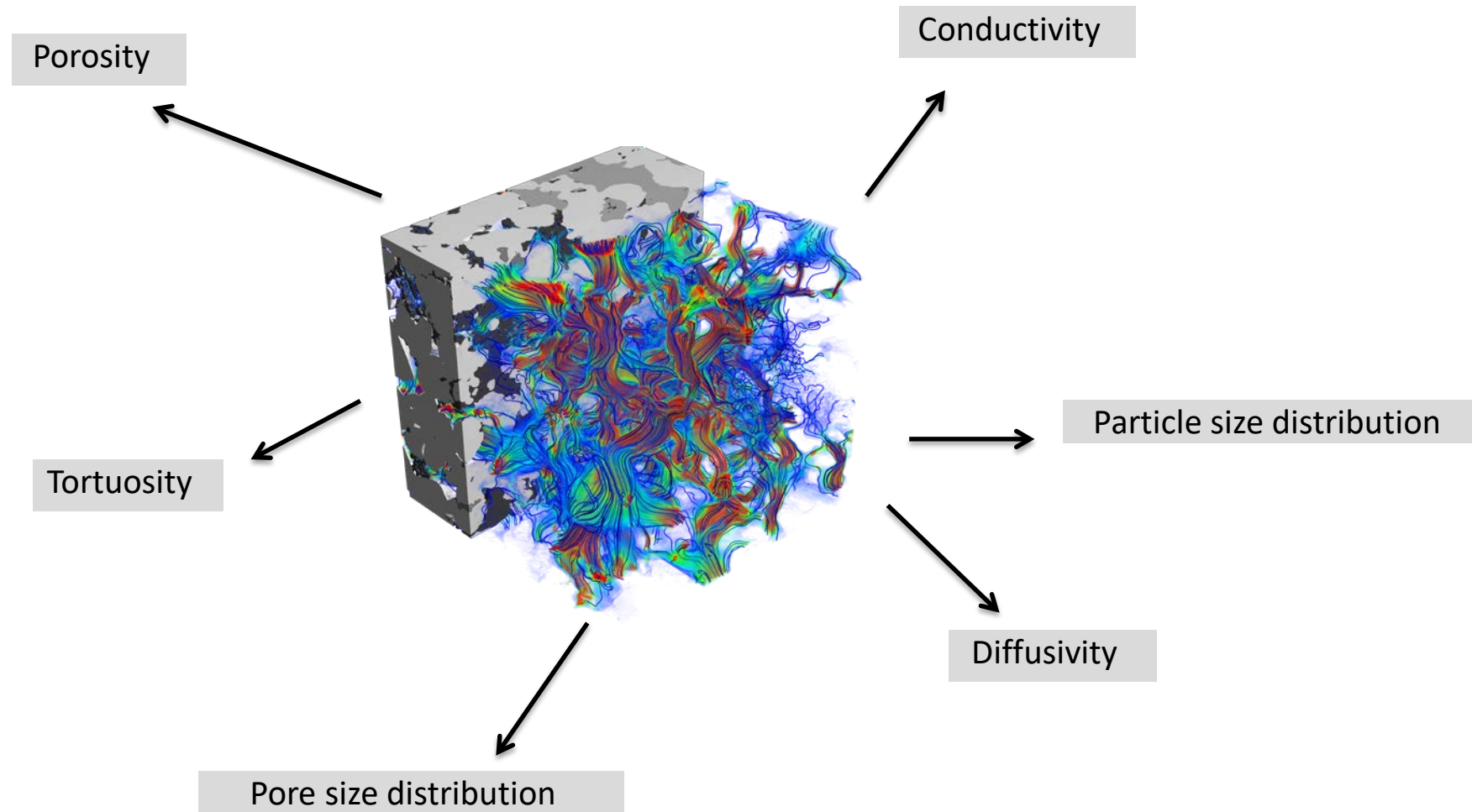
Scan and segmentation by KIT (Karlsruhe Institute of Technology)



Transportation is crucial

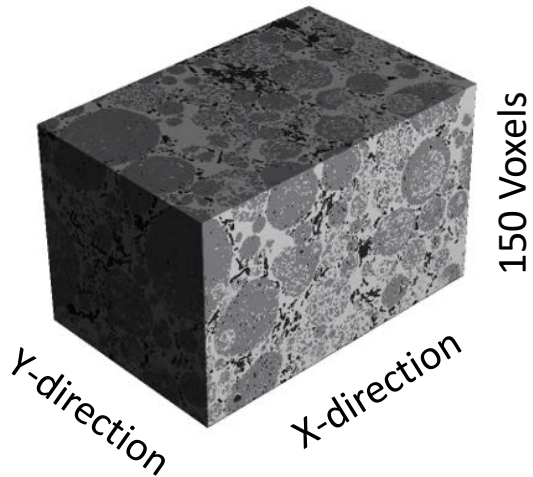


The microstructure defines macroscopic properties



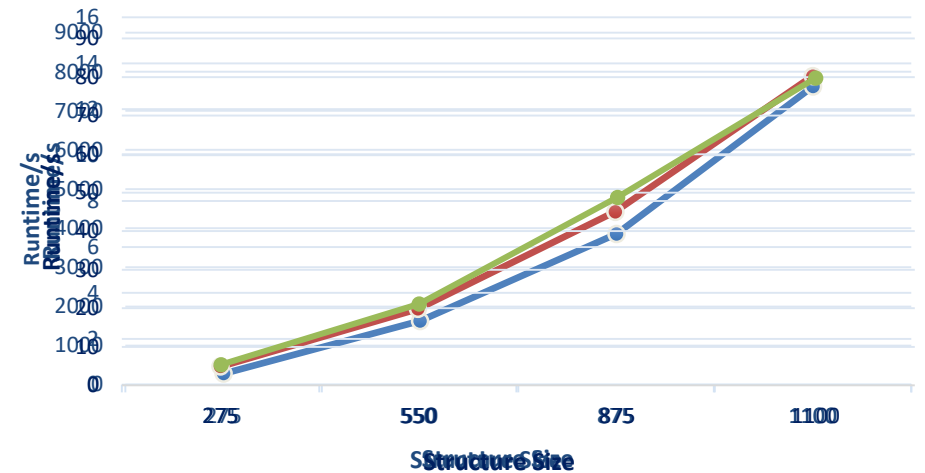
Runtime for the microstructure analysis

Structure Size in x and y	Runtime for Tortuosity	Runtime for Grain Size Distribution	Runtime for Specific Surface Area
275	~5 min	5 s	0.8 s
550	~0.5 h	21 s	3.3 s
875	~1 h	49 s	7.5 s
1100	~2 h	~1.25 min	13.4 s



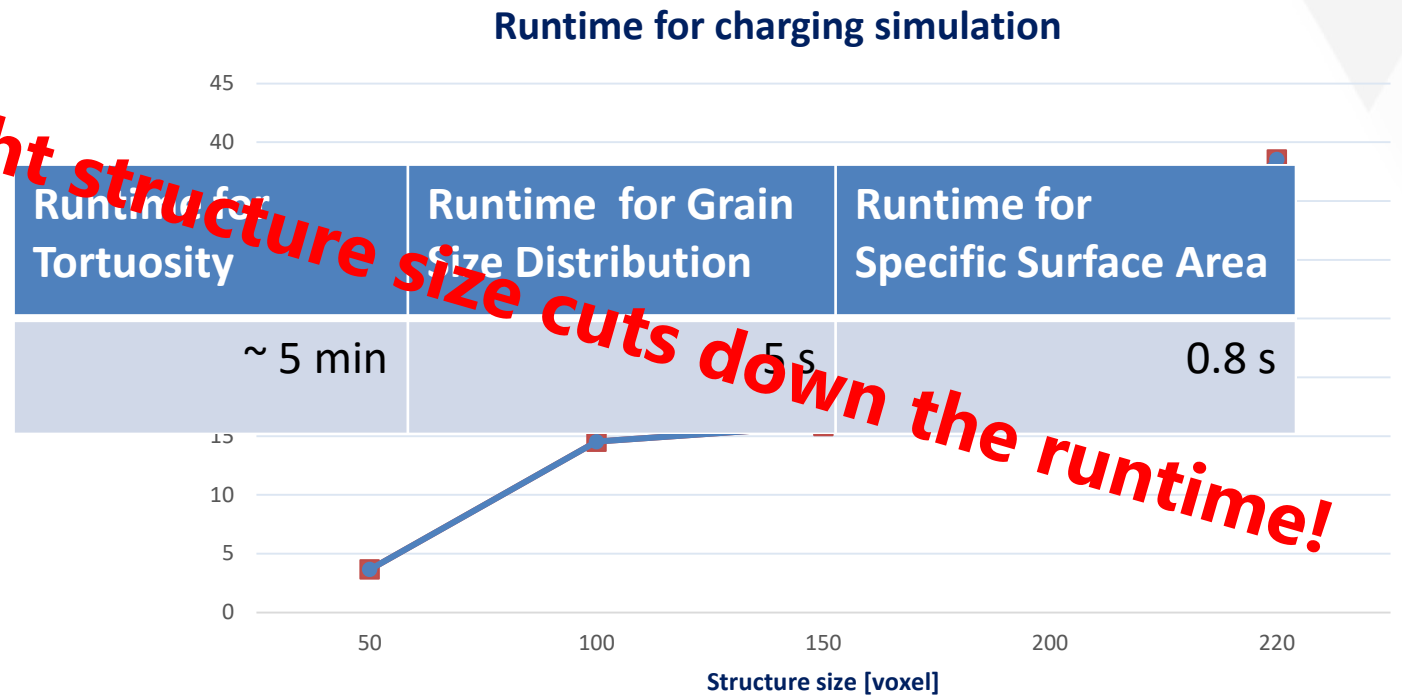
8 parallel processes used

Runtime for Specific Surface Area
Runtime for Grain Size Distribution



Runtime for charging simulations

Structure Size in x und y	Runtime for charging simulation
50 voxel	3.7 h
100 voxel	14.5 h
200 voxel	22.2 h
400 voxel	43.9 h



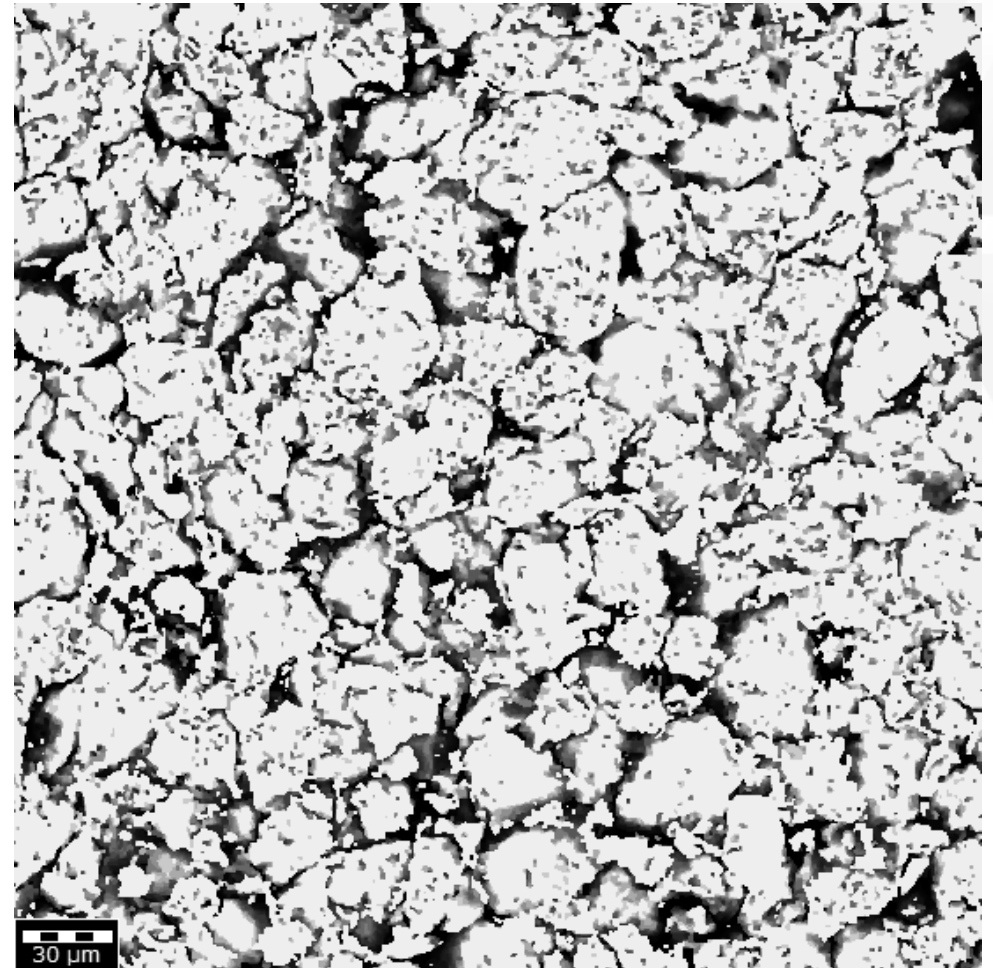
Analyzed structure: Anode: same structure size as cathode, voxel length = 0.325 μm , C-rate = 1, CPU = 16



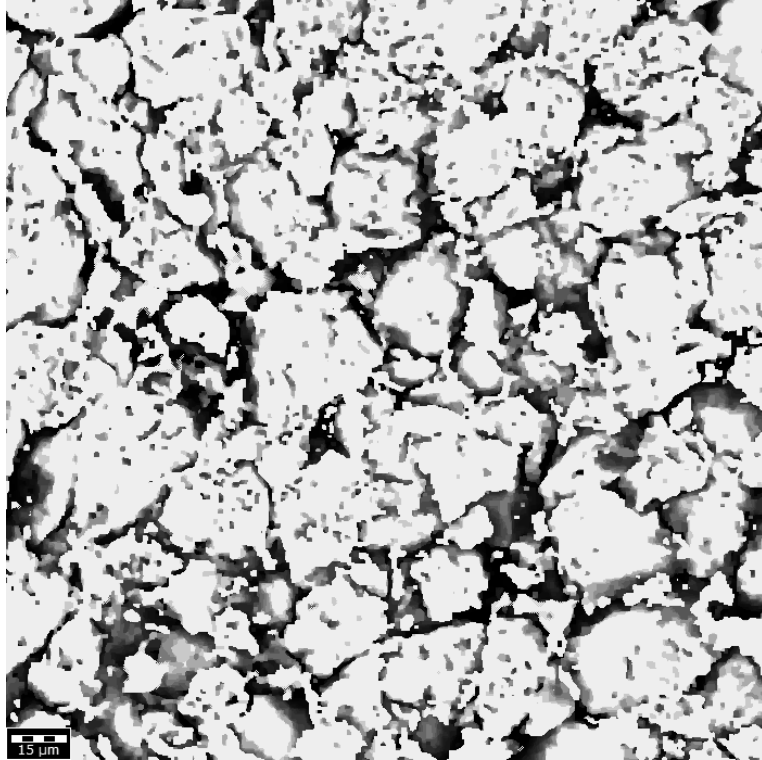
How large does the structure need to be?

Sample

- Cathode scan from ETH-Zürich, V. Wood et al.
- Segmented by ETH
- Structure size:
1100 x 1100 x 150 voxels
- Described in Müller et al. 2018



What is the right structure size?



Hexagonal array Unit cell

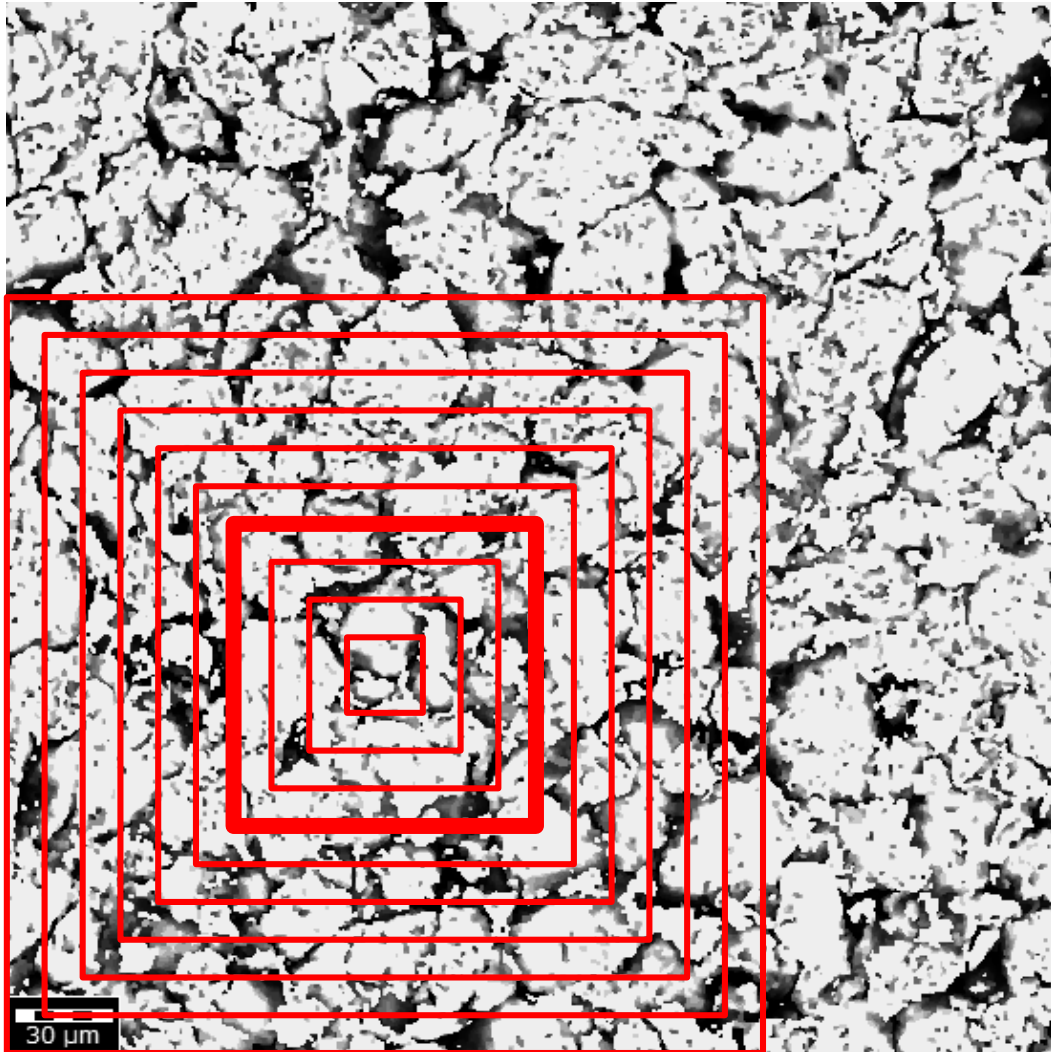
Analyzed electrode structure

We need a region large enough to obtain the same statistical values for different locations of the region on the entire structure.

Definition: Representative volume element
RVE

the region is representative for the entire structure

Choosing regions to analyze



- We chose a starting region, with similar size and geometric properties as in Müller et al. 2018, (200 x 200 x 150 voxel)
- Next testing regions are concentric squares with 50 voxel less or 50 voxel more in x and y

Computed geometrical properties

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

Computed geometrical properties

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

Tortuosity: How “tortuous” (curved) is the path?

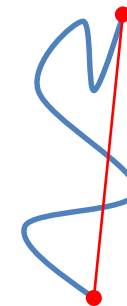


← Low tortuosity,
 $\tau \sim 1$

High tortuosity,
 $\tau \gg 1$



Tortuosity (τ) is the ratio of length of the path (L) to the distance between the ends (C):



$$\tau = \frac{L}{C}$$



courtesy of Jeff Gelb,
Zeiss 2017

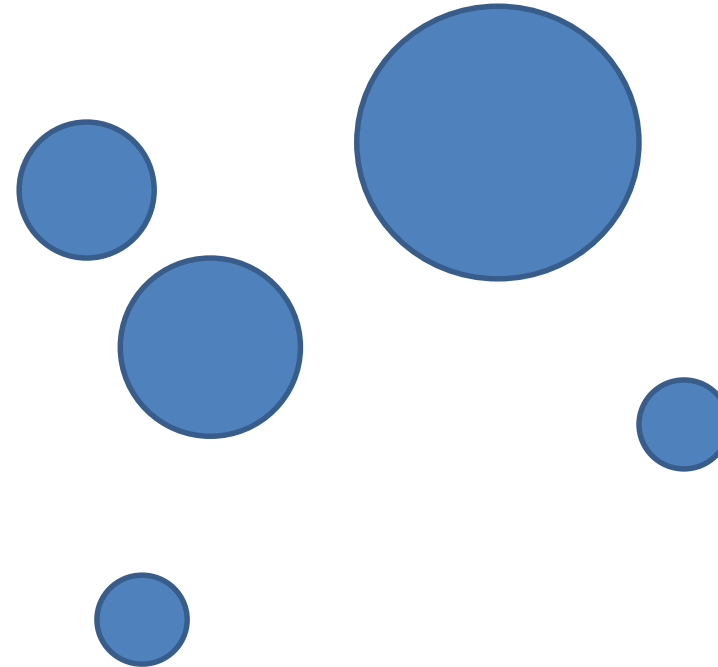
Computed geometrical properties

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

Computed geometrical properties

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

D50: How large is the “normal” particle?



D50 (median) means that there are as many particles that are larger than this value and smaller than this value

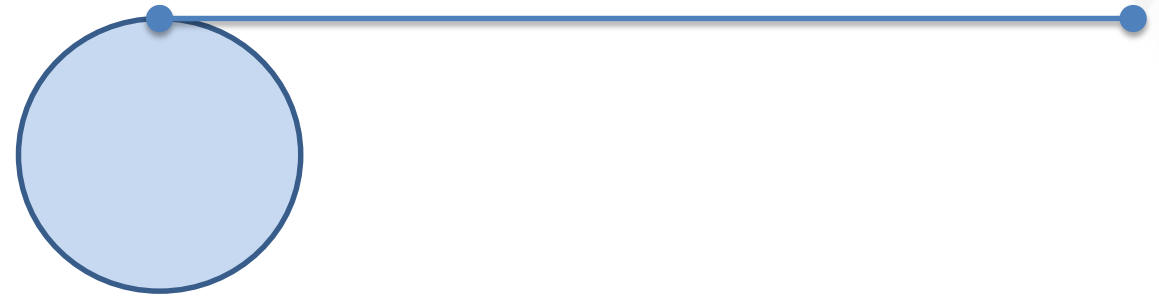
Computed geometrical properties

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

Computed geometrical properties

Specific Surface Area:
How much of the solid phase touches the pore space?

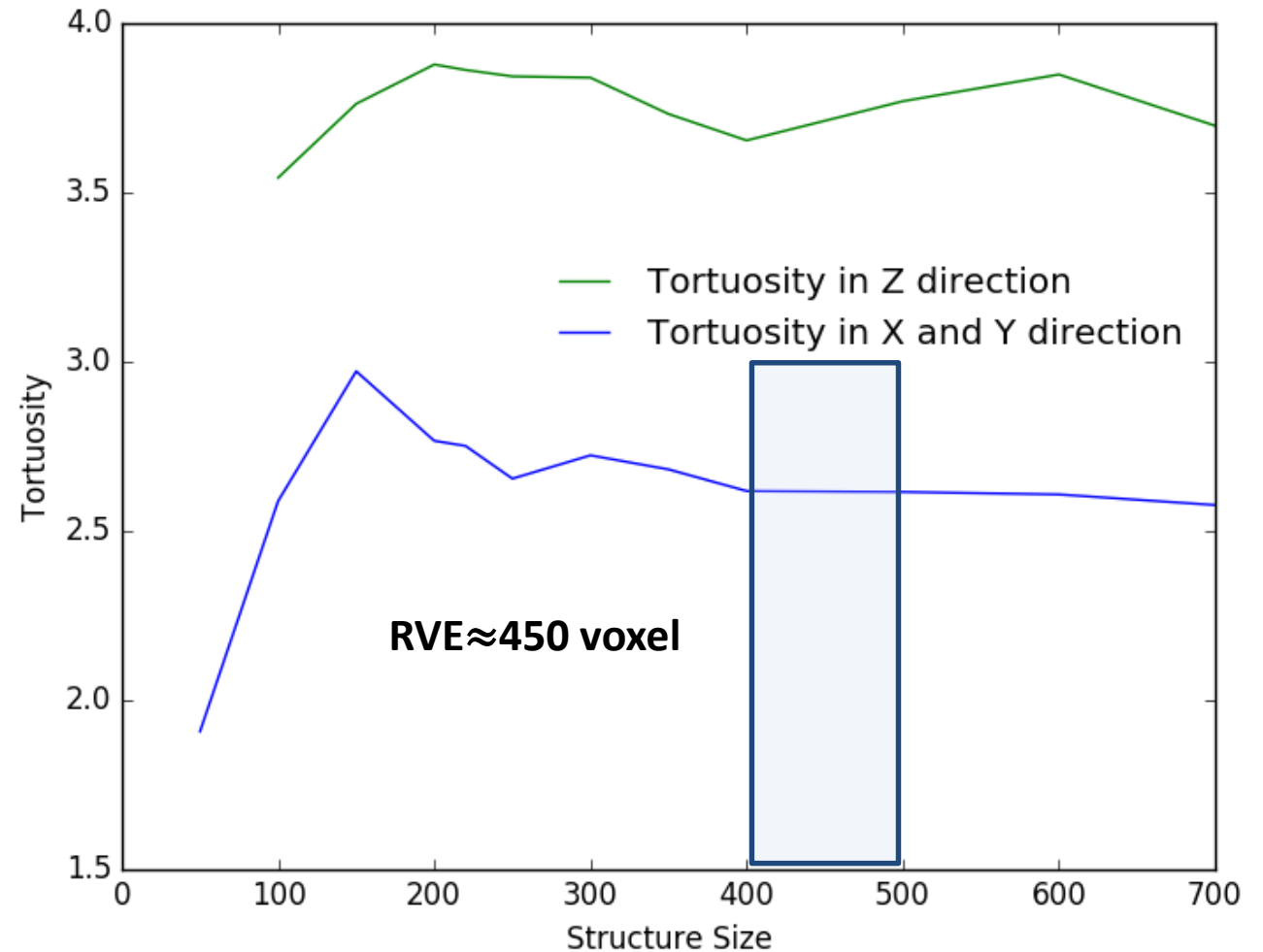
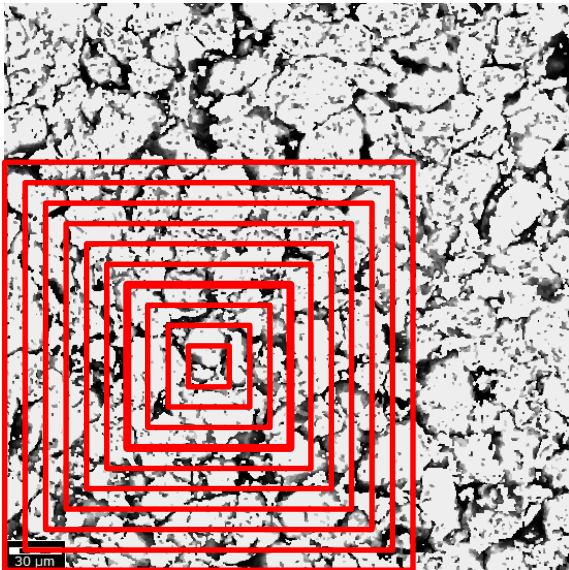
- Tortuosity
- D50 of grain sizes
- Specific Surface Area



The **specific surface area** is the total surface area of a material per bulk volume (units of m^2/m^3 or m^{-1}).

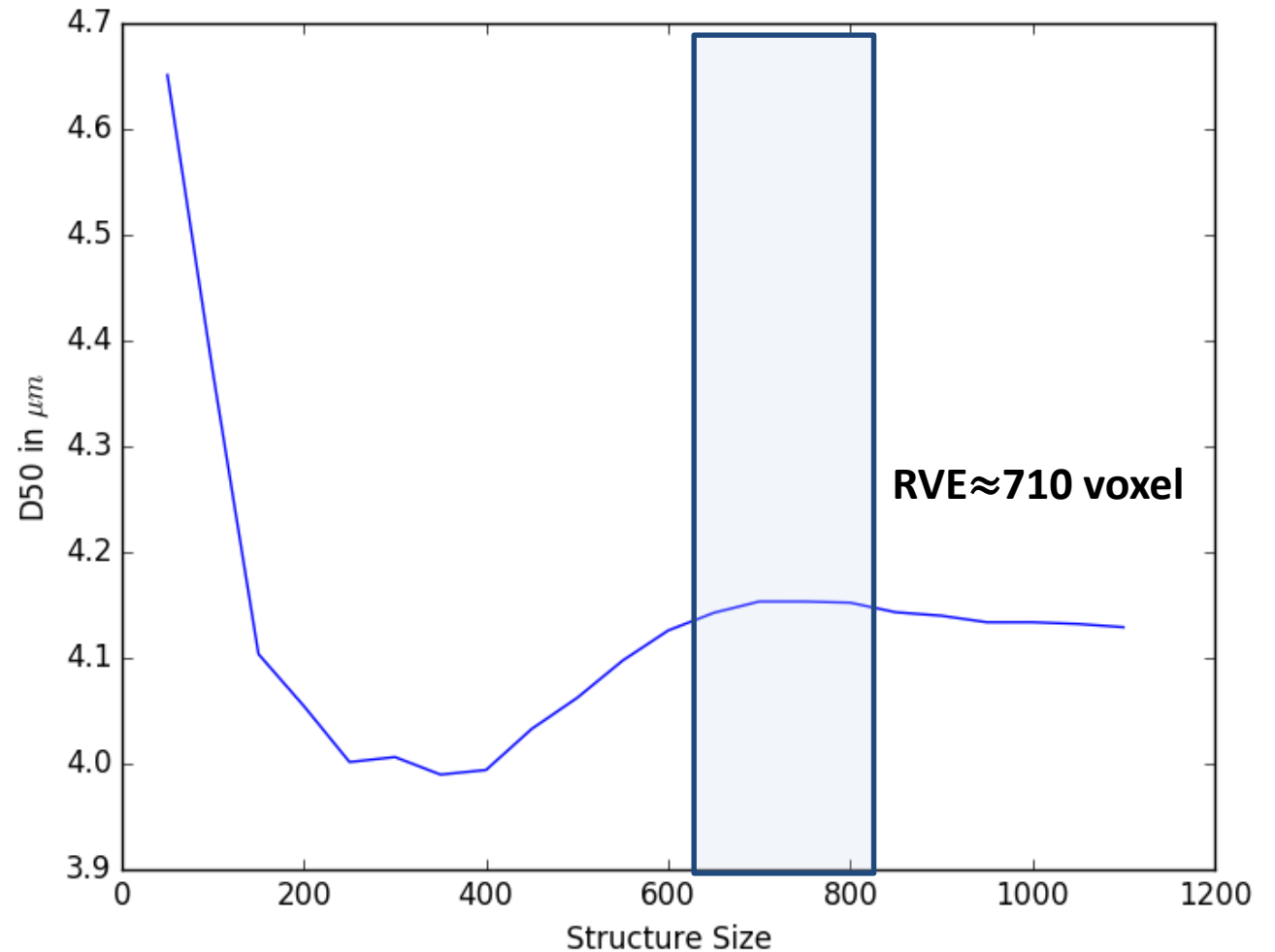
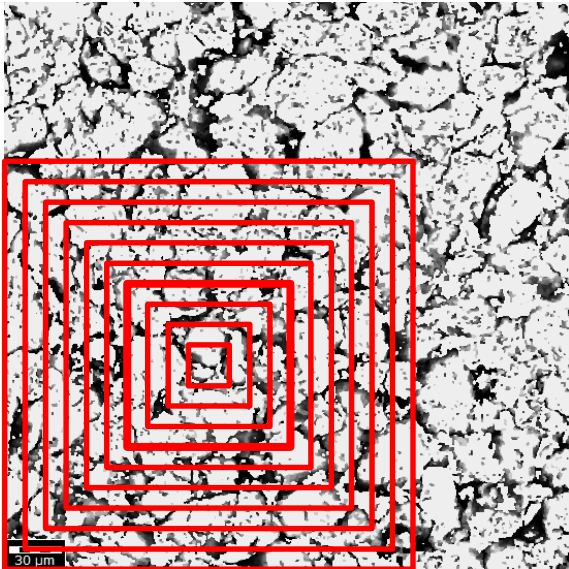
Variation of the properties for different regions

- Tortuosity
- D50 of grain sizes
- Specific Surface Area



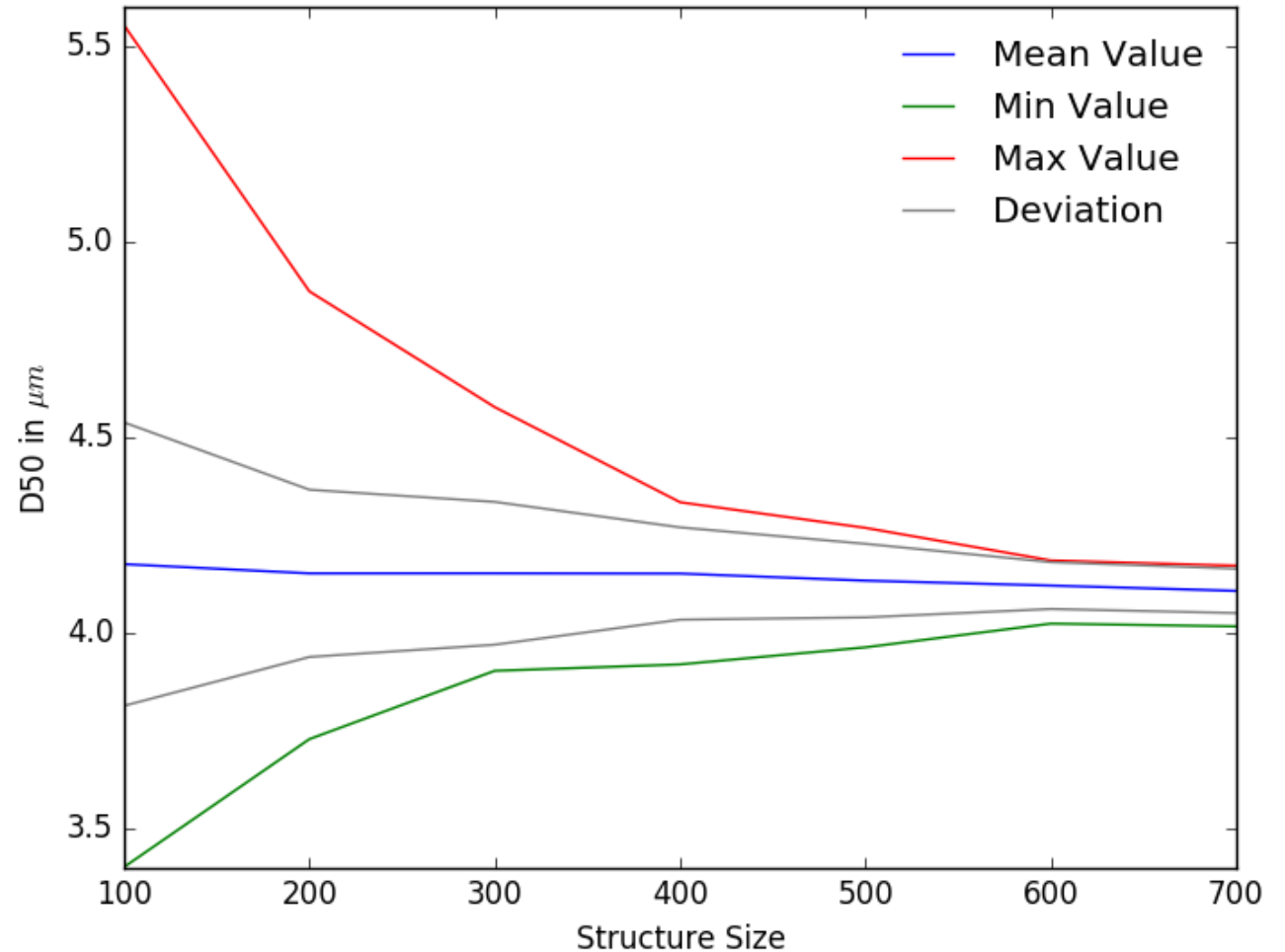
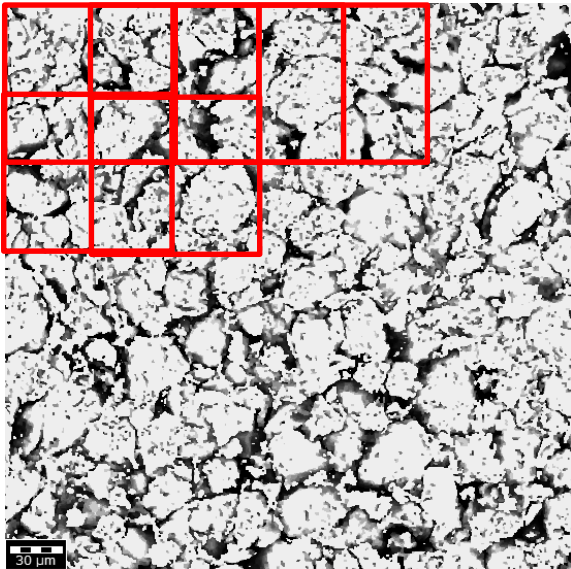
Variation of the properties for different regions

- Tortuosity
- D50 of grain sizes
- Specific Surface Area



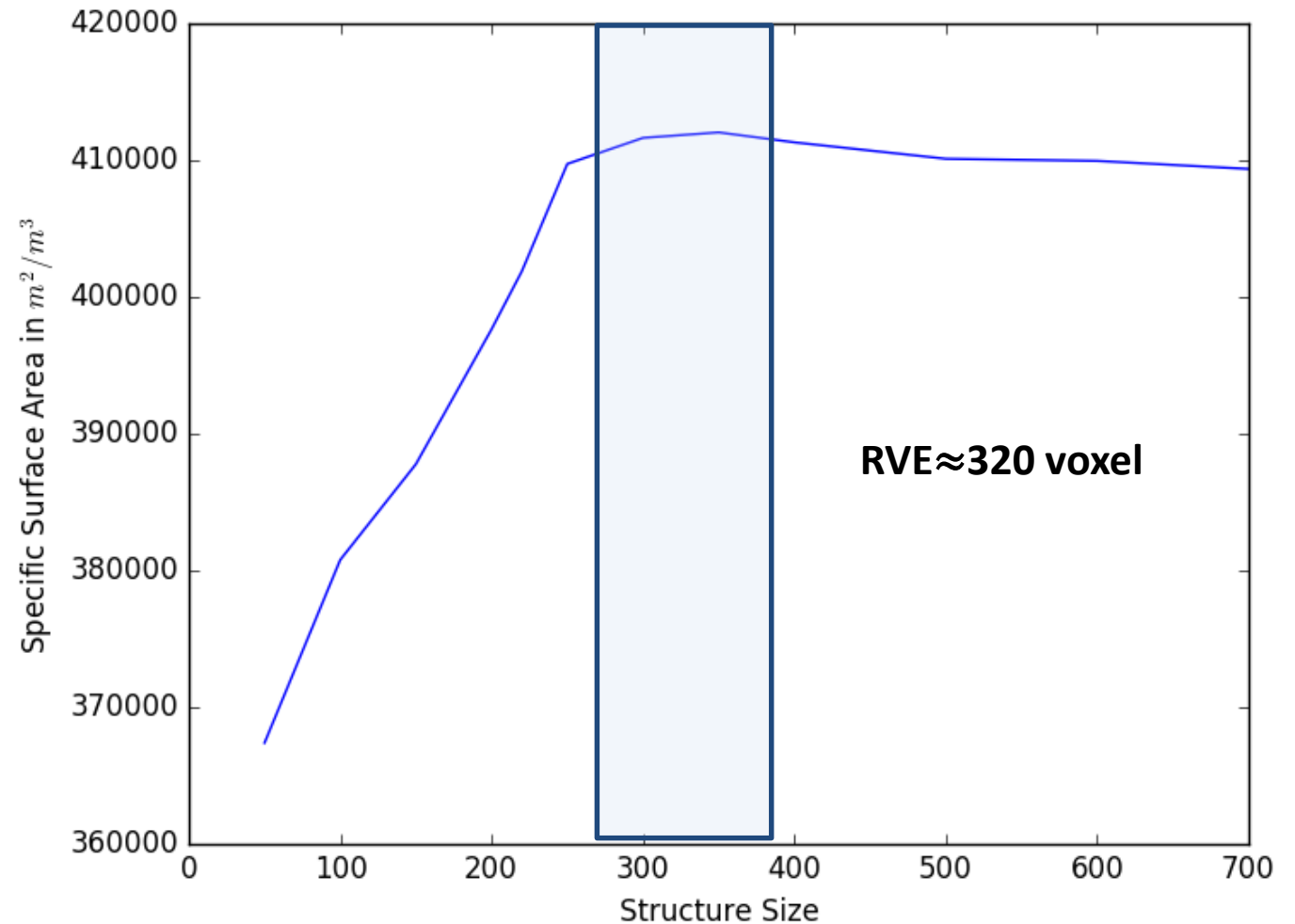
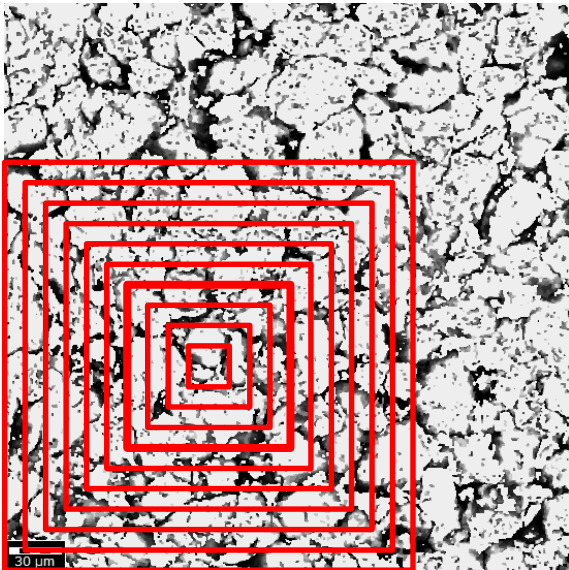
Variation of the properties for different regions

- Tortuosity
- D50 of grain sizes
- Specific Surface Area



Variation of the properties for different regions

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

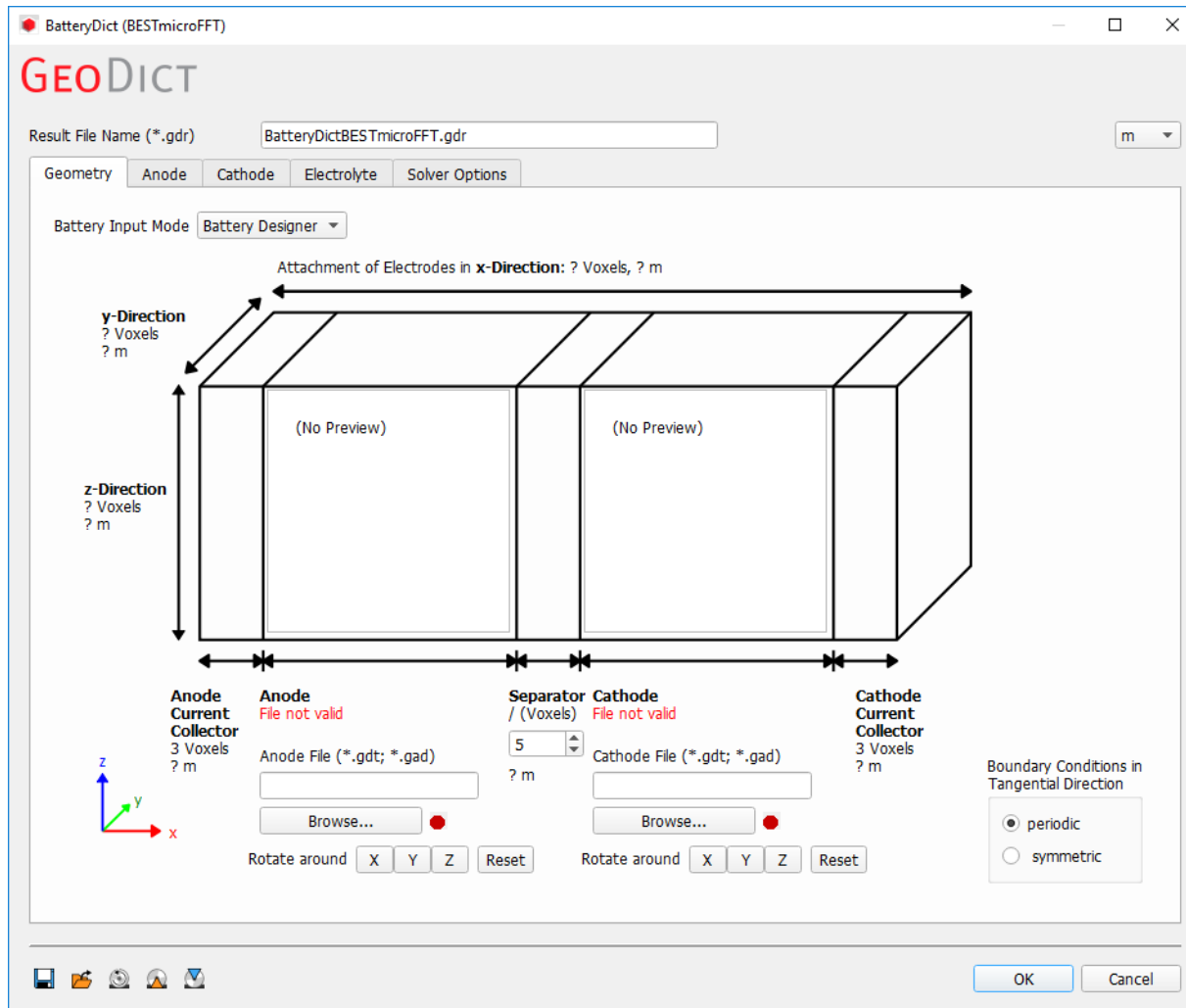


Resulting RVE for micro-scale properties

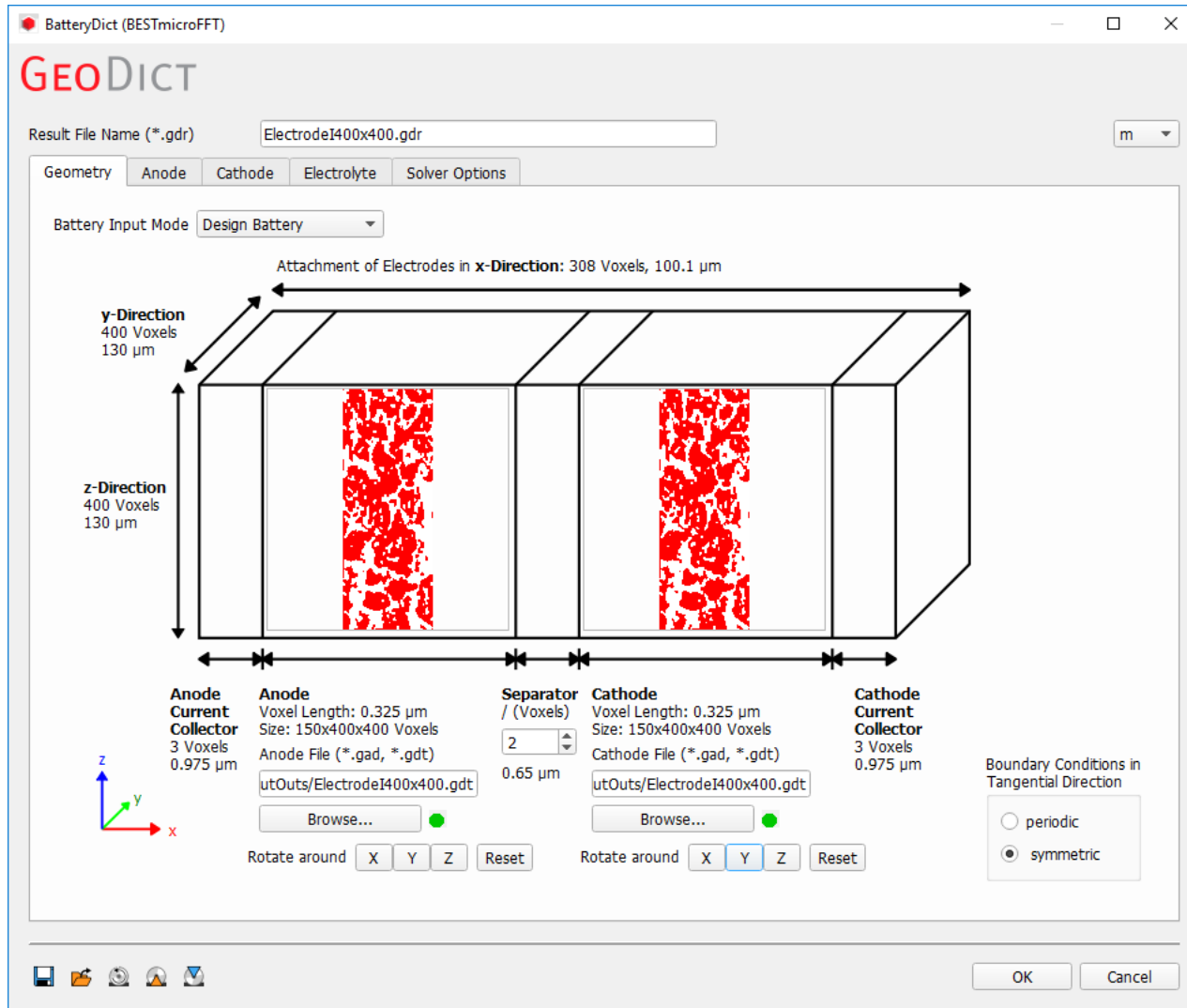
Property	Structure size for RVE in x and y [voxel]
Tortuosity	450
D50 of grain sizes	710
Specific Surface Area	320

Battery Charging Simulations

Input for BatteryDict module

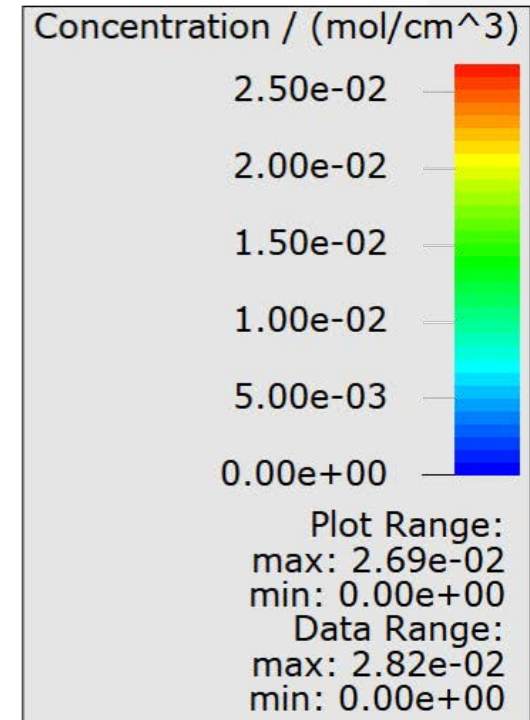
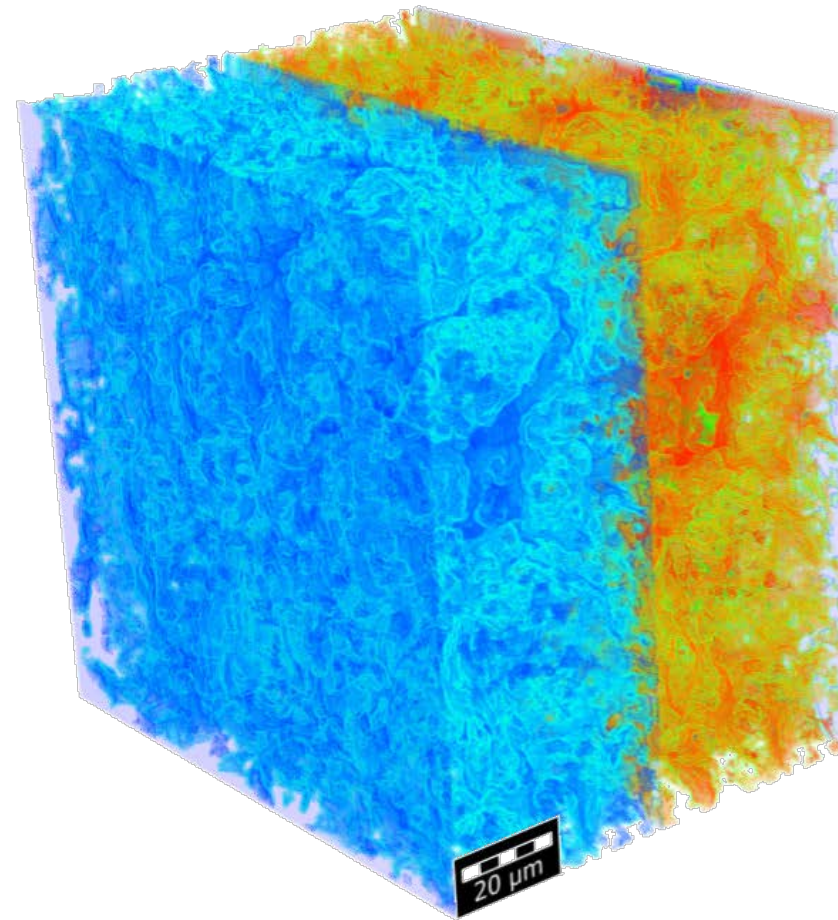


Input for BatteryDict module



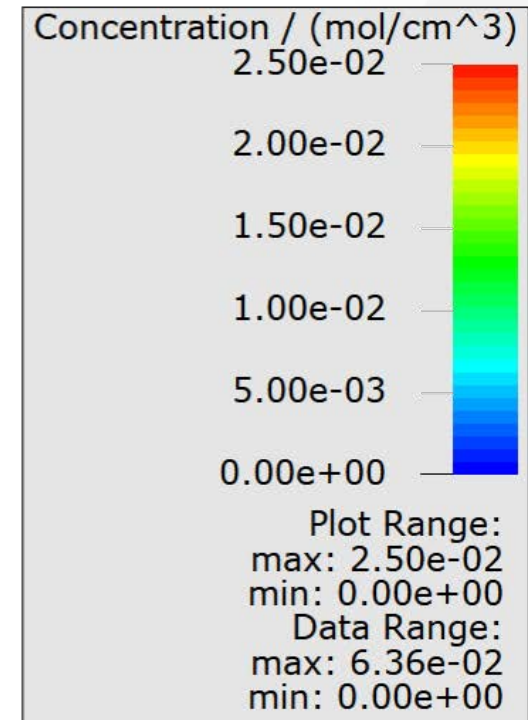
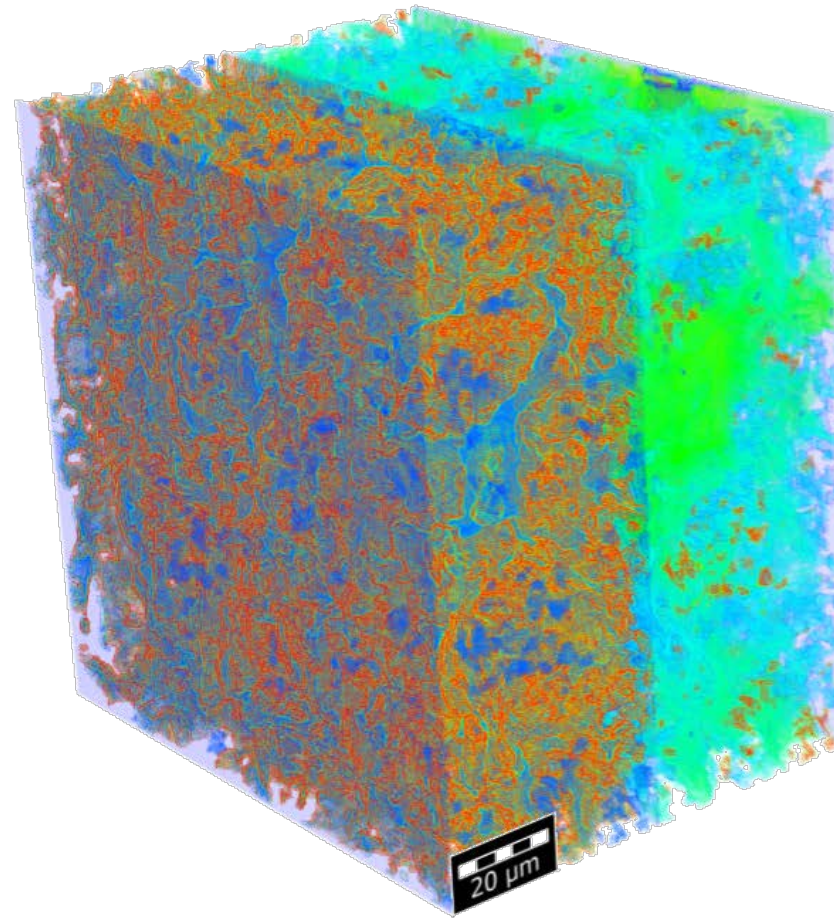
Result of BatteryDict module

Li-ion concentration at 20% SOF

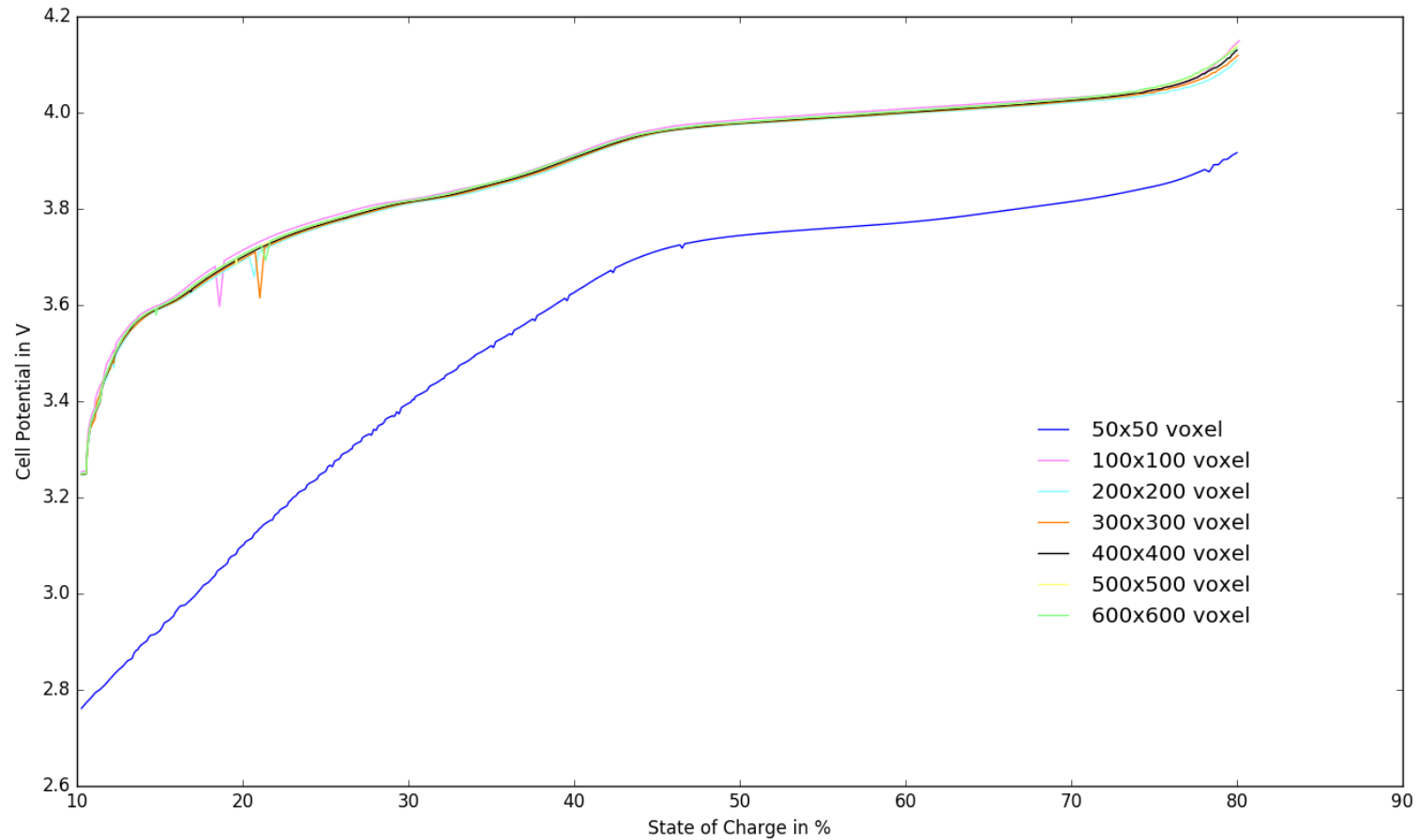


Result of BatteryDict module

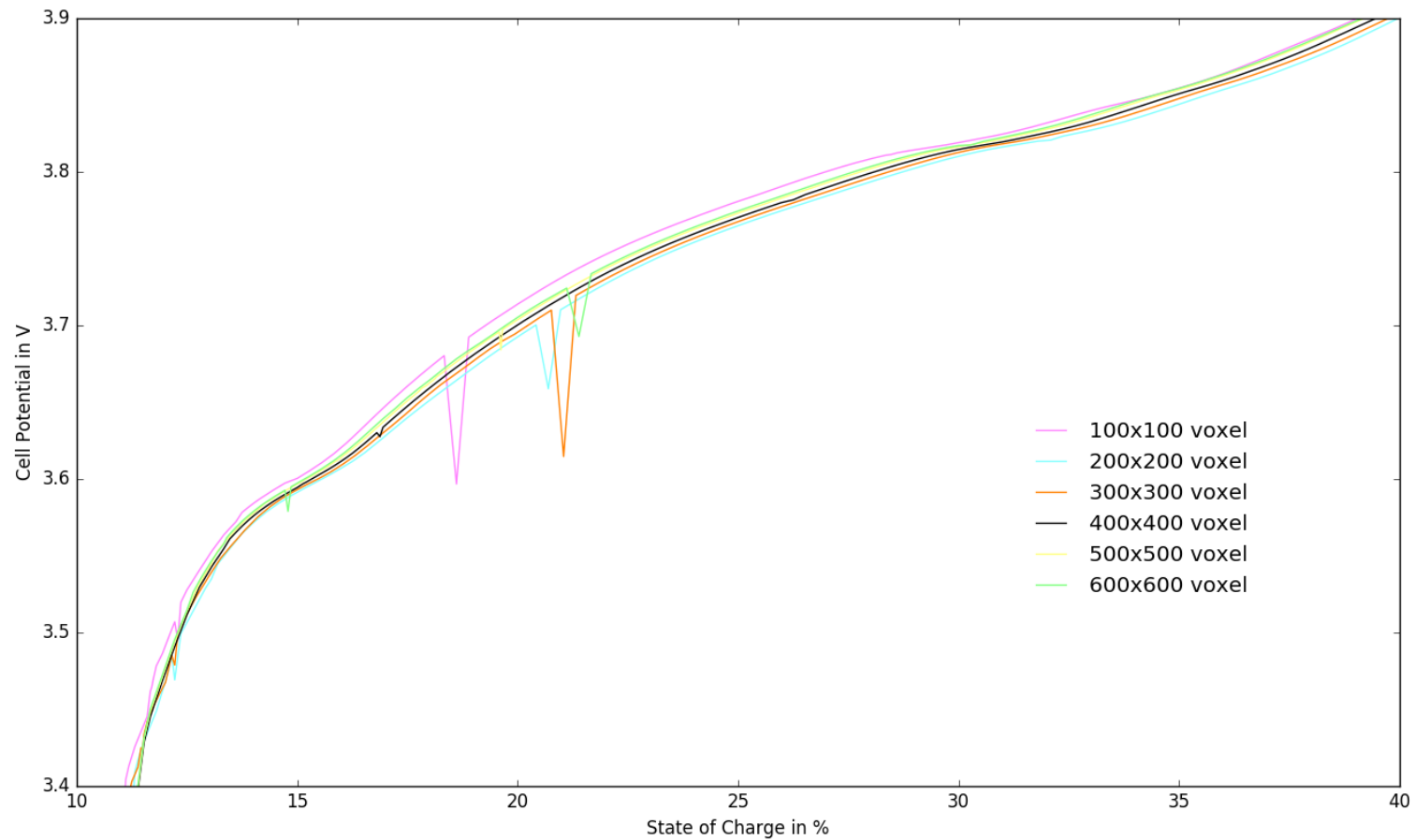
Li-ion concentration at 70% SOF



Charge curves for differently sized regions



Charge curves for differently sized regions



Resulting RVE for charging simulation

Property	Structure Size for RVE in x and y [voxel]
Tortuosity	450
D50 of grain sizes	710
Specific Surface Area	320
Charging simulation	400

Resulting RVE for charging simulation

Property	Structure Size for RVE in x and y [voxel]	Runtime for RVE
Tortuosity	450	<0.5h
D50 of grain sizes	710	<1.5min
Specific Surface Area	320	<3.5s
Charging simulation	400	~43h

Conclusions

- RVEs for different properties are not necessarily equal
- For our sample, the RVE for tortuosity and the RVE for charging simulation are of similar size
- Using the RVE for tortuosity to choose the RVE for charging simulations may shorten simulation runtime
- Next step: get more significant statistics

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Digital Engineering

Thank You!



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