OPTIMUM REGION-SIZE FOR BATTERY CHARGING SIMULATIONS ON THE MICROSCALE

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(Math2Market)
Li-Ion Batteries: A Complex, Multi-Scale Problem
What is GeoDict?

**GeoDict® 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
Introduction
Schematic of a Li-Ion battery

Anode

Cathode

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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
LiFePO$_4$ - cathode

Scan and segmentation by KIT (Karlsruhe Institute of Technology)
Transportation is crucial
Transportation is crucial
The microstructure defines macroscopic properties

- Porosity
- Conductivity
- Tortuosity
- Particle size distribution
- Pore size distribution
- Diffusivity
## Runtime for the microstructure analysis

<table>
<thead>
<tr>
<th>Structure Size in x and y</th>
<th>Runtime for Tortuosity</th>
<th>Runtime for Grain Size Distribution</th>
<th>Runtime for Specific Surface Area</th>
</tr>
</thead>
<tbody>
<tr>
<td>275</td>
<td>~5 min</td>
<td>5 s</td>
<td>0.8 s</td>
</tr>
<tr>
<td>550</td>
<td>~0.5 h</td>
<td>21 s</td>
<td>3.3 s</td>
</tr>
<tr>
<td>875</td>
<td>~1 h</td>
<td>49 s</td>
<td>7.5 s</td>
</tr>
<tr>
<td>1100</td>
<td>~2 h</td>
<td>~1.25 min</td>
<td>13.4 s</td>
</tr>
</tbody>
</table>

8 parallel processes used
## Runtime for charging simulations

<table>
<thead>
<tr>
<th>Structure Size in x und y</th>
<th>Runtime for charging simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 voxel</td>
<td>3.7 h</td>
</tr>
<tr>
<td>100 voxel</td>
<td>14.5 h</td>
</tr>
<tr>
<td>200 voxel</td>
<td>22.2 h</td>
</tr>
<tr>
<td>400 voxel</td>
<td>43.9 h</td>
</tr>
</tbody>
</table>

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?

For a regular array, the unit cell is sufficient to get all geometrical information about the entire 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?

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

\[ \tau = \frac{L}{C} \]

Low tortuosity, \( \tau \sim 1 \)

High tortuosity, \( \tau >> 1 \)

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

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

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

The **specific surface area** is the total surface area of a material per bulk volume (units of m²/m³ or m⁻¹).
Variation of the properties for different regions

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

![Diagram showing variation of tortuosity with structure size and RVE of 450 voxel]
Variation of the properties for different regions

- Tortuosity
- D50 of grain sizes
- Specific Surface Area

$$\text{RVE} \approx 710 \text{ voxel}$$
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

![Image of grain structure]

\[ RVE \approx 320 \text{ voxel} \]
## Resulting RVE for micro-scale properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Structure size for RVE in x and y [voxel]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tortuosity</td>
<td>450</td>
</tr>
<tr>
<td>D50 of grain sizes</td>
<td>710</td>
</tr>
<tr>
<td>Specific Surface Area</td>
<td>320</td>
</tr>
</tbody>
</table>
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

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<tr>
<td>Charging simulation</td>
<td>400</td>
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### Resulting RVE for charging simulation

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<th>Runtime for RVE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tortuosity</td>
<td>450</td>
<td>&lt;0.5h</td>
</tr>
<tr>
<td>D50 of grain sizes</td>
<td>710</td>
<td>&lt;1.5min</td>
</tr>
<tr>
<td>Specific Surface Area</td>
<td>320</td>
<td>&lt;3.5s</td>
</tr>
<tr>
<td>Charging simulation</td>
<td>400</td>
<td>~43h</td>
</tr>
</tbody>
</table>
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
Thank You!

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