DIGITAL 3D RECONSTRUCTION FROM 2D SCAN OF A LI-ION CATHODE

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1. What is GeoDict and Data for this talk

2. Motivation

3. Step 1: NMC cathode recreation using GeoDict only

4. Step 2: NMC cathode recreation using GeoDict and optiSLang
What is GeoDict and Data for this talk

Motivation

Step 1: NMC cathode recreation using GeoDict only

Step 2: NMC cathode recreation using GeoDict and optiSLang
CORE CAPABILITIES OF GEODict®

MODEL & DESIGN MATERIALS

ANALYZE & SIMULATE MATERIAL PROPERTIES

EXPLORE THE BEHAVIOR OF MATERIALS

DEVELOP NOVEL MATERIALS

OPTIMIZE PROCESSES
<table>
<thead>
<tr>
<th><strong>GeoDict® Solutions for...</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Filtration</strong></td>
</tr>
<tr>
<td>For a clean environment</td>
</tr>
<tr>
<td><strong>Electrochemistry</strong></td>
</tr>
<tr>
<td>For electromobility</td>
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<tr>
<td><strong>Structural Materials</strong></td>
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<tr>
<td>For lightweight applications</td>
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<tr>
<td><strong>Digital Rock Physics</strong></td>
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<tr>
<td>For efficient energy production</td>
</tr>
</tbody>
</table>
**Typical Workflow with GeoDict®**

1. **Import**
   - Import of 3d images captured by μCT or FIB/SEM techniques
   - Digital Material

2. **Analyze**
   - In-depth digital analysis and evaluation of material properties
   - Quantification of geometrical, structural, and physical material properties
   - Digital Twin

3. **Model**
   - Digital material design based on the statistical material properties
   - Digital Prototypes

4. **Design**
   - Design by varying the statistics of the geometry that govern the material properties
   - Digital Prototypes
The structural statistical information output of GrainFind is the input for GrainGeo and FiberGeo, the GeoDict® modules for the generation digital twins of the material.

- **GrainGeo**
  - Creates models of granular materials
  - Here, it is used to model the structure of the active material

- **FiberGeo**
  - Creates models of fibrous materials
  - Here, it is used to model the fibrous binder

➤ **Result: Digital Twin**
Digital prototypes
Digital prototypes are quickly designed by varying the statistics of the geometry that govern the material properties.

Many digital prototypes of the cathode are swiftly and directly analyzed on the computer.

Result: Selection of digital prototypes with different volume fractions
GeoDict modules and simulations used

- **ImportGeo** to process the image data
- **GrainGeo** to generate artificial cathode structures
- **GrainFind** to analyze granular structures for its geometrical properties
- **DiffuDict** to predict diffusivity and tortuosity
For this talk we use a data set kindly provided by:

KIT (Karlsruhe Institute of Technology)

Nickel Cobalt Manganese (NMC) cathode

These data and further information such as tortuosity values can be found in *Tortuosity Anisotropy in Lithium-Ion Battery Electrodes*[^1],

[^1]: Tortuosity Anisotropy in Lithium-Ion Battery Electrodes: Martin Ebner, Ding-Wen Chung, R. Edwin García and Vanessa Wood
GEOMETRIC ANALYSIS TOOL GRAINFIND

- Some of the results per grain:
  - Volumes and diameters of volume-equivalent sphere
  - Diameters of inscribed spheres
  - Sheppard sphericities and Krumbein sphericities
  - Fit shape’s diameters, direction, and orientation

- Statistics about grains
  - Volume statistics
  - Diameter statistics
  - Sphericity statistics
  - Fit-shape direction statistics

- Classification of grain shapes
**Cathode Creation Tool GrainGeo**

- **GrainGeo** generates granular structures.
- Different kinds of grains can be generated:
  - Spheres and ellipsoids (described by their diameters)
  - Convex polyhedrons (described by diameters of enclosing ellipsoid)
  - Many others
- Objects can be randomly created.
- Overlapping objects can be created.
- Or overlap can be removed.
DiffuDict simulates diffusion experiments of Bulk and Knudsen diffusion:

- Effective diffusivity
- Tortuosity:
  - For a curve (blue) in space, the tortuosity of this curve is the quotient between the length of the curve $L$ and the length of the straight line $l$ between the curve’s endpoints (red), $\tau = \frac{L}{l}$
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**Motivation for Digital Experiments**

- To reduce time and costs in cathode development processes:
  - Experiments can be performed digitally
  - Testing digital prototypes allows to only produce the most promising
- Use digital twin of cathode to understand real cathode better
  - Use this twin to see how changes to this cathode alter the performance
  - Develop the next generation cathode based on real cathode

→ But therefore we need the digital twin
- Obtain it by importing 3d FIB-SEM image stack
- Or use single 2d SEM image
For digital experiments reliable digital representatives of the cathode material is needed:

- Import sample from FIB-SEMs
  + This yields exact digital representative
  - More expensive
  - Sample is destroyed in the process

- Import sample from single SEM image
  + Sample is not destroyed
  + Cheaper than 3d scans
  - No 3d representation

→ Develop methodology to create 3d digital twin from a single SEM image with optiSLang and GeoDict.
Main Problem is that **Information is missing!**

Where to get information for reliable 3d reconstruction?

- Knowledge from similar cathodes
- Knowledge from manufacturers
- Experimental Input:
  - Porosimetry by mercury intrusion
  - Porosity
  - Tortuosity
  - Permeabilities

→ Obtain geometric information of 2d scan by GeoDict and combine with external inputs
3D RECONSTRUCTION FROM 2D SCAN

METHODODOLOGY VALIDATION

1. Use 3d scan of NMC cathode
2. Take 2d slice as “SEM scan”
3. Reconstruct 3d digital cathode
4. Validate results with 3d scan from 1.
AGENDA

1. What is GeoDict and Data for this talk

2. Motivation and methodology

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**STEP 1: NMC RECREATION TOOLS AND PREREQUISITES**

For the NMC cathode in *Tortuosity Anisotropy in Lithium-Ion Battery Electrodes*[^1], *tortuosity* values are given.

**Workflow:**

1. Use GrainFind on 2d scan
2. Recreate 3d cathode with 2d GrainFind information
   - Use GrainGeo for creation of artificial cathodes
3. Compare cathodes for their *tortuosities* from [^1] and *porosity*

[^1]: *Tortuosity Anisotropy in Lithium-Ion Battery Electrodes*: Martin Ebner, Ding-Wen Chung, R. Edwin García and Vanessa Wood
**STEP 1: NMC RECREATION WITH GRAINFIND**

Take 2d slice of NMC scan

Use GrainFind to identify grains and obtain statistics

And create artificial cathode
**Step 1: NMC Validation of 3D Representation**

3d scan

Digital cathode

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<table>
<thead>
<tr>
<th></th>
<th>Tortuosity x</th>
<th>Tortuosity y</th>
<th>Tortuosity z</th>
<th>Porosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.212</td>
<td>1.38</td>
<td>1.21</td>
<td>1.22</td>
<td>49.97 %</td>
</tr>
<tr>
<td>1.22</td>
<td></td>
<td></td>
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**Step 1: NMC Validation of 3D Representation**

- Take 2d slice of 3d scan
- Take 2d slice of digital cathode

**Compute:**
Geometry statistics

<table>
<thead>
<tr>
<th>Diameter Type</th>
<th>Mean (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shortest Diameter</td>
<td>4.98</td>
</tr>
<tr>
<td>Intermediate Diameter</td>
<td>6.52</td>
</tr>
<tr>
<td>Longest Diameter</td>
<td>12.94</td>
</tr>
<tr>
<td>Mean of shortest Diameter</td>
<td>7.42</td>
</tr>
<tr>
<td>Mean of intermediate Diameter</td>
<td>10.64</td>
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<tr>
<td>Mean of longest Diameter</td>
<td>15.47</td>
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**Step 1: NMC Recreation with GrainFind Validation Results**

Comparison of computed calibration parameters

<table>
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<th>Relative Error /(%)</th>
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<td>63</td>
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<td>Mean of longest Diameter</td>
<td>12.94 µm</td>
<td>15.47 µm</td>
<td>20</td>
</tr>
<tr>
<td>Tortuosity x</td>
<td>1.212</td>
<td>1.38</td>
<td>12</td>
</tr>
<tr>
<td>Tortuosity y</td>
<td>1.22</td>
<td>1.21</td>
<td>0.2</td>
</tr>
<tr>
<td>Tortuosity z</td>
<td>1.24</td>
<td>1.22</td>
<td>2</td>
</tr>
<tr>
<td>Porosity</td>
<td>49.97 %</td>
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→ Physical properties almost good, geometric properties not sufficiently accurate
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GeoDict Workflow is basis for Sensitivity analysis:

Input parameters for Sensitivity analysis:
- Porosity
- Grain diameters in x, y and z direction (Assume 3 different kind of grains)
- Grain orientations

As responses use geometric and physical properties.
- **Tortuosity** and **porosity** (physical properties)
- **GrainFind** results (geometric properties)

Later apply optimization routine on the obtained MOP
optiSLang workflow is simple and does not need large complexity:
150 designs calculated + 1 validator system
**STEP 2: NMC ANALYSIS BY OPTISSLANG: SENSITIVITY**

Orientation in y direction is dependend on:
- Input orientation in y direction
- Input orientation in z direction
→ Expected and necessary criterion!

Tortuosity in x direction:
- Orientation in x direction
- Acceptable coefficient of prognosis
→ For later studies more designs should be calculated
Knowledge from Step 1:

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Improve the Diameter results → set those as constrains: rel. error ≤ 20%

Improve the physical results:
- Already pretty good so set constrained with rel. error ≤ 10%
- Tortuosity in x direction as optimization variable
STEP 2: NMC ANALYSIS BY OPTISSLANG:
RESULTING CATHODE

sample of NMC cathode

artificial reconstruction of NMC cathode
**Step 2: NMC Validation of 3D Representation**

3D scan

Digital Cathode

Compute: Porosity and tortuosity

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<td></td>
<td>1.28</td>
<td></td>
<td></td>
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<tr>
<td>Tortuosity z</td>
<td></td>
<td></td>
<td>1.30</td>
<td></td>
</tr>
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<td></td>
<td></td>
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**STEP 2: NMC VALIDATION OF 3D REPRESENTATION**

Take 2d slice of 3d scan

![Image of 2D slice of 3D scan]

Take 2d slice of digital cathode

![Image of 2D slice of digital cathode]

Compute: geometry statistics

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As criteria we use results from Step 1:

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All constraints and optimization variables are within bounds!

Some are at their limit, but did not exceed it

→ This artificial cathode is a digital twin for tortuosity and diffusivity
Recreating an artificial cathode with standalone GrainFind and GrainGeo tools already yields good results.

But in combination with optiSLang results are improved:
- More designs for Sensitivity should be considered.

This methodology is applicable to homogenous cathodes very good.

But:
- For inhomogeneous cathode this methodology can work but:
  - Needs more inputs.
  - Needs to be extended and validated.
THANK YOU FOR YOUR ATTENTION!