Study of the impact of microstructure on electrical properties in lithium-ion batteries; simulations on actual microstructures and generation of numerical architectures

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Li-ion batteries are interesting for multiple applications because of their power and energy densities. However there is still a gap to be bridged between theoretical models like Newman’s and experiments. One of the reasons for that is the difficulties to understand the links between microstructure and effective properties within the positive electrodes also named cathodes.

Cathode composition:
- clusters of active material (AM), energy storage;
- blend of polymer with conductive additive (mechanical coherence and main electronic conduction);
- porosity/electrolyte (ionic conduction)

⇒ complex multiphase composite that have a huge impact on effective properties like conduction.

The aim of this work is to investigate this microstructure in 3D and use this data to conduct simulations for effective properties.

### Volume acquisition

**X-ray tomography**
- Non destructive technique
- Lab tomography at 0.3µm resolution
- Synchrotron tomography at 0.05µm resolution
- Polymetric phase non visible

**FIB/SEM tomography**
- Destructive technique
- 10nm resolution
- 10x10x10µm maximum
- Special preparation
- All phases visible
- Zeiss Nvision 40 and Fibirics software

Very good description of the microstructure except for ROI size (representativity), setup complexity and time consuming.

### Numerical simulations

**Finite elements simulations**
- Meshing: Avizo and GMSH
- Simulation: Abaqus
- Complex microstructure: meshing difficult
- Small volumes only

**FFT simulations**
- Morphomm software from F. Willot
- Useful for test campaigns and property determinations
- RVE notion is important => Representativity
- Bulk phase properties can be estimated
- Can be a basis for comparison with experimental and simulation data

**Discrete elements simulations**
- LIGGHTS software
- Collaboration with SIMAP laboratory and C.L. Martin
- Very versatile ans promising tool
- Heat transfer feasible then electric conduction too
- 2 ways for simulations:
  - Classic: 1 numerical particle = 1 physical particle
  - => works, have been done
  - 1 physical particles = multiple numerical particles with global simulation laws => possibilities for complex behaviour
- Work in progress
  - Models to be developed

### Conclusion:
- 2 imaging technologies and 3 simulation ways investigated
  - RX tomography shows some limitations (resolution and phase description) which reduce its interest for simulation while FIB/SEM tomography allows a precise description of the microstructure. However it is time consuming and more difficult to setup and post-process.
  - FFT simulation seems particularly unadapted due to the difficulties to perform the meshing. On the contrary FFT simulation is an easier way to perform calculation as long as a segmented volume is available. The DEM simulation gathers good possibilities and should be a good way to conduct complex behaviour simulations.
- Prospects:
  - There is mostly two major leads for the short time works:
    - Develop the DEM models and simulations
    - Improve the segmentation method

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