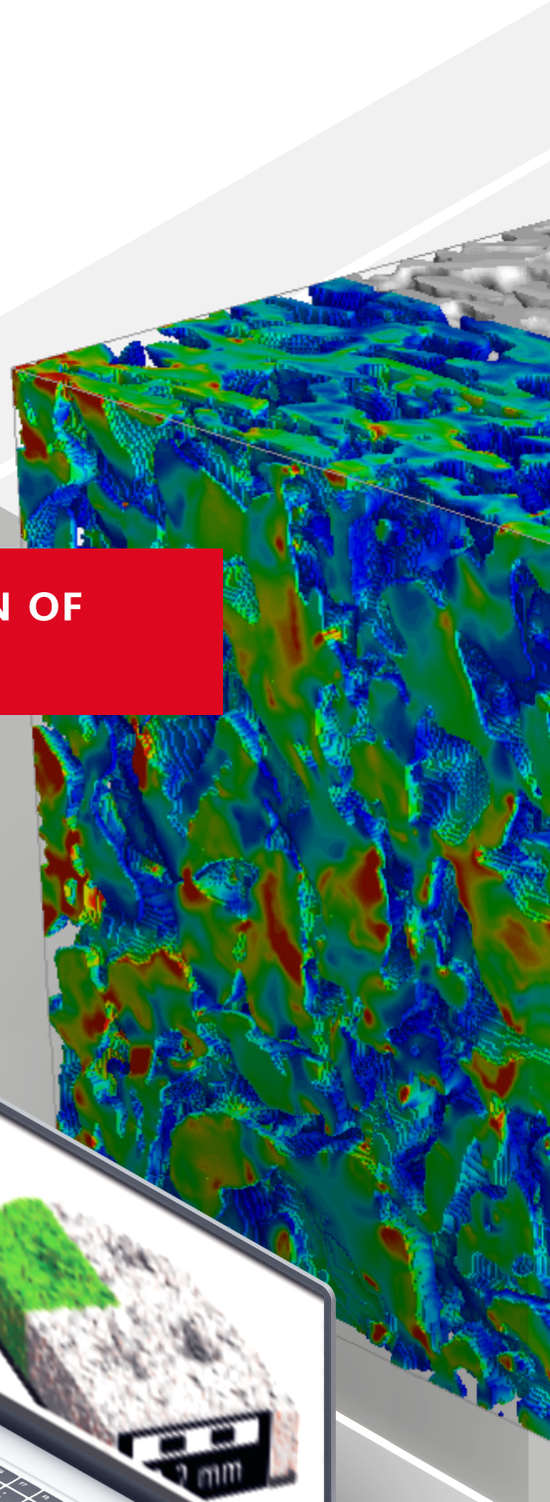
GeoDict

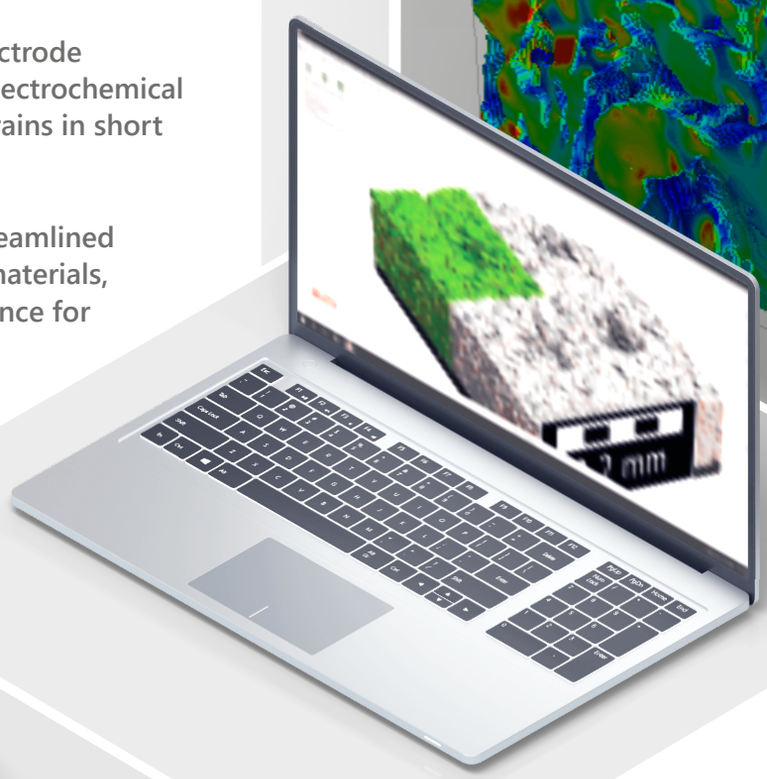
The Digital Material Laboratory



GeoDict Workflow for Battery R&D

Experimentally Validated Simulation of Strain-Induced Battery Aging

- Obtaining structural data on the microscale during cycling is complex and expensive.
- GeoDict's BatteryDict-Degradation add-on couples electrochemical and mechanical simulations using realistic material parameters.
- It provides insightful data for electrode development and will simulate electrochemical cycling with local stresses and strains in short time.
- Reliable simulations allow for streamlined material engineering of energy materials, improving lifetime and performance for e-mobility and energy storage.



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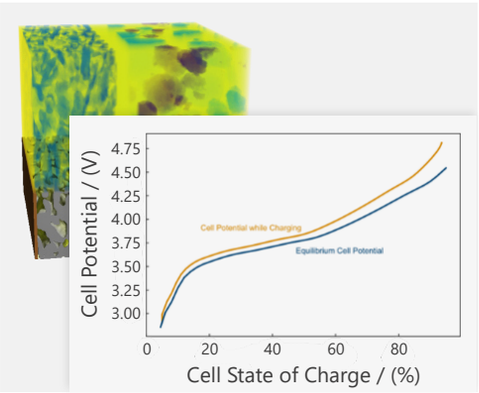
GeoDict Workflow for Digital Battery Development

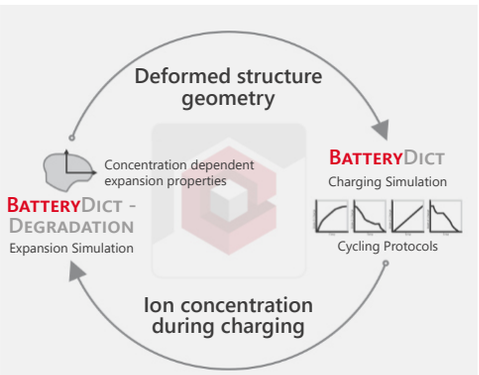
1 Electrochemical Simulation



- A battery charging simulation is performed to understand the local movement of electrons and ions within the active materials, the electrolyte, and binder.
- Lithium intercalation causes mechanical expansion and structural aging in batteries.
- Local lithium concentration determines the extent of expansion and damaging effects.
- Battery degradation simulation calculates local lithium concentration to understand mechanical stresses and aging effects.

Result: Local lithium concentration

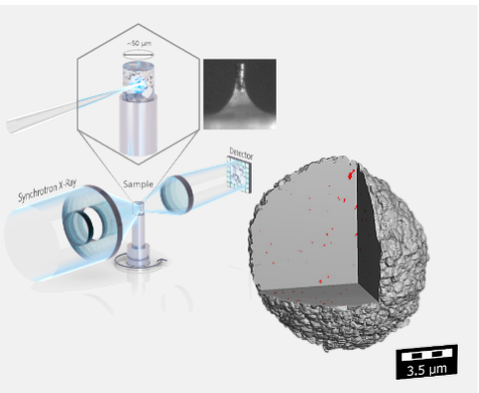
2 Mechanical Simulation



- Battery degradation occurs due to microstructural changes during cycling, where local stress and strain of the electrode material is simulated in relation to the Li-intercalation reaction.
- Simulate local volumetric changes using GeoDict software based on lithium concentration.
- Implement coupling of electrochemical and mechanical simulation in the software.

Result: Stress, strain, and displacement indicating cell damage during cycling.

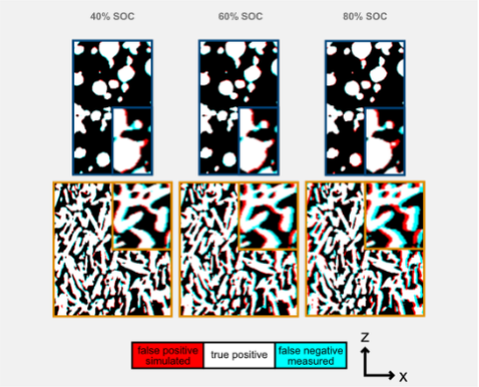
3 Measurements



- SOLVED! project tracked battery microstructure during cycling via in-operando XTM using the TOMCAT beamline[1].
- Anode and cathode expansion coefficients were extracted and imported into the simulation tool.
- Simulation validated by comparison with in-operando XTM of Li(NiMnCo)O_2 cathode and graphite anode.
- Electrochemical characterization used to parametrize simulation.

Result: Dataset for validation

4 Validation



- Validation of full-cell simulation for a battery consisting of graphite anode and NMC811 cathode.
- Simulation of cut-out of graphite anode was validated with in-operando measurement, showing total expansions of 10% and 9.8%.
- Quantitative agreement between simulation and experiment was calculated from voxel congruence.
- 2D cross sections of simulated and imaged electrodes at different SOC were overlaid to visualize congruence, with black voxels for pores and white voxels for agreement between measurement and simulation[2].

Result: Validated digital approach for battery R&D

[1] Pietsch and Wood (2017), DOI 10.1146/annurev-matsci-070616-123957

[2] Wenzler et al. (2023), DOI 10.1149/1945-7111/acb5c9

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