

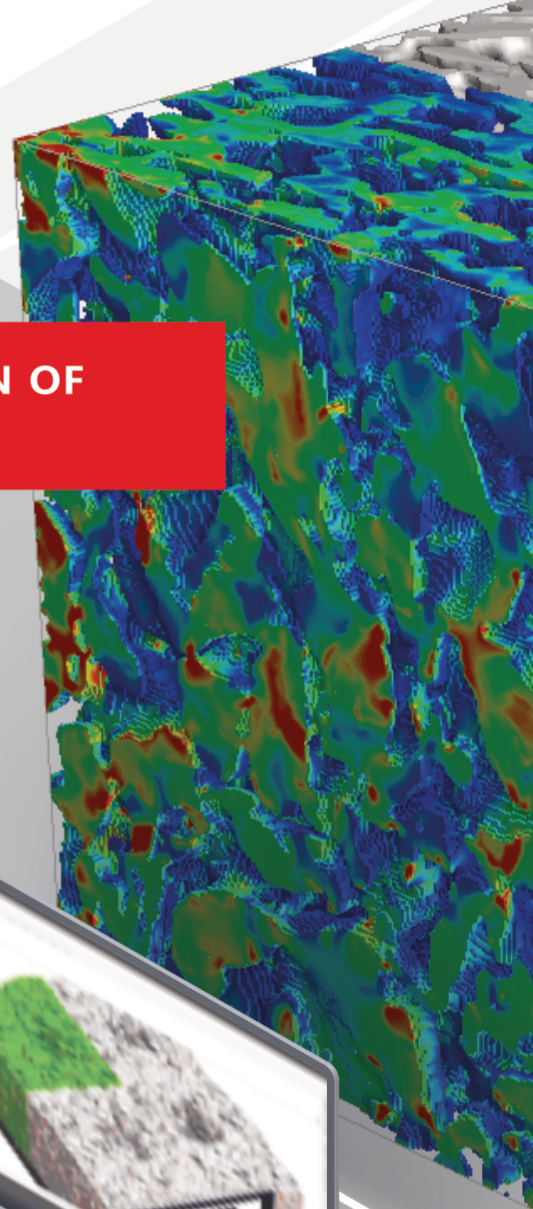
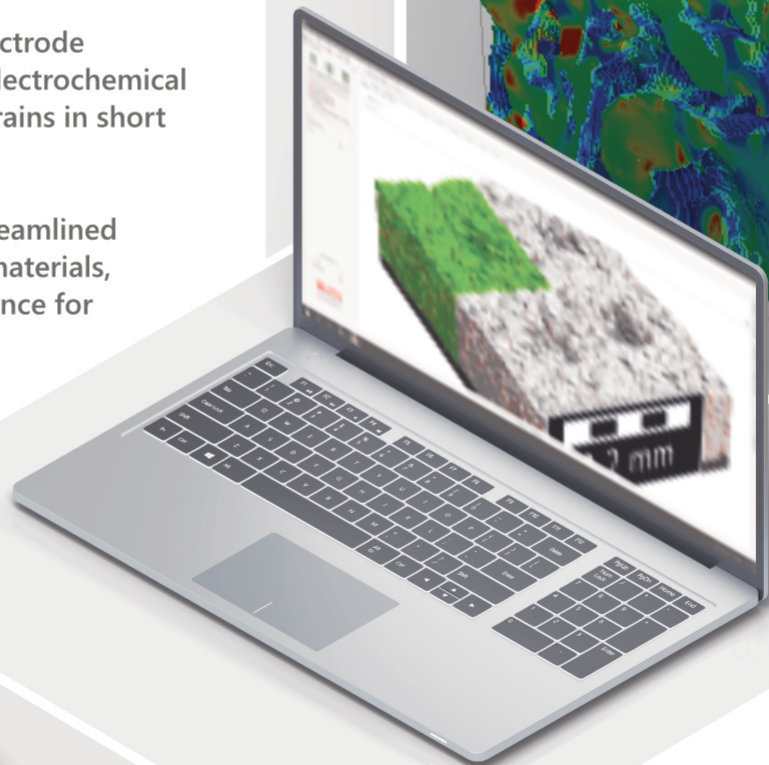
GEODict

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.

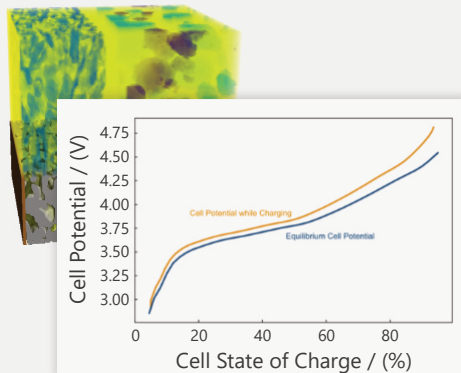


MATH
2 MARKET

GeoDict Workflow for Digital Battery Development

1

Electrochemical Simulation

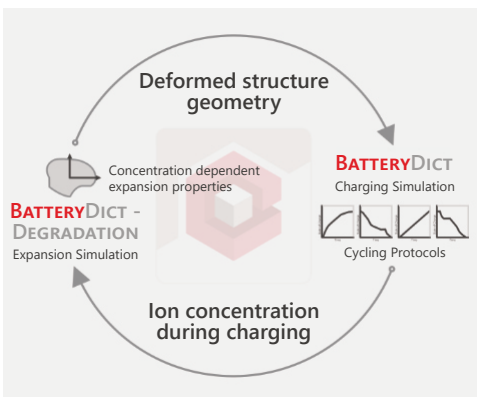


- A battery charging simulation is performed to understand the local movement of electrons and ions within the active materials, the electrolyte, and binder.
- Lithium intercalation causes mechanical expansion and structural aging in batteries.
- Local lithium concentration determines the extent of expansion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

Result: Local lithium concentration

2

Mechanical Simulation

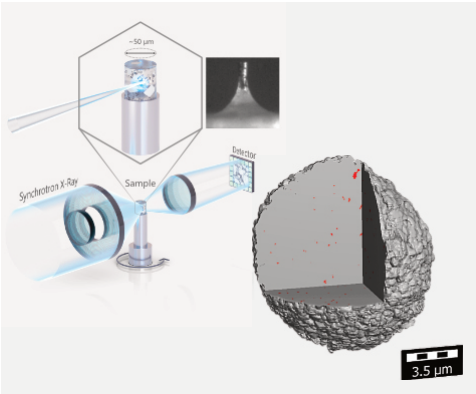


- Battery degradation occurs due to microstructural changes during cycling, where local stress and strain of the electrode material is simulated in relation to the Li-intercalation reaction.
- Simulate local volumetric changes using GeoDict software based on lithium concentration.
- Implement coupling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

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

3

Measurements

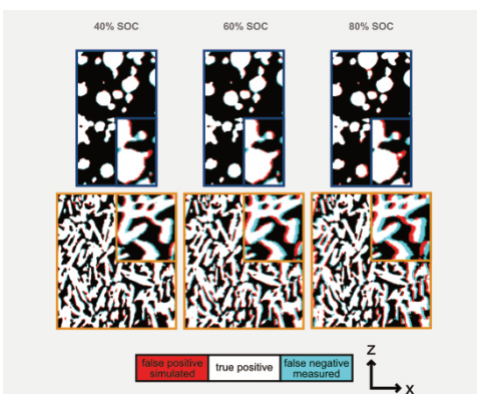


- SOLVED! project tracked battery microstructure during cycling via in-operando XTM using the TOMCAT beamline^[1].
- Anode and cathode expansion coefficients were extracted and imported into the simulation tool.
- Simulation validated by comparison with in-operando XTM of Li(NiMnCo)O₂ cathode and graphite anode.
- Electrochemical characterization used to parametrize simulation.

Result: Dataset for validation

4

Validation



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

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

Result: Validated digital approach for battery R&D