Computational Mechanics Group
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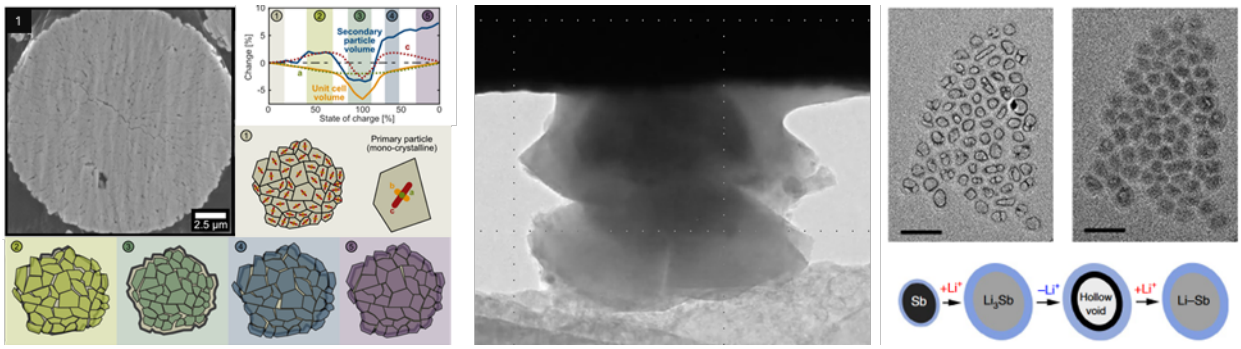
Master's thesis / Semester project

Numerical Modeling of Lithium-Ion Particle Degradation using the Finite Element Method

To meet the rising demand of durable batteries, continuous attempts are made to use higher capacity materials such as Nickel Manganese Cobalt cathodes (*NMC*) or Silicon (*Si*) / Antimony (*Sb*) anodes since their theoretical capacity is ten times higher than the conventional electrodes. Yet, during early charging cycles, these materials undergo high mechanical degradation due to their large volumetric expansion. This results in fracture and delamination of the electrode and rapid capacity fading.

To investigate this problematic, we develop a comprehensive Finite Element Model to analyze diffusion, phase separation, and mechanical deformations during lithium (de)intercalation in high-capacity material particles. The numerical model will help pinpoint reasons for rapid degradation and explore material property modifications to prevent premature mechanical failure. Different topics can be defined upon meeting, depending on the student's interest as well as the current research state. Topic examples would be:

- Modelling the anistropic diffusion in *NMC*-secondary particle coupled with elastoplastic deformation during the first delithiation-lithiation cycle [1].
- Introducing a damage (void) growth model or phase-field for fracture model for a *NMC*-secondary particle to capture the particle irreversible volumetric change [1].
- Coupling phase-separation and fracture at a single *Si*-primary particle [2].
- Study of an oxide shell in limiting particle degradations (buckling) [3].
- ...



[1] Defragmentation of *NMC* secondary particle during a discharging cycle. **[2]** Cracking of a *Si* primary particle during lithiation. **[3]** Hollowing and filling of a *Sb* primary particle with an oxide layer during charging-discharging cycles.

References

[1] N. Wenzler, "Characterization and Simulation of Mechanical Transformations in Lithium Ion Battery Anodes and Cathodes," Doctoral Thesis, ETH Zurich, 2022. doi: 10.3929/ethz-b-000592217.
[2] X. H. Liu, L. Zhong, S. Huang, S. X. Mao, T. Zhu, and J. Y. Huang, "Size-Dependent Fracture of Silicon Nanoparticles During Lithiation," ACS Nano, vol. 6, no. 2, pp. 1522–1531, Feb. 2012, doi: 10.1021/nn204476h.
[3] M. G. Boebinger et al., "Spontaneous and reversible hollowing of alloy anode nanocrystals for stable battery cycling," Nat. Nanotechnol., vol. 15, no. 6, pp. 475–481, Jun. 2020, doi: 10.1038/s41565-020-0690-9.

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