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Lithium-ion battery degradation: how to model it

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Available on arXiv: <u>https://arxiv.org/abs/2112.02037</u>

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Background: Why degradation? Why now?





Background: What is battery degradation?



Energy





Our coupled degradation model





Our coupled degradation model





Results: diffusion-limited SEI growth only

PyBaMM's SEI growth model assumes SEI to have two layers, but in this work it is simplified to include only one layer.



Effect of varying solvent diffusivity in SEI far exceeds that of including two SEI layers instead of one

Results: SEI growth and lithium plating



$$\frac{\partial c_{Li}}{\partial t} = -aN_{Li} - \gamma_0 c_{Li} \frac{\delta_{SEI}(0)}{\delta_{SEI}} \qquad N_{Li} \equiv k_{Li} \left[c_{Li} \exp\left(\frac{\alpha_a F}{RT} \eta_{Li}\right) - c_e \exp\left(-\frac{\alpha_c F}{RT} \eta_{Li}\right) \right] \qquad \eta_{Li} \equiv \phi_s - \phi_e - J_{int} \delta_{SEI} \rho_{SEI}$$

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Results: SEI growth on particle cracks





Results: SEI growth on particle cracks



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Results: Loss of active material only





Results: all mechanisms





Results: all mechanisms







Key conclusions



- For diffusion-limited SEI growth, varying the solvent diffusivity has a far greater effect than switching between one and two SEI layers
- A new partially reversible Li plating model is proposed. Both rate constants affect capacity loss in different ways
- SEI on cracks consumes more lithium than SEI on initial surface, in agreement with other models in the literature
- Pore clogging from SEI growth on cracks can cause sudden failure
- Loss of active material parameters require experimental validation
- Extreme temperatures cause more degradation than high currents
- Better physics than existing models, but more parameters to find



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