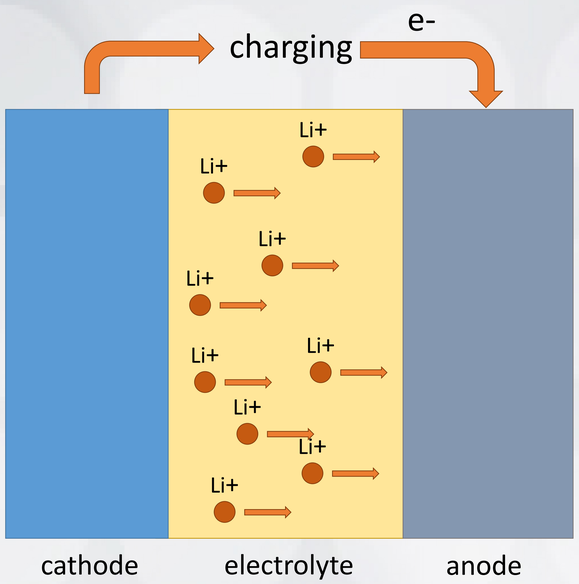
Modelling Electrochemical Devices

Chris Gritton, James Guilkey, Justin Hooper, Dmitry Bedrov, Robert M. Kirby, Martin Berzins

Silicon offers a theoretical <u>10x Improvement</u> in charge capacity over traditional lithium Ion battery materials.

Anode Material	Theoretical Charge Capacity
Graphite	350 $mAhg^{-1}$
Silicon	3500 $mAhg^{-1}$

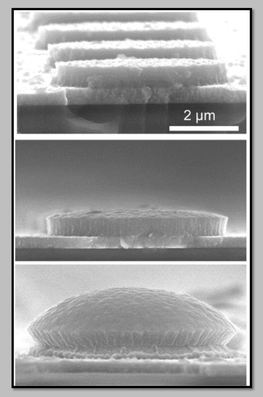
Battery Model



The material point method and the finite volume method are used to model the three different physical processes of <u>electrostatics</u>, <u>chemical diffusion</u>, and <u>mechanical deformation</u>.

Issues Associated With Silicon

280% Expansion at Full Lithiation



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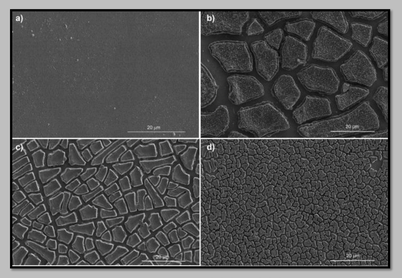
Cracking after Multiple Lithiation/Delithation Cycles



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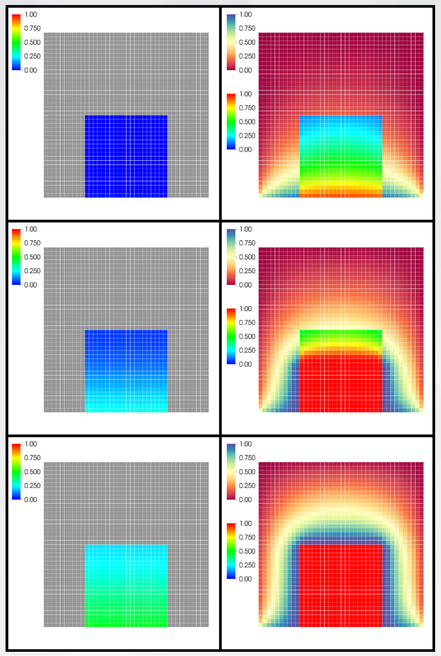
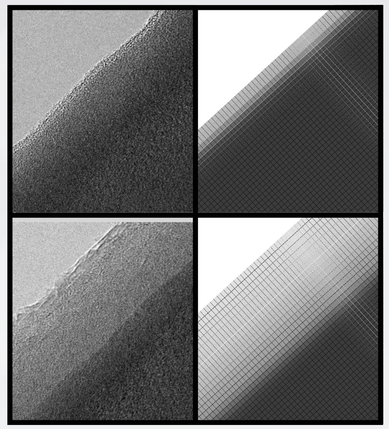
Can we use computer simulations to predict the Behavior of a silicon anode undergoing the lithiation process?

Coupled Multi-physics Computer Simulation Of Silicon Anode

Electrostatics



Chemical Diffusion



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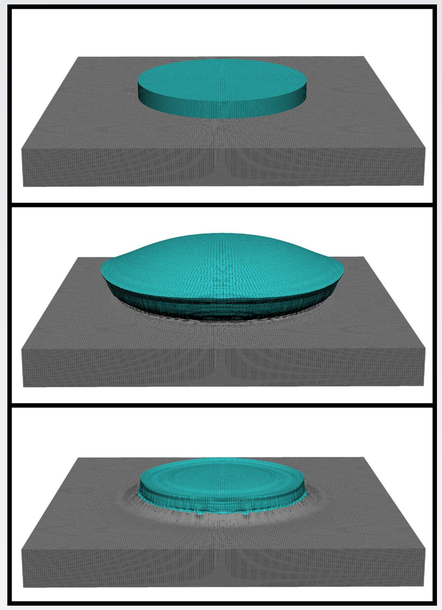
Mechanical Deformation



The implementation of the numerical methods along with the coupling between the physical processes is done using Uintah computational framework.

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- Juchuan Li et al. J. Electrochem. Soc. 2011;158:A689-A694
- Jiang Wei Wang et al. *Nano Lett.* 2013, 13, 709-715.