Introduction to Computational Materials Science and Materials Data Science (590400)

Hui-Chia Yu 游輝嘉
Department of Computational Mathematics, Science and Engineering
Department of Chemical Engineering and Materials Science
Michigan State University

Course description

This course is designed as a gateway course for graduate students. It will showcase modeling and simulation methods for mesoscale and microscale morphology evolution in materials, covering topics such as diffusion, phase transformation, precipitation, solidification, grain growth, eutectic growth, crystal growth, sintering, electrodeposition, spinodal decomposition, and crack propagation. First, students will be exposed to atomic-scale simulation methods, such as density functional theory (DFT), molecular dynamics (MD), and Monte Carlo (MC) methods, and extend to microstructure evolutions. We will then focus on continuum-scale methods, specifically phase-field approaches, to simulate mass transport and phase transformation based on kinetic and thermodynamic descriptions. Finally, we will study emerging data science modeling methods for material phenomena. Students will learn these materials science modeling techniques via hands-on coding exercises.

Teaching method: This course will be taught using both lectures and hands-on coding exercise: approximately 2/3 of class meeting time for lectures and the remaining 1/3 for coding practices. The coding labs will be conducted in a flipped classroom format; i.e., Students are required to complete pre-class assignments to gain basic knowledge for the respective in-class coding assignments.

Tentative topics

- Intro to DFT and MD simulations with simple hands-on coding practices
- Intro to MC simulations with Random walk, Ising model, and Diffusion limited aggregation
- Basics of finite difference method
- Time stepping methods (e.g., Euler and Runge-Kutta)
- Thermodynamics free energy
- Allen-Cahn (Ginzburg-Landau) phase field model for nucleation and growth
- Cahn-Hilliard phase field model for spinodal decomposition
- Solidifications, Eutectic transformation
- Grain growth, Sintering, Solid-solid phase transformation
- Crystal growth
- Crack propagation
- Emerging machine learning methods on materials science applications.

Grading policy

- Homework assignments and coding lab reports -- 45%
- Semester project
  - Report – 25%
  - Oral presentation – 10%
- Quiz/exam – 15%
- Participation – 5%

AI policy: Students are encouraged to use AI, but references are required.

THIS COURSE WILL GIVE YOU...

- Some background mathematics and relevant science
- Some overview of modeling and simulation methods in materials science
- Introduction to methods such as Phase Field Model, Finite Difference Method, Fourier Spectrum Method, Finite Element Method, Molecular Dynamics, Monte Carlo Method
- Practice in using CMS tools and scientific computing through homework, projects, and lab sessions.

What to Expect

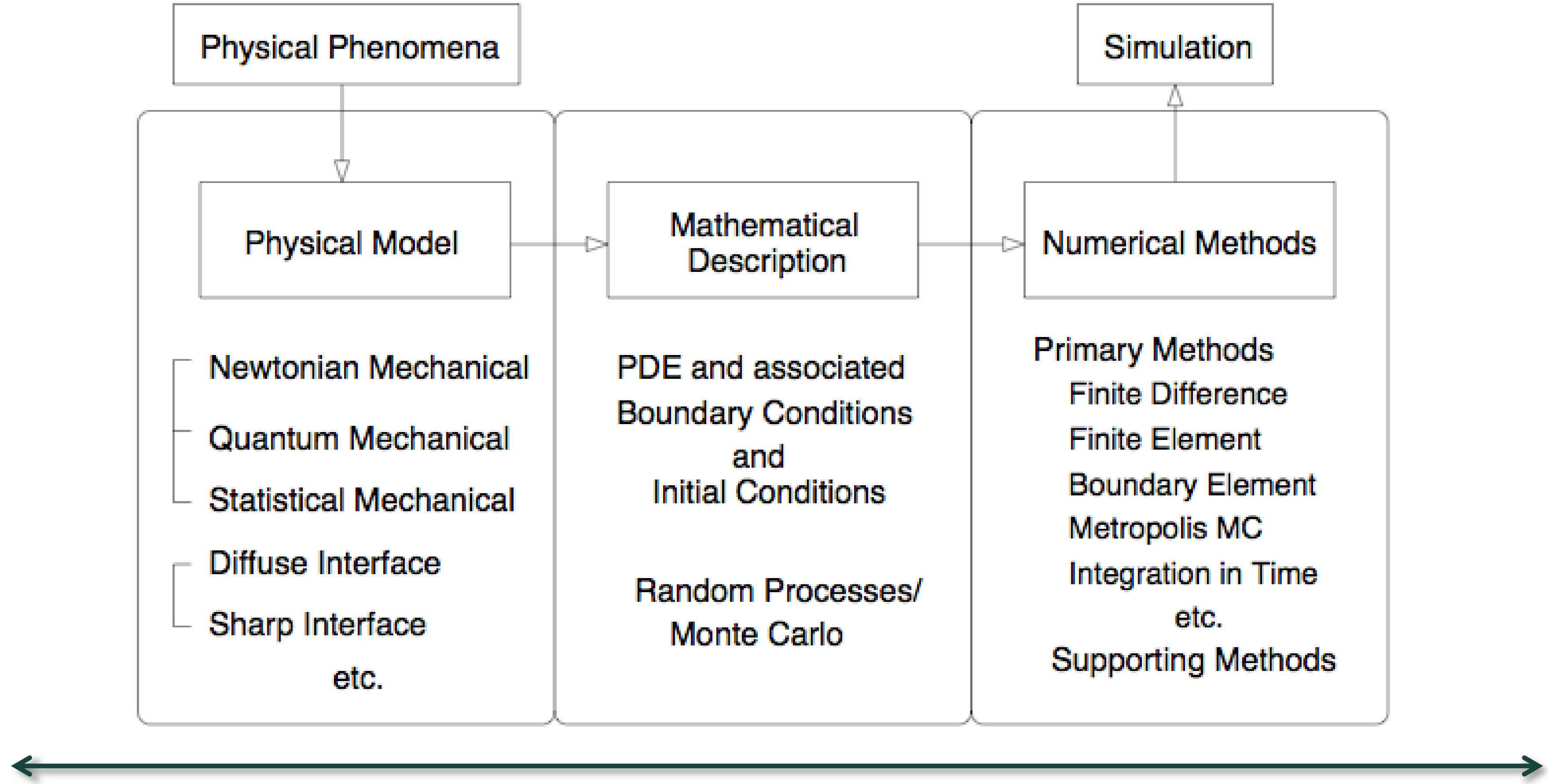
- Feedback is welcome.
- The basic materials may be boring, but you will likely appreciate it later.
- If not familiar with programming and math, it may be tough at the beginning, but the training is very useful (even outside of programming).
- We will cover a lot of different topics/methods (and thus not in depth).

What is Computational MS?

- Materials are governed by their underlying physics
- Their complexity often requires modeling and simulation
  - Modeling: determination of important physics
  - Simulation: prediction based on the model
- Computational MSE: studies of materials by modeling and simulations

What can we do with Computational MS?

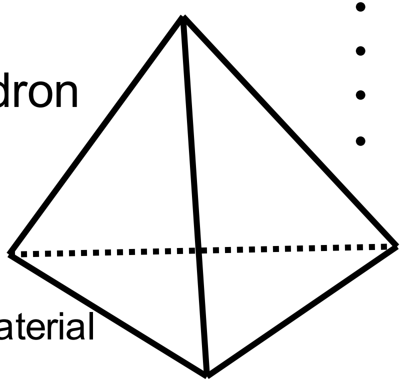
Material design, material fraction & processing, material properties, stress-strain, fatigue and fracture, ….


Physical Phenomena
Simulation
Physical Model
Mathematical Description
Numerical Methods
Newtonian Mechanical
Quantum Mechanical
Statistical Mechanical
Diffuse Interface
Sharp Interface
etc.
PDE and associated
Boundary Conditions
and
Initial Conditions
Random Processes/
Monte Carlo
Primary Methods
Finite Difference
Finite Element
Boundary Element
Metropolis MC
Integration in Time
etc.
Supporting Methods

What can we do with Computational MS?

Material design, material fraction & processing, material properties, stress-strain, fatigue and fracture, ….

Materials science tetrahedron



structure

- arrangement of internal components
- subatomic
- atomic
- microscopic
- macroscopic

processing

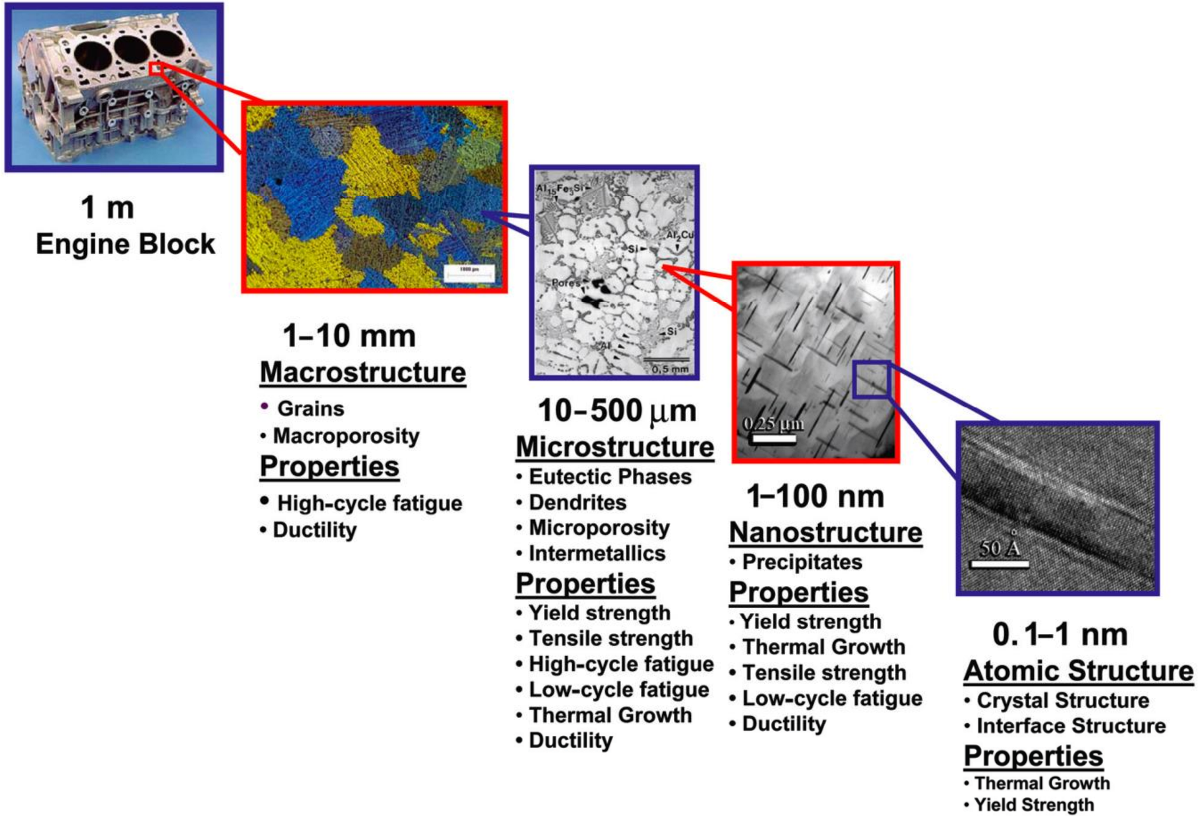
- method of preparing material

properties

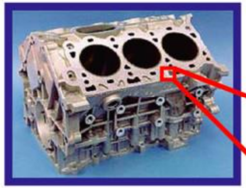
- material characteristic
- response to external stimulus
- mechanical, electrical, thermal, magnetic, optical, deteriorative

performance

- behavior in a particular application

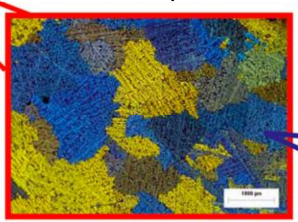

1 m
Engine Block
1–10 mm
Macrostructure
• Grains
• Macroporosity
Properties
• High-cycle fatigue
• Ductility
10–500 μm
Microstructure
• Eutectic Phases
• Dendrites
• Microporosity
• Intermetallics
Properties
• Yield strength
• Tensile strength
• High-cycle fatigue
• Low-cycle fatigue
• Thermal Growth
• Ductility
1–100 nm
Nanostructure
• Precipitates
Properties
• Yield strength
• Thermal Growth
• Tensile strength
• Low-cycle fatigue
• Ductility
0.1–1 nm
Atomic Structure
• Crystal Structure
• Interface Structure
Properties
• Thermal Growth
• Yield Strength
0,5 mm
0.25 μm
50 Å

Continuum-level models

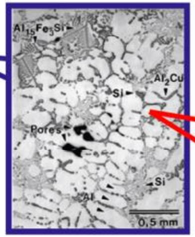


FEM/FDM
simulations:
-mechanics
-flow
-temperature

Continuum-level models
(at microstructural scale)



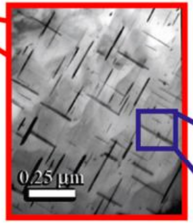
FEM/FDM
simulations:
-grain growth



Phase
equilibrium

FEM/FDM
-solidification
-processing

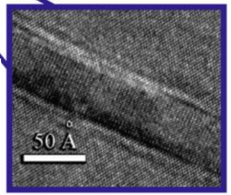
Meso-scale models
(dislocations in plasticity, etc.)



Phase
equilibrium

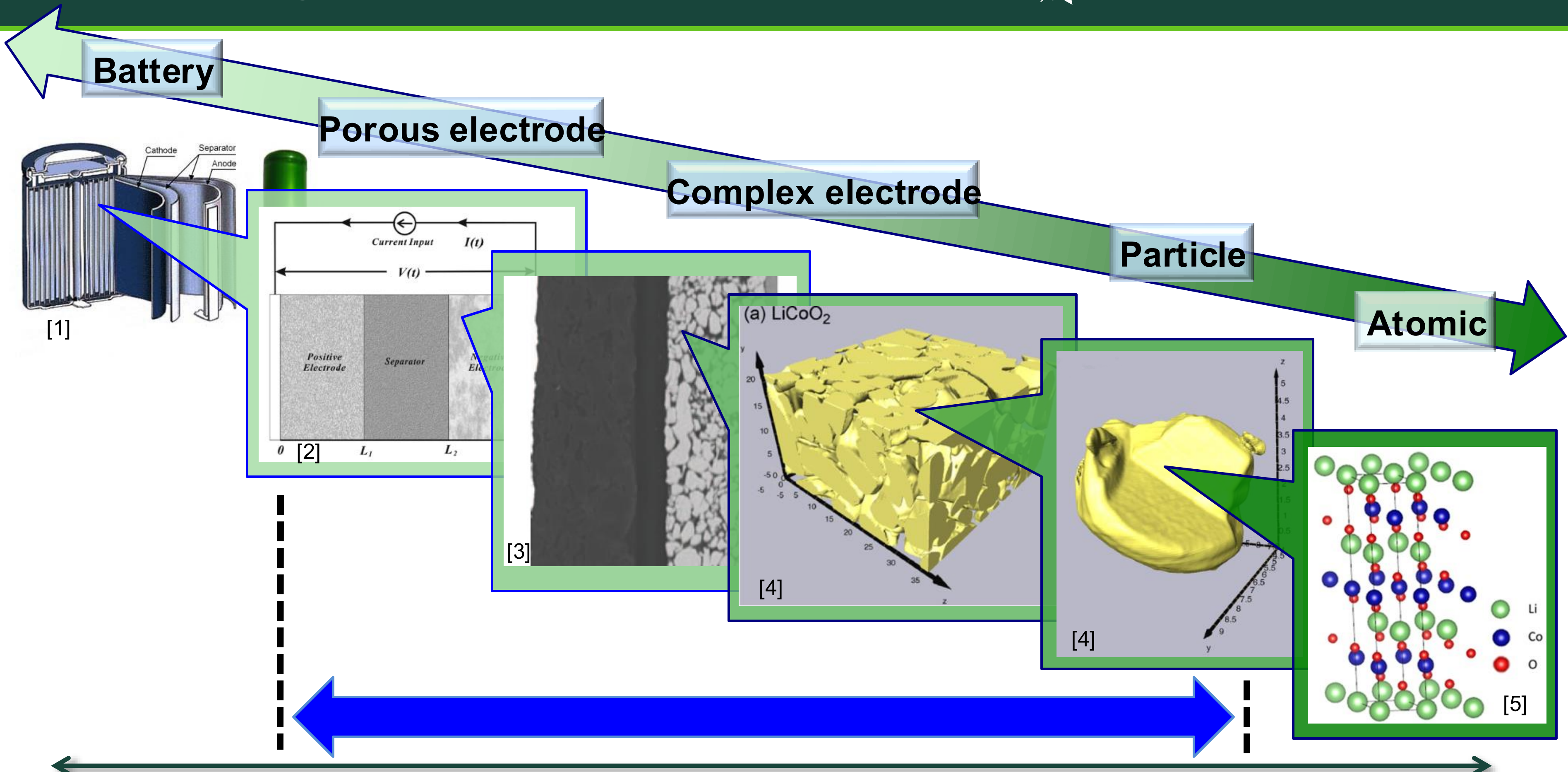
FEM/FDM
-processing

Atomic-scale models
(atomic structure, dynamics)



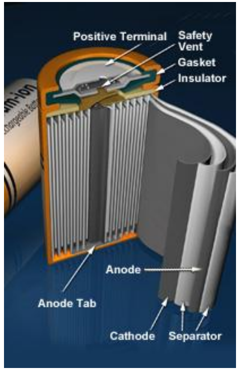
MD
Ab initio

Parallel in many problems

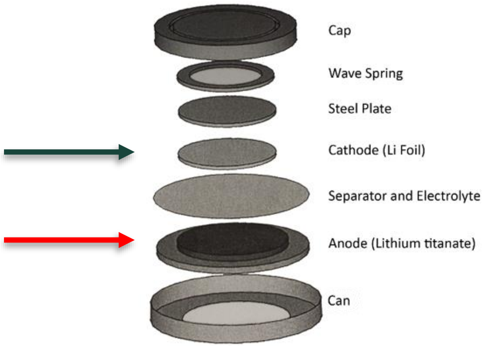


[1] A. Poullikkas, *Renew Sust Energ Rev* 27 (2013) 778; [2] Z. Shen *et al.*, *Dyn Sys Meas Cont* 135 (2013) 041011 ; [3] M. Smith *et al.*, *J Electrochem Soc* 11 (2009) A896; [4] J. Wilson *et al.*, *J Power Source* 196 (2011) 3443; [5] L. Wu & .J Zhang, *J Appl Phys* 118 (2015) 225101

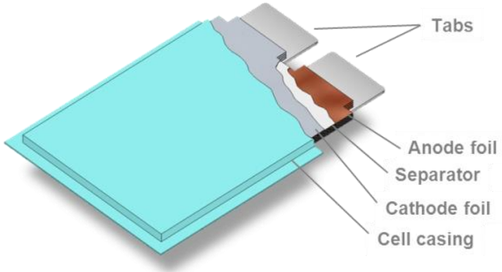
Swiss-roll cells



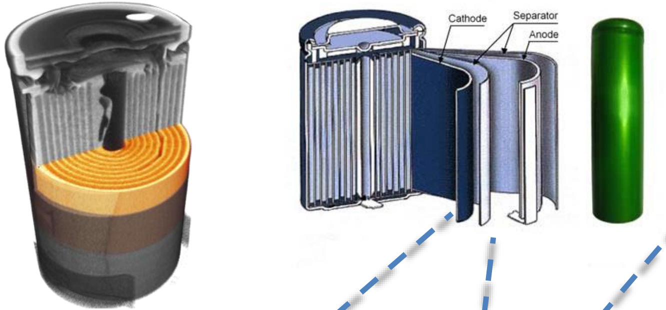
Coin cell

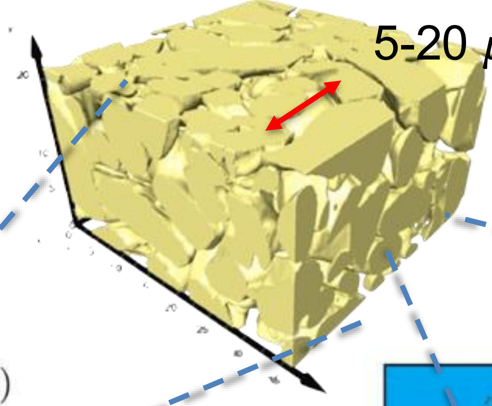


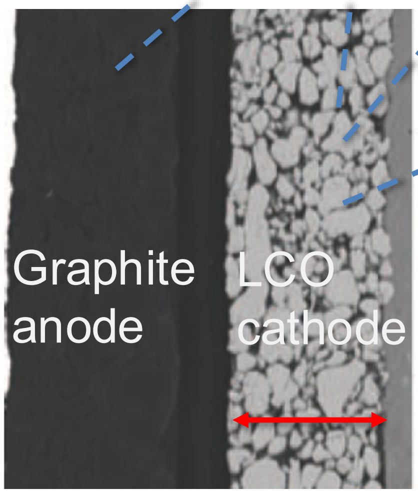
Pouch cell



Electrochemical governing equations



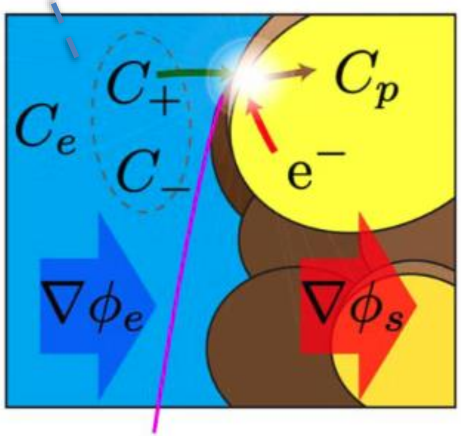




(a)

$$\frac{\partial C_e}{\partial t} = \nabla \cdot (D_e \nabla C_e) - \frac{\mathbf{i}_e \cdot \nabla t_+}{z_+ \nu_+ F}$$

$$\nabla \cdot [(z_+ m_+ - z_- m_-) F C_e \nabla \phi_e + (D_+ - D_-)] = 0$$



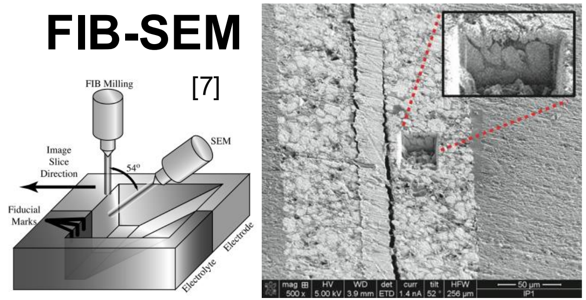
$$\frac{\partial C_p}{\partial t} = \nabla \cdot (D_p \nabla C_p)$$

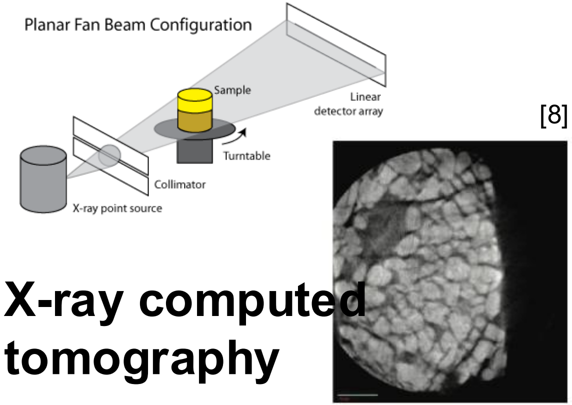
$$\nabla \cdot (\kappa_s \nabla \phi_s) = 0$$

$$r_{xn} = k_f C_+ \exp\left(\frac{-\alpha z_+ F}{RT} [\phi]_e^p\right) - k_b C_p \exp\left(\frac{(1-\alpha) z_+ F}{RT} [\phi]_e^p\right)$$

FIB-SEM

[7]

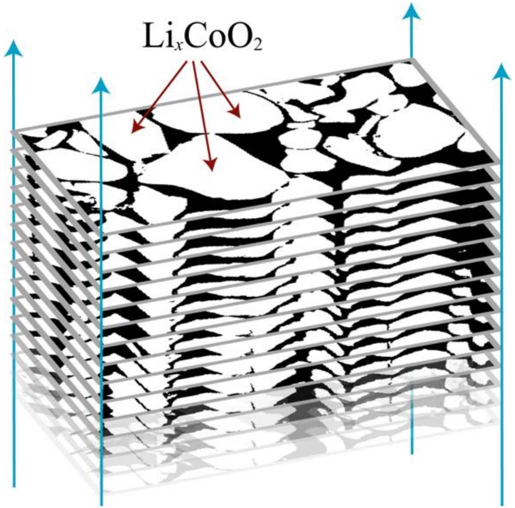




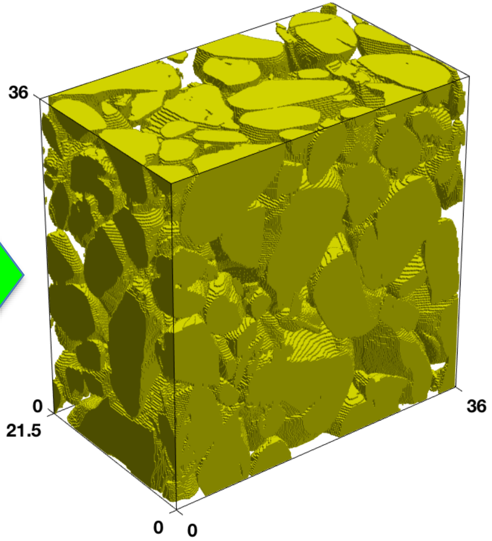
[8]

X-ray computed tomography

Combing series of images



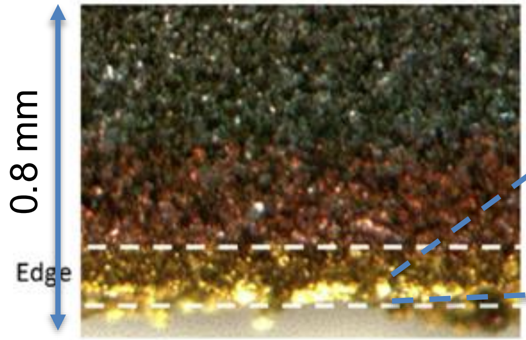
Voxel microstructure

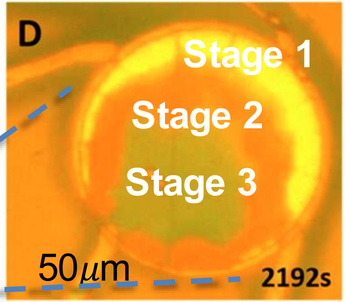


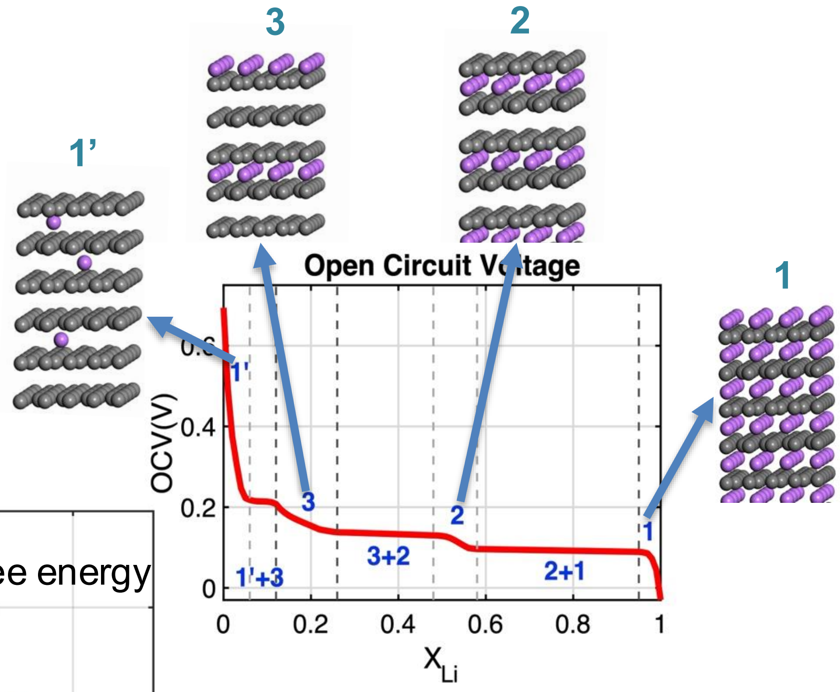
[7] J. Wilson *et al.*, *ECS Trans* 7 (2007) 1879; [8] B Yan et al, *Journal of The Electrochemical Society*, **159** (10) A1604-A1614 (2012)

Phase separating electrode (graphite)

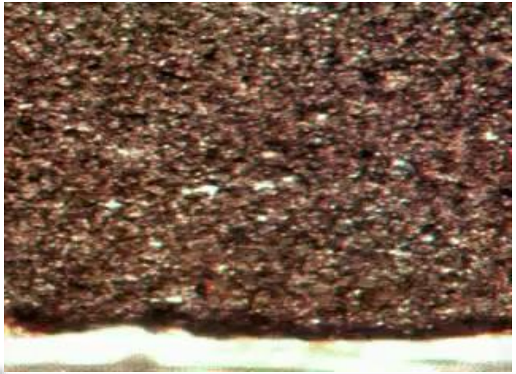
MICHIGAN STATE UNIVERSITY

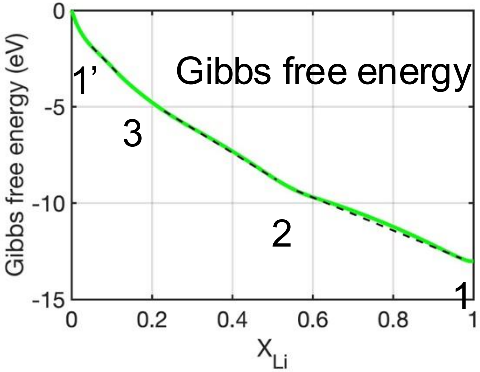






As more and more Li gets intercalated into Graphite, it goes through phase transformations.





[1] Harris *et al.*, Direct in-situ measurements of Li transport in Li-ion battery negative electrodes, 2009; [2] Ender et al., Anode microstructures from high-energy and high-power lithium-ion cylindrical cells obtained by X-ray nano-tomography, 2014

Phase field model for phase transition in graphite

graphite disk

Phase transition

$$\frac{\partial X_p}{\partial t} = \frac{1}{\psi_p}\nabla\cdot\psi_p M_p \nabla\left(\mu_p(X) - \varepsilon\nabla^2 X_p\right) + \frac{1}{\psi_p}\frac{|\nabla\psi_p|}{\rho} r_{xn}$$

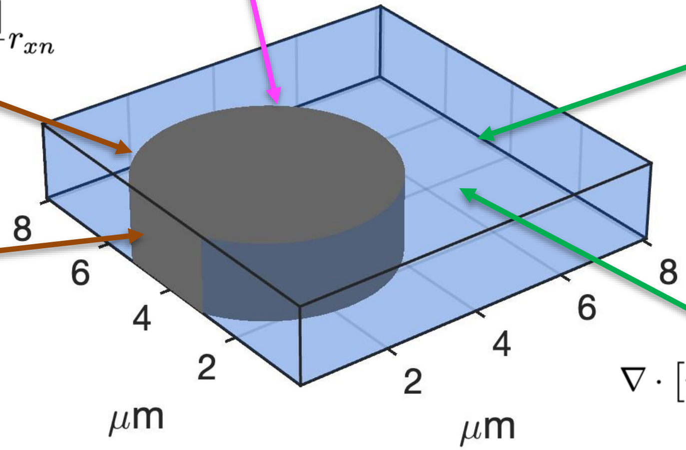
electropotential

$$\nabla\cdot(\psi_p \kappa_p \nabla\phi_p) - |\nabla\psi_p| z_+ F r_{xn} = 0$$

Particle surface

Butler-Volmer

$$r_{xn} = k_f C_e \exp\left[\frac{-\alpha z_+ F}{RT}[\phi]_e^p\right] - k_b C_p \exp\left[\frac{(1-\alpha) z_+ F}{RT}[\phi]_e^p\right]$$



Electrolyte region

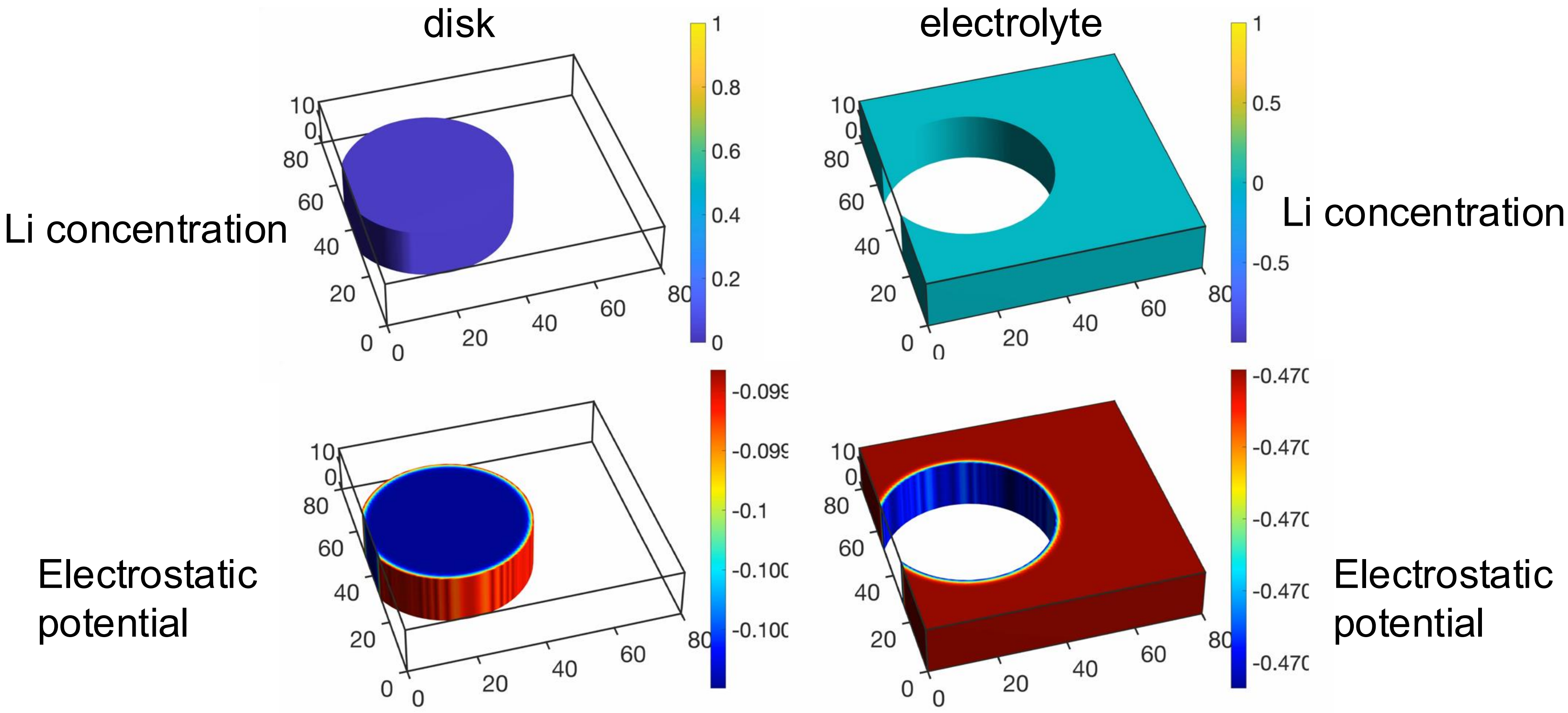
Salt diffusion

$$\frac{\partial C_e}{\partial t} = \frac{1}{\psi_e}\nabla\cdot(\psi_e D_e \nabla C_e) + \frac{|\nabla\psi_e|}{\psi_e}\frac{r_{xn} t_-}{\nu_+} - \frac{\mathbf{i_e}\cdot\nabla t_+}{z_+\nu_+ F}$$

electropotential

$$\nabla\cdot\left[\psi_e\left(z_+ m_+ - z_- m_-\right) F C_e \nabla\phi_e\right] + |\nabla\psi_e|\frac{r_{xn}}{\nu_+} = \nabla\cdot\left[\psi_e\left(D_- - D_+\right)\nabla C_e\right]$$

A. Malik et al, in preparation


disk
electrolyte
Li concentration
Li concentration
Electrostatic potential
Electrostatic potential
1
0.8
0.6
0.4
0.2
0
1
0.5
0
-0.5
-0.099
-0.099
-0.1
-0.100
-0.100
-0.470
-0.470
-0.470
-0.470
-0.470
0
20
40
60
80
10
0

PROGRESS REPORT

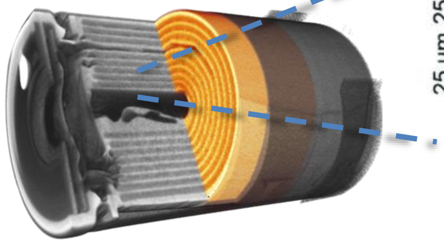
ADVANCED ENERGY MATERIALS

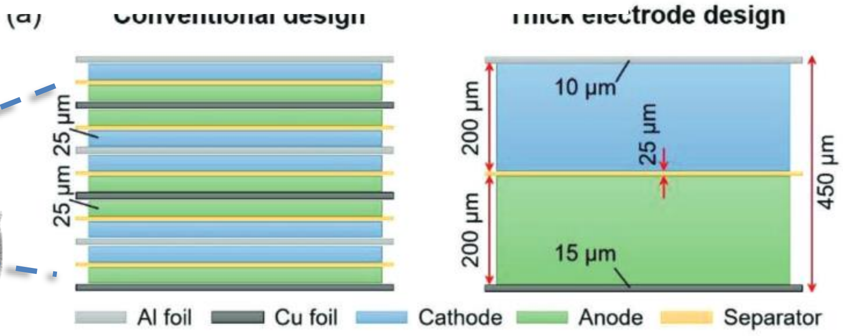
Electrode Materials

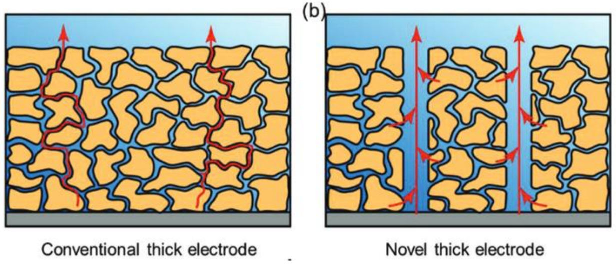
www.advenergymat.de

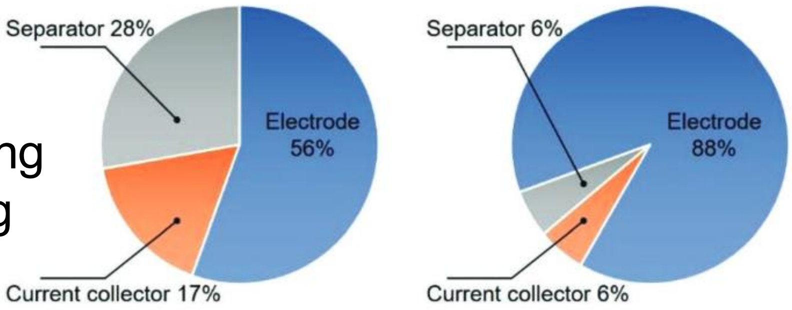
Thick Electrode Batteries: Principles, Opportunities, and Challenges

Yudi Kuang, Chaoji Chen, Dylan Kirsch, and Liangbing Hu**







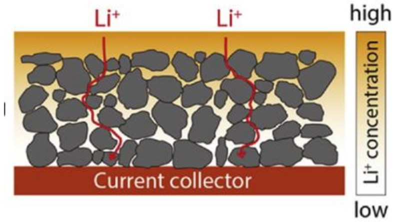


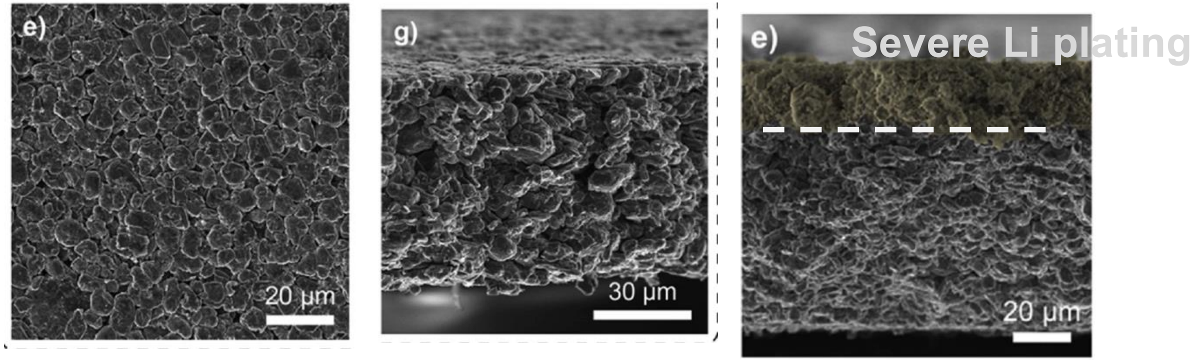
Increase energy density by removing inactive packaging materials.

- Increase energy density by removing inactive packaging materials.
- Using tunnels to enhance transport is required for thick electrodes.

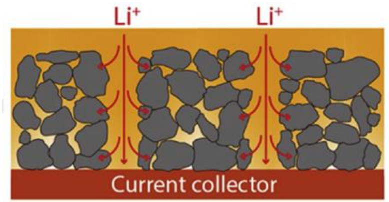
Laser ablated tunnels

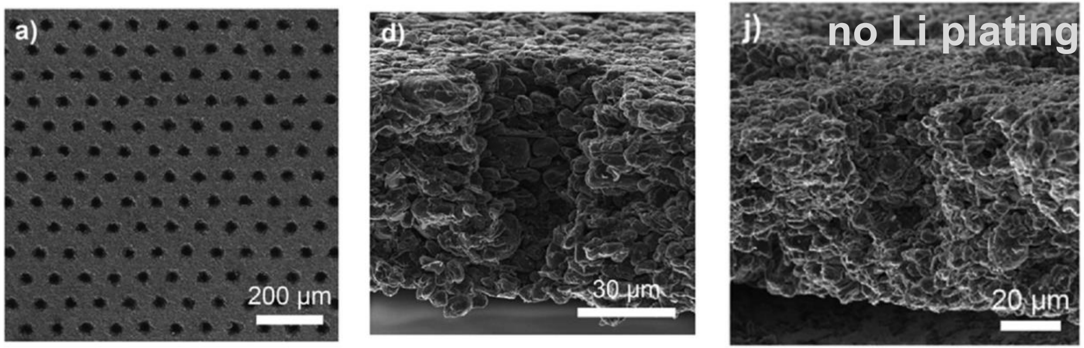
original





With tunnels





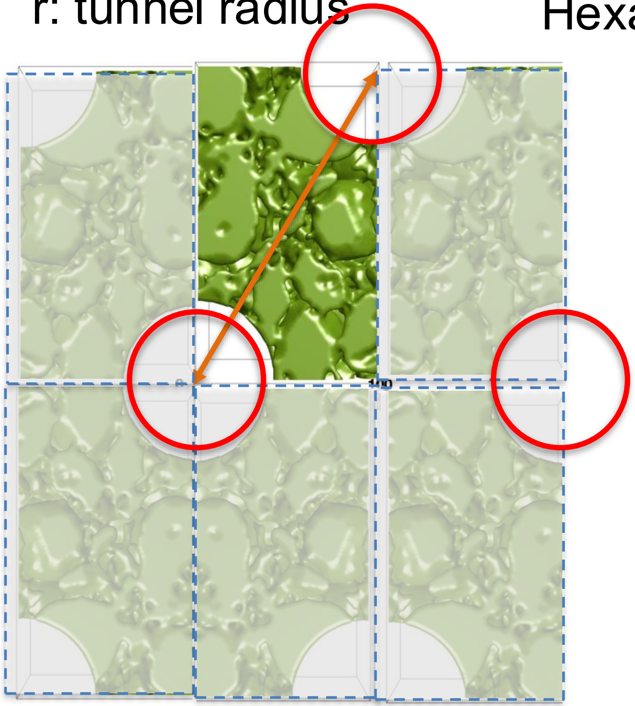
Using laser ablated tunnels to mitigate Li-plating

[14] K H Chen et al., JPS 471 (2020) 228475

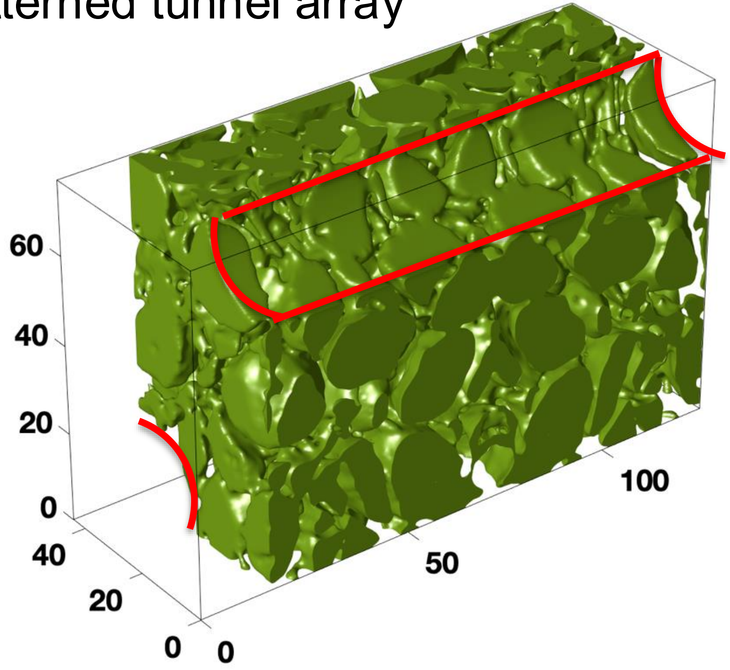
Create tunnels on voxel microstructures: setting voxel value to be zero.

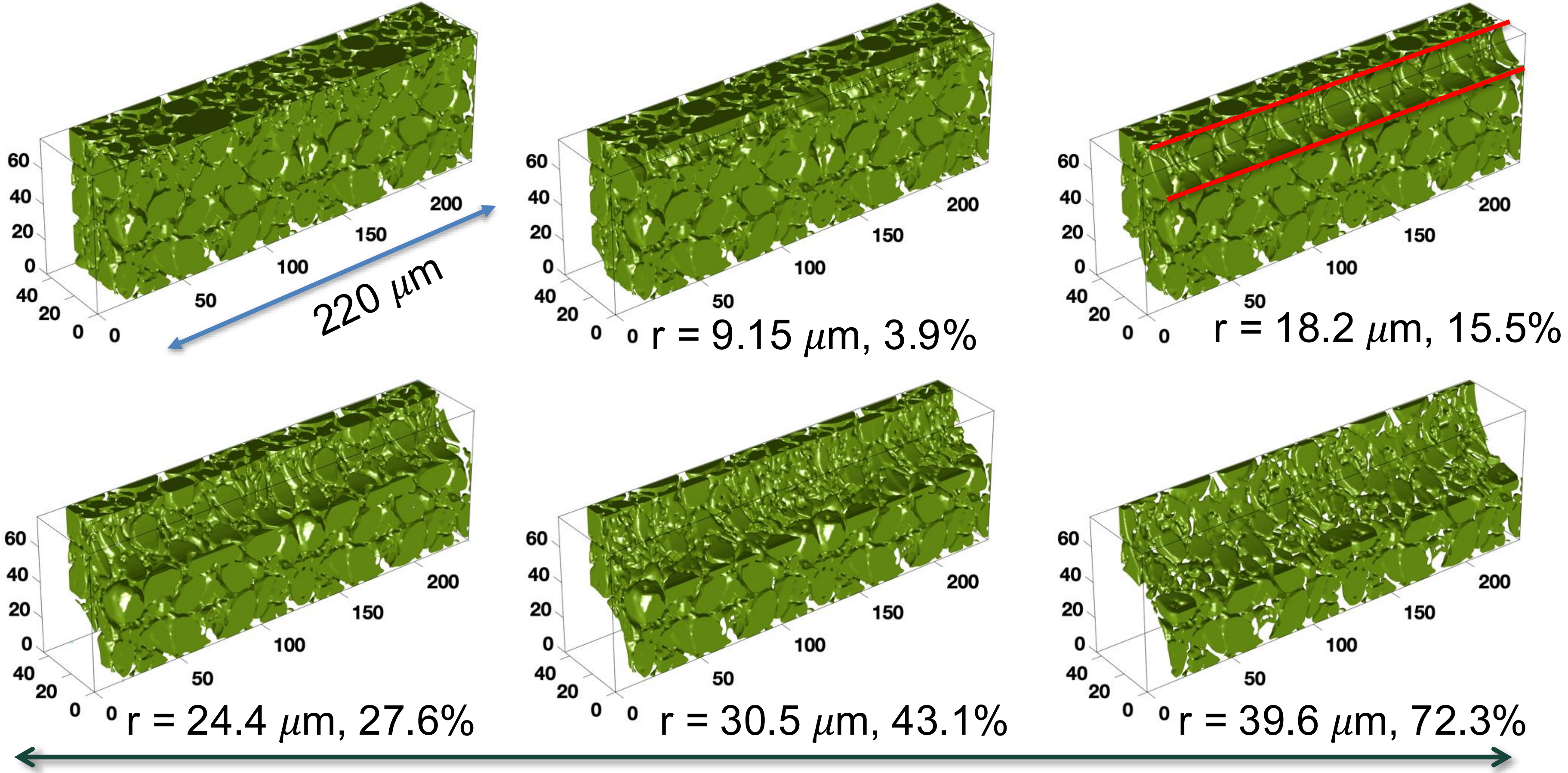
d: inter-tunnel distance

r: tunnel radius

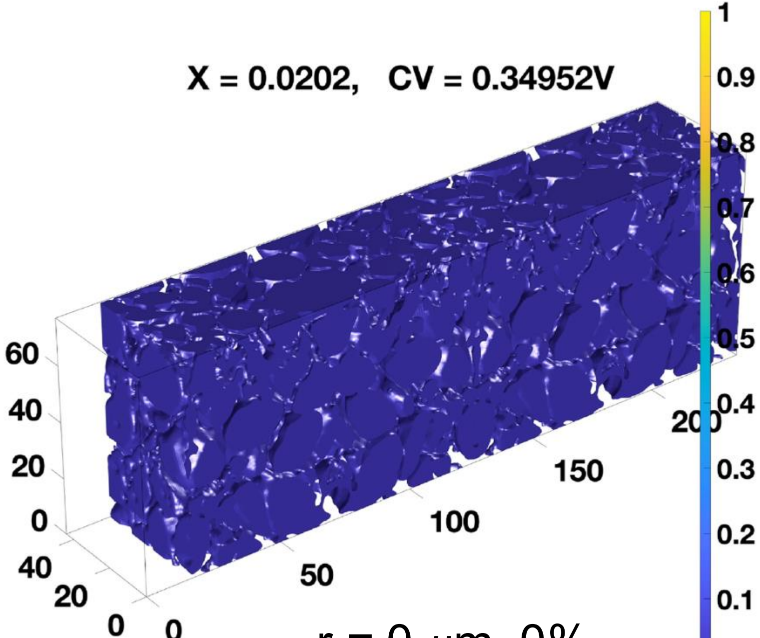


Hexagonal-patterned tunnel array



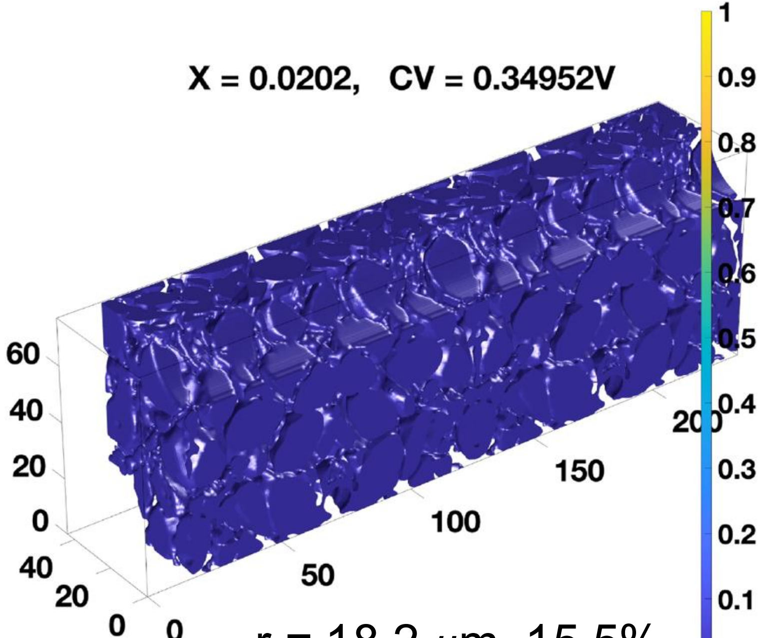

220 μm
r = 9.15 μm, 3.9%
r = 18.2 μm, 15.5%
r = 24.4 μm, 27.6%
r = 30.5 μm, 43.1%
r = 39.6 μm, 72.3%

MICHIGAN STATE UNIVERSITY



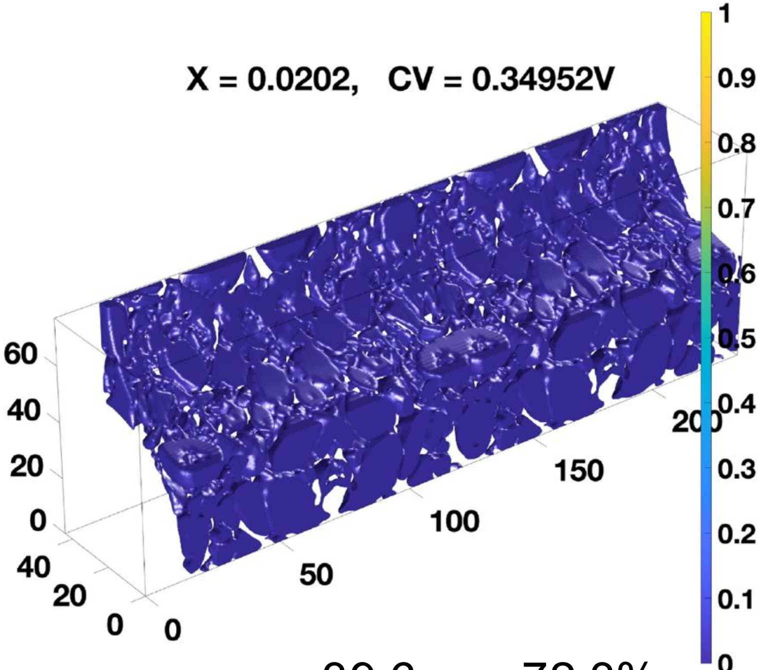
r = 0 μm, 0%

SoC: 0.23; 3.53e-9 mol



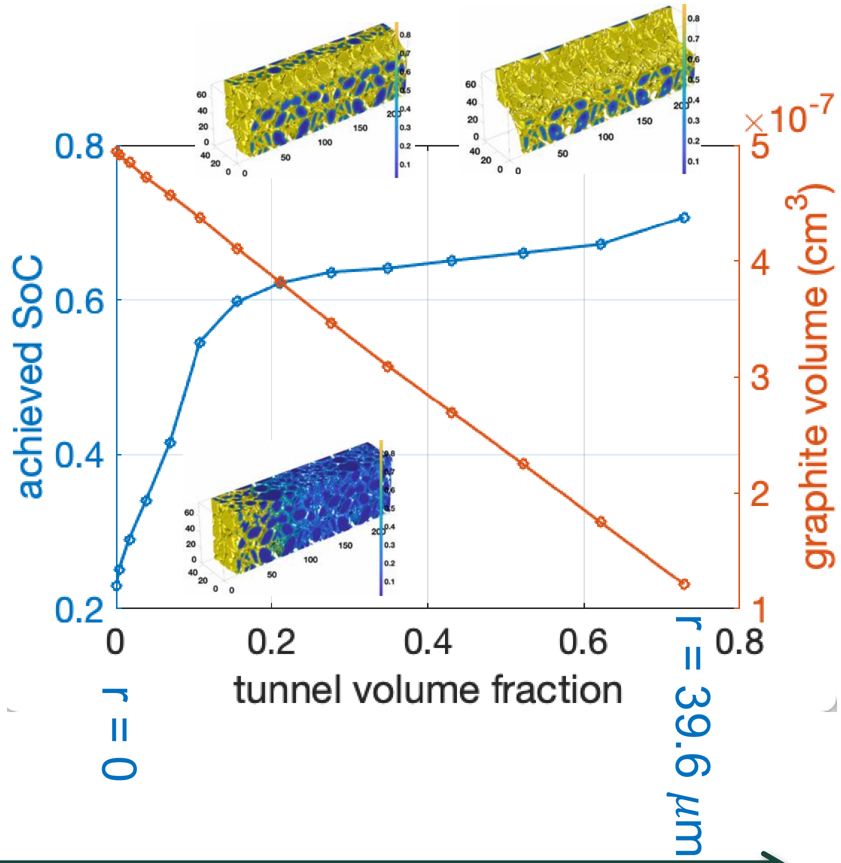
r = 18.2 μm, 15.5%

SoC: 0.60; 7.66e-9 mol



r = 39.6 μm, 72.3%

SoC: 0.71; 2.68e-9 mol



Optimal radius

Hexagonal arrang., d = 87.7 μm