Battery Safety Science Webinar Series

Advancing safer energy storage through science

June 14, 2021

Multiphysics and Multiscale Modeling of Lithium-ion Battery Safety Issues

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BACKGROUND

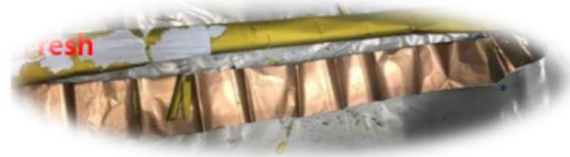
Battery Crash Safety

Fire/explosion after car crash

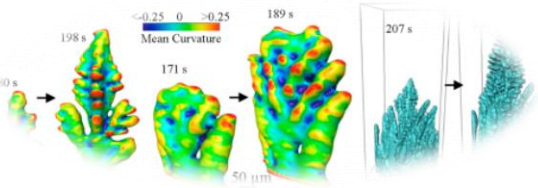
Cell-phone battery explosion after penetration

Large-scale energy storage system safety

Battery Degradation



Li-plating



Li-dendrite

- Mechanical abusive loading
- Li plating
- Li dendrite
- Particle crack

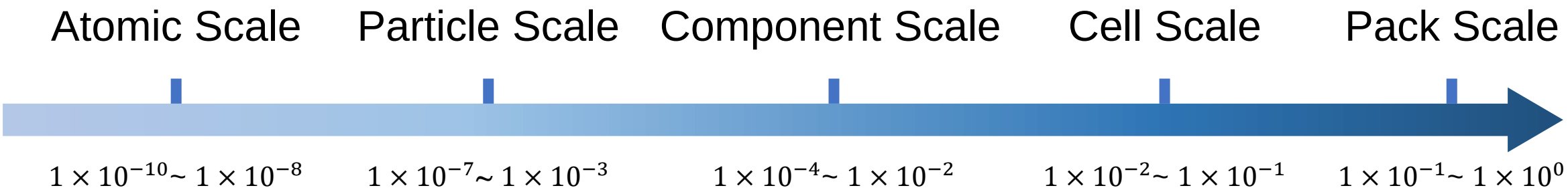
Internal short circuit → Thermal runaway → Explosion/fire

Voltage recovery *Discharge only*

Silent thermal runaway

Explosion/fire

(Liu, et al. *Energy Storage Materials,* 2020)


Atomic Scale
Particle Scale
Component Scale
Cell Scale
Pack Scale
$1 \times 10^{-10} \sim 1 \times 10^{-8}$
$1 \times 10^{-7} \sim 1 \times 10^{-3}$
$1 \times 10^{-4} \sim 1 \times 10^{-2}$
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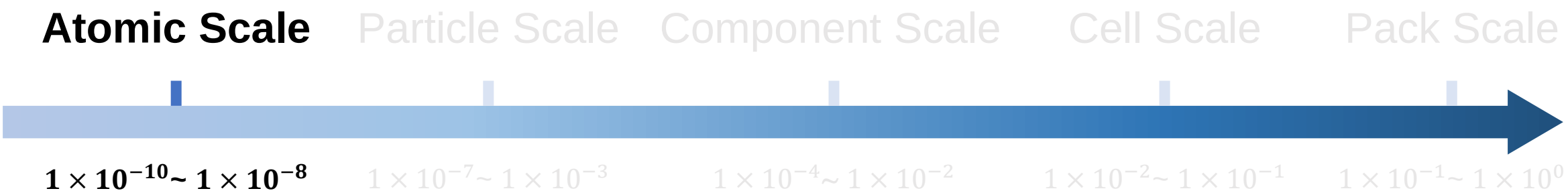
$1 \times 10^{-1} \sim 1 \times 10^{0}$

Unit: m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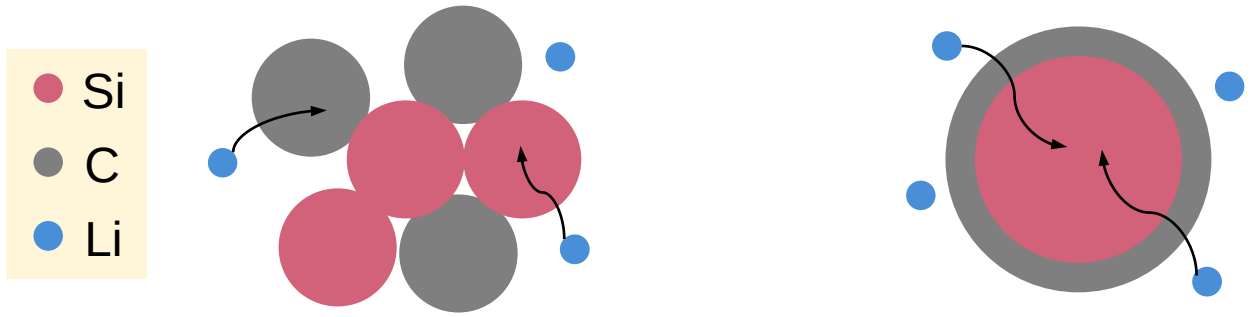
Unit: m

AN INTERESTING QUESTION

Li diffusion mechanism in Si/C system

Two representative Si/C mixing modes



Mixture mode

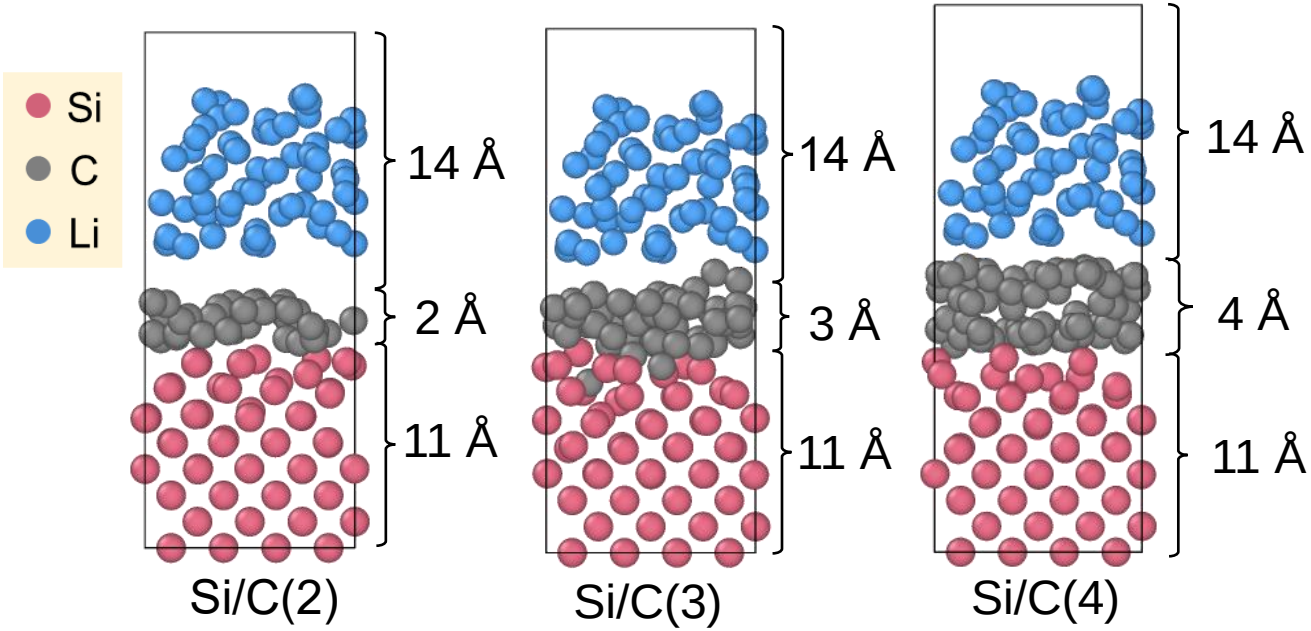
Core-shell mode

1. Li diffusion in Si first or C first?
2. How the composite configuration affects diffusion? ➡ DFT simulation
3. How the C material affects Li diffusion in Si?

Method

DFT simulation

Si/C with various C layer thicknesses

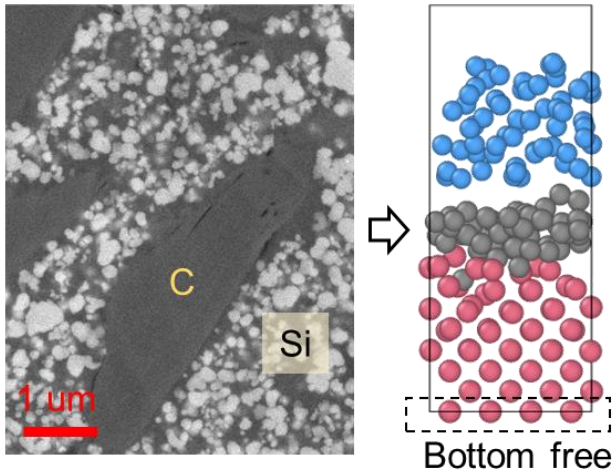


AIMD simulation:

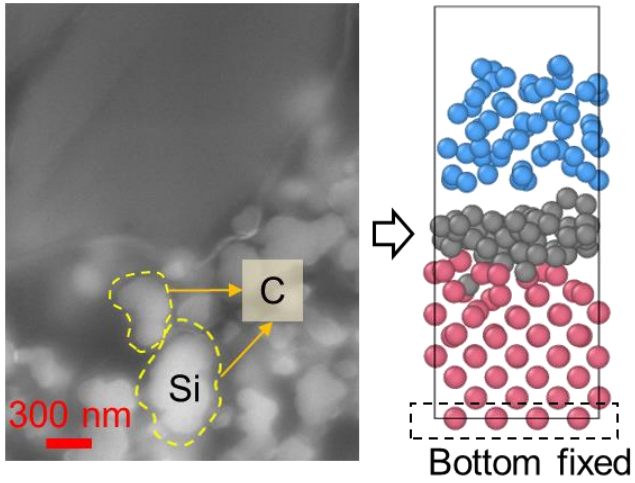
1200 K, 0.01 eV/Å, 10^{-4} eV

(Gao, et al. *ACS Applied Material & Interfaces,* 2021)

Two representative Si/C configuration modes



Mixture mode

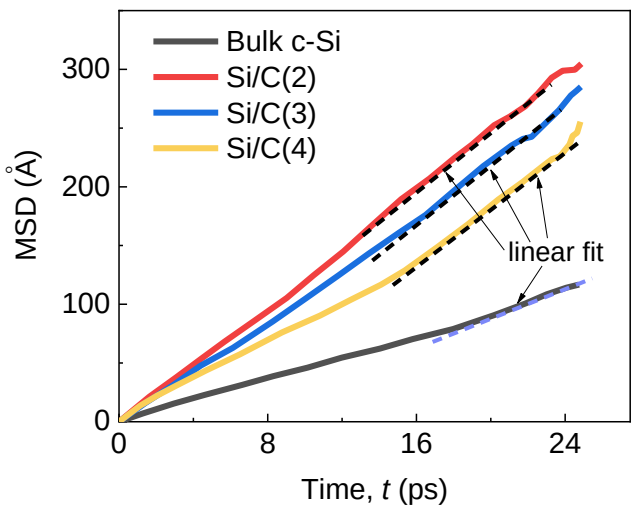


Core-shell mode

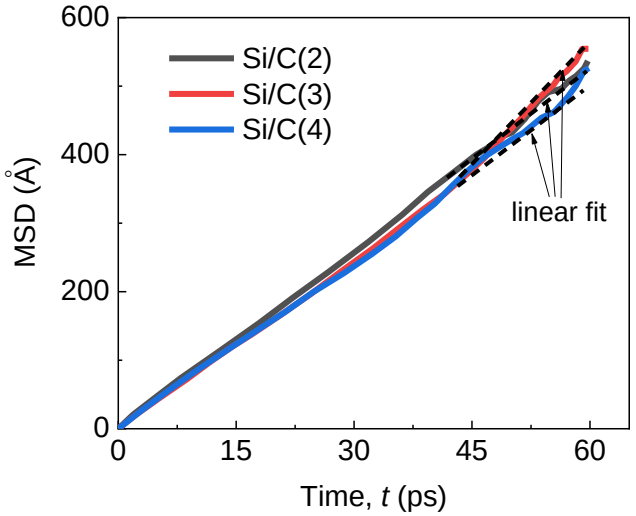
Discussion

Diffusivity analysis

Core-shell mode

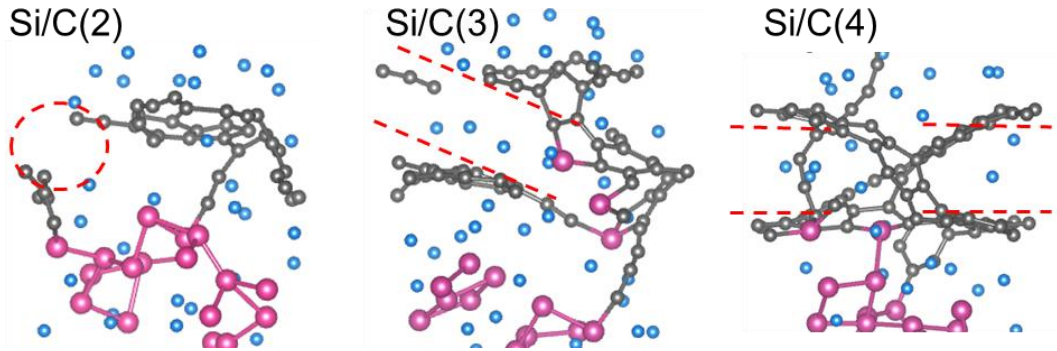


Mixed mode



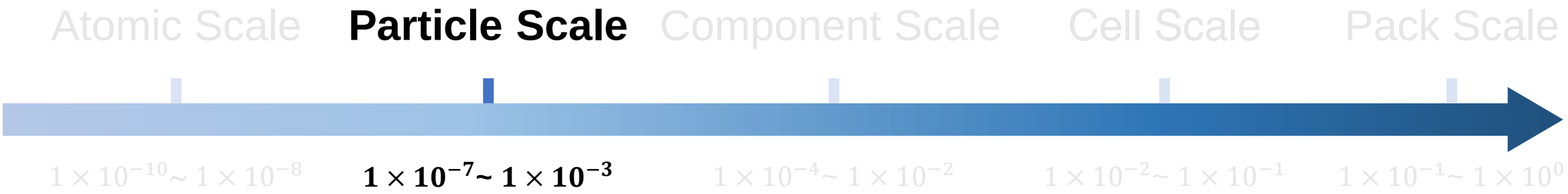
Type	Bulk c-Si	Si/C (2)	Si/C (3)	Si/C (4)
Mixture mode	7.75e-5	2.097e-4	2.028e-4	2.003e-4
Core-shell mode	\	1.545e-4	1.953e-4	1.435e-4

Core-shell mode



- A thicker C layer slightly decreases the Li diffusivity in Si
- The overall Li diffusivity in mixture mode is almost same
- Li diffusivity in core-shell mode highly depends on the C layer atomic structure
- Li diffusivity in core-shell mode is commonly lower than in mixture mode

(Gao, et al. *ACS Applied Material & Interfaces*, 2021)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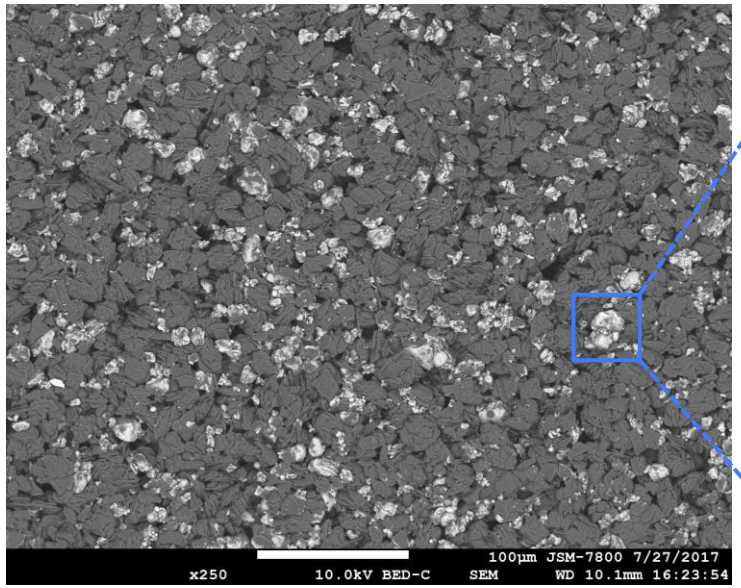
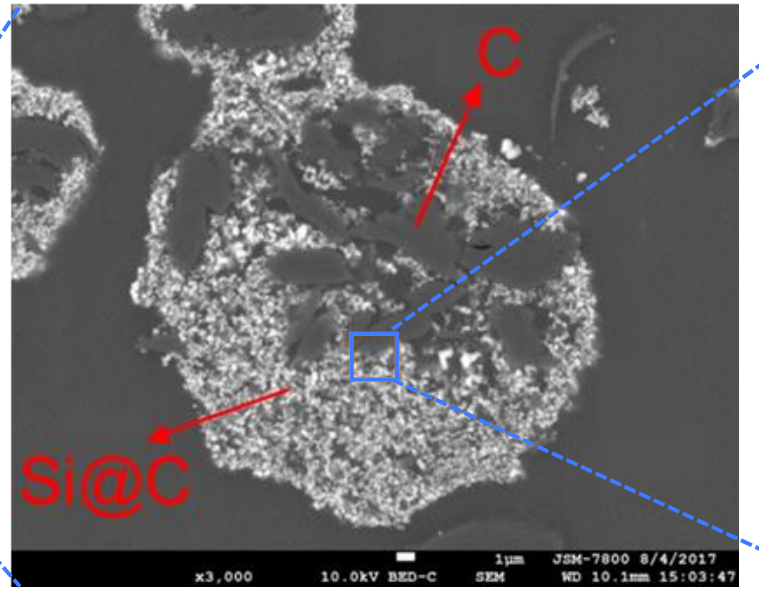
Unit: m

SI/C COMPOSITE ANODE PARTICLE

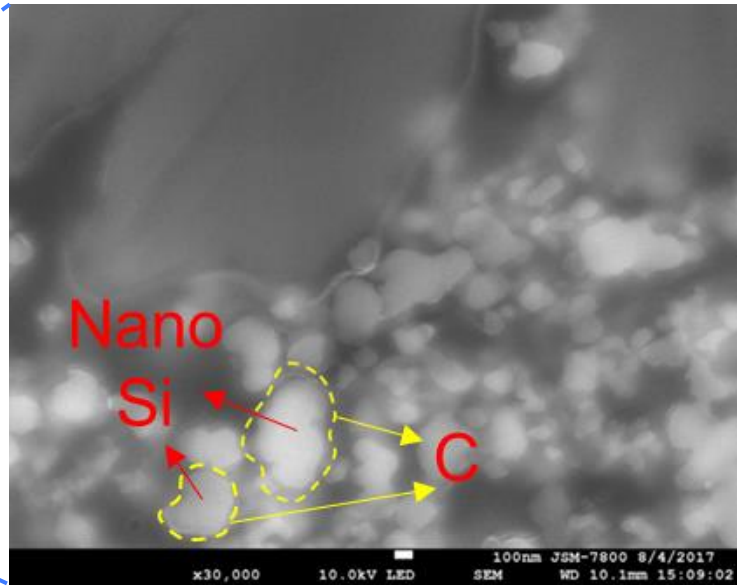
SEM images of Si/C composite anode



Si/C composite anode



Si/C composite particle



Si/C core-shell structure (Si@C)

1mm → 100nm

Micro-scale

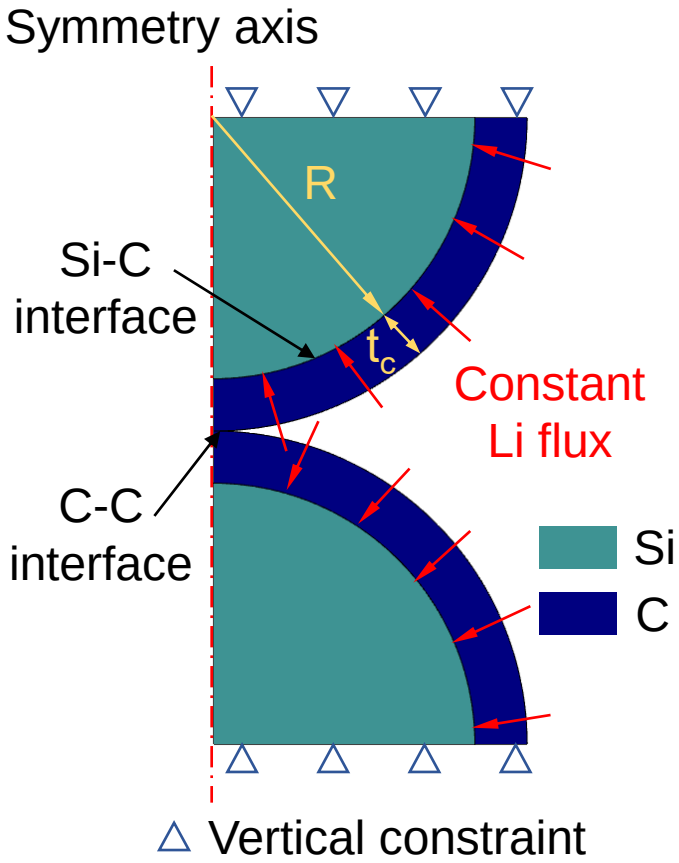
Nano-scale

Si/C composite anode shows a complex multiscale structure property

PART I: CONTACT BEHAVIOR

Modeling: Si-C core-shell particles

- FEM model settings



- Governing equations

COMSOL module

- Mechanical model

Total true strain $\varepsilon_{ij} = \varepsilon_{ij}^{l} + \varepsilon_{ij}^{e} + \varepsilon_{ij}^{p}$

Governing equation

$\varepsilon_{ij}^{l} = \ln(1+\alpha\bar{c})/3$: Lithiation induced strain

α is related to state of Li_xSi_y, $Li_{15}Si_4 \rightarrow \alpha$=2.75

$\varepsilon_{ij}^{e} = \left[(1+\nu)\sigma_{ij} - \nu\sigma_{kk}\delta_{ij}\right]/E$: Elastic strain

Based on Hooke's law

$d\varepsilon_{ij}^{p} = \lambda S_{ij}^{p}$: Plastic strain increment

Generalized form, S_{ij}^{p} is deviatoric stress

Invasive extension

Structural mechanics

- Electrochemical model

Diffusion equation

Partial differential equation

$$\frac{\partial c}{\partial t} - D\nabla\cdot\left(\nabla c - \frac{\Omega c}{RT}\nabla\sigma_h\right) = 0$$

$$\bar{c} = c/c_{max}$$

$$E(\bar{c}) = E_0 + \bar{c}(E_1 - E_0)$$

$$\sigma_y(\bar{c}) = \sigma_y^0 + \bar{c}(\sigma_y^1 - \sigma_y^0)$$

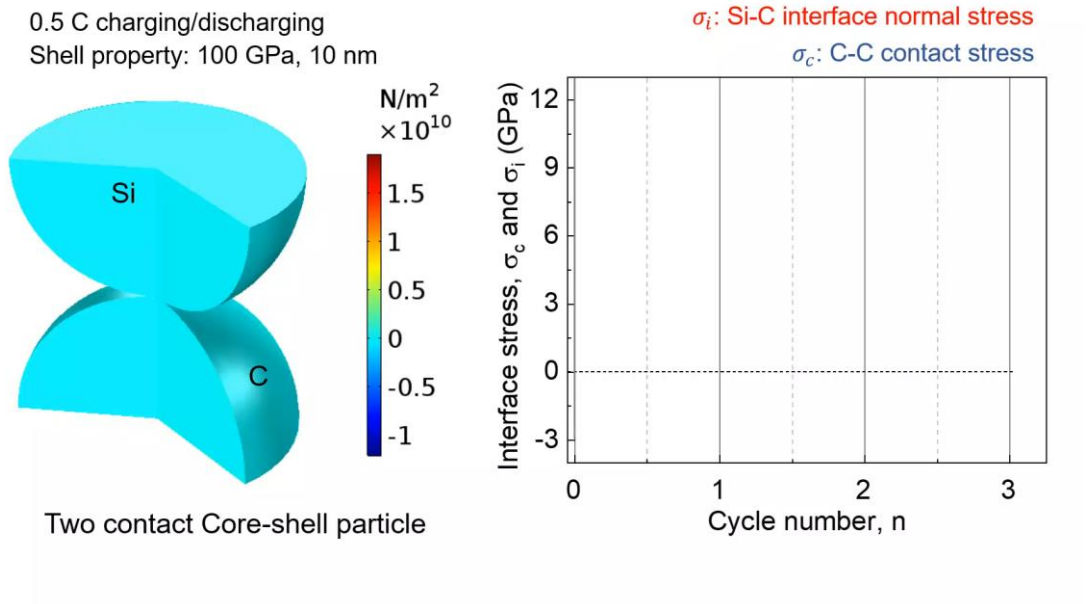
Mechanical parameters related to Li^+ concentration c

(Gao, et al. *Energy Storage Materials*, 2019)

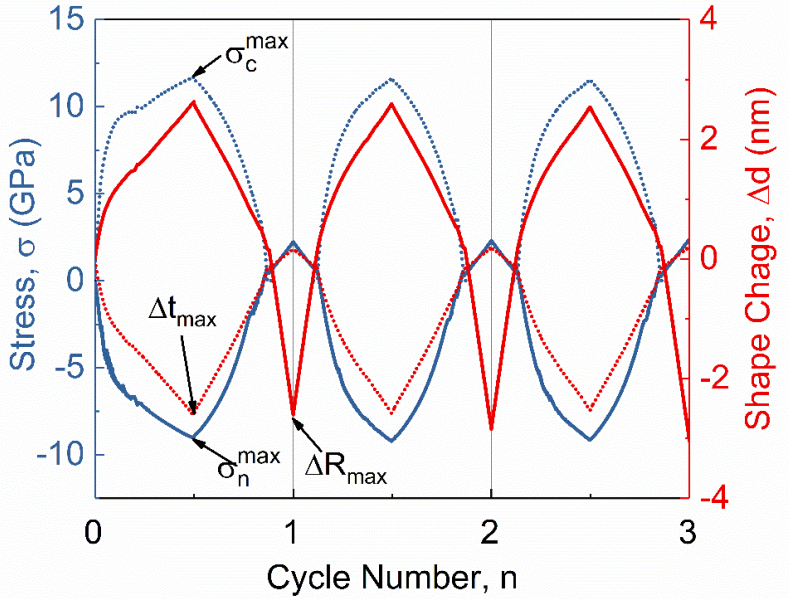
PART I: CONTACT BEHAVIOR

Simulation: Stress analysis

- Stress evolution and distribution



- Parameter definition



- ➢ **Plastic contact** mainly occur in first cycle
- ➢ **Tensile stress** produced in every cycle end

σ_n^{max} maximum Si-C interface normal stress

σ_c^{max} maximum C-C contact stress

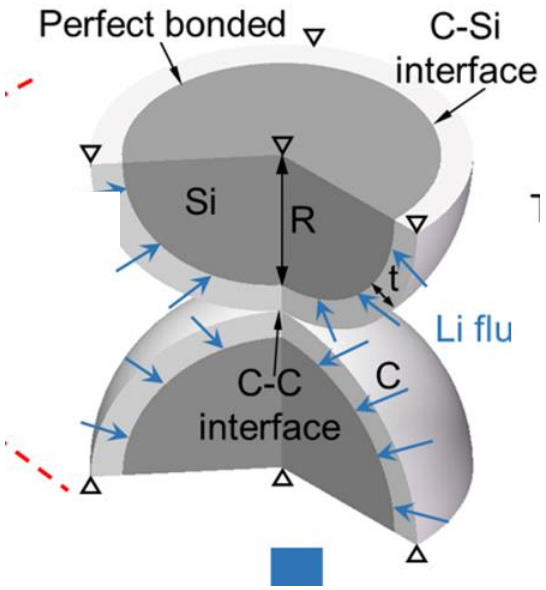
$R / R_0 = (R_0 + \Delta R_{max}) / R_0$ maximum Si radius change

$(t / t_0)_{max} = (t_0 + \Delta t_{max}) / t_0$ maximum C thickness change

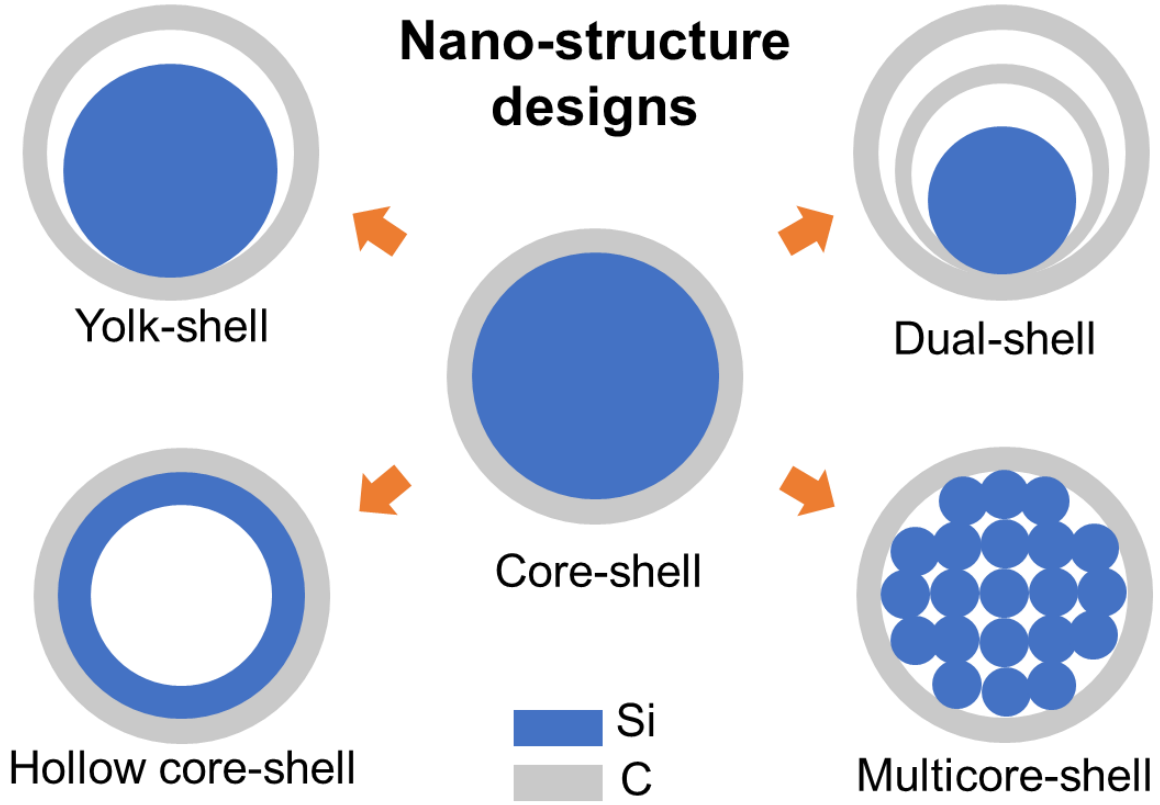
(Gao, et al. *Energy Storage Materials*, 2019)

PART II: SI/C CORE-SHELL STRUCTURES

Modeling: Si-C core-shell particles



Core-shell structure studied in previous slides



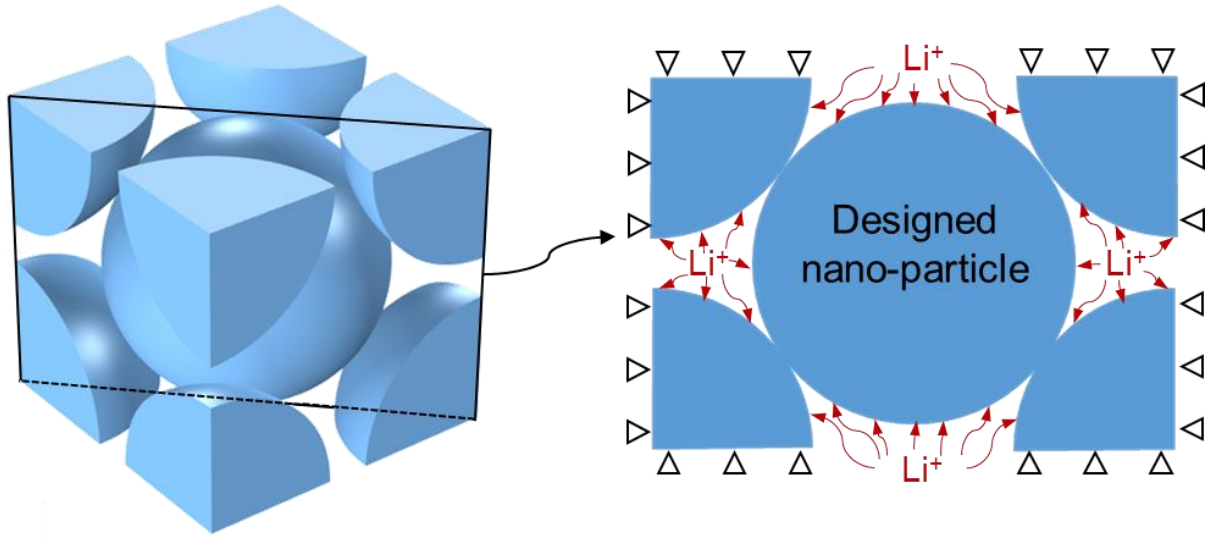
The best one?

(Gao, et al. *Nano Energy*, 2021)

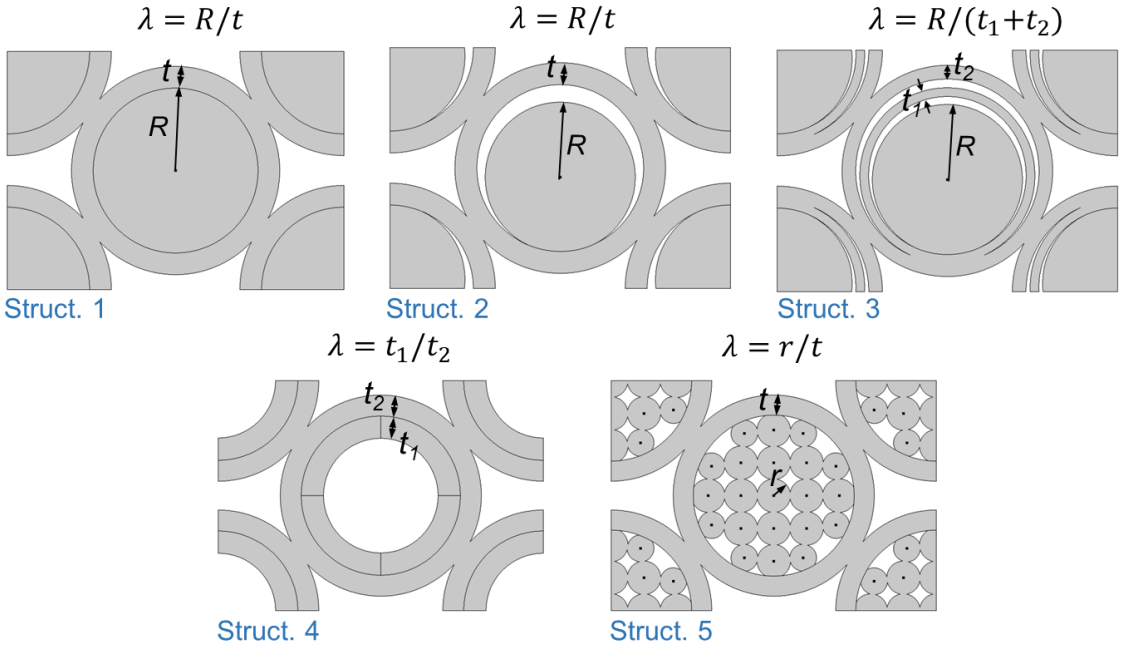
PART II: SI/C CORE-SHELL STRUCTURES

Modeling: FEM model settings

Geometry and boundary



Five structures



- Same governing equations were adopted
- Each structure has three different λ values

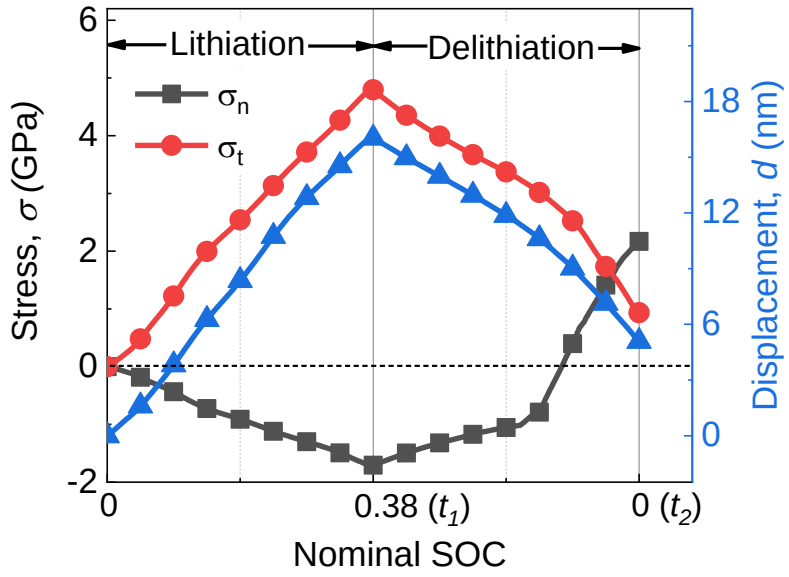
(Gao, et al. *Nano Energy*, 2021)

Gao et al., *Nano Energy*, 2020

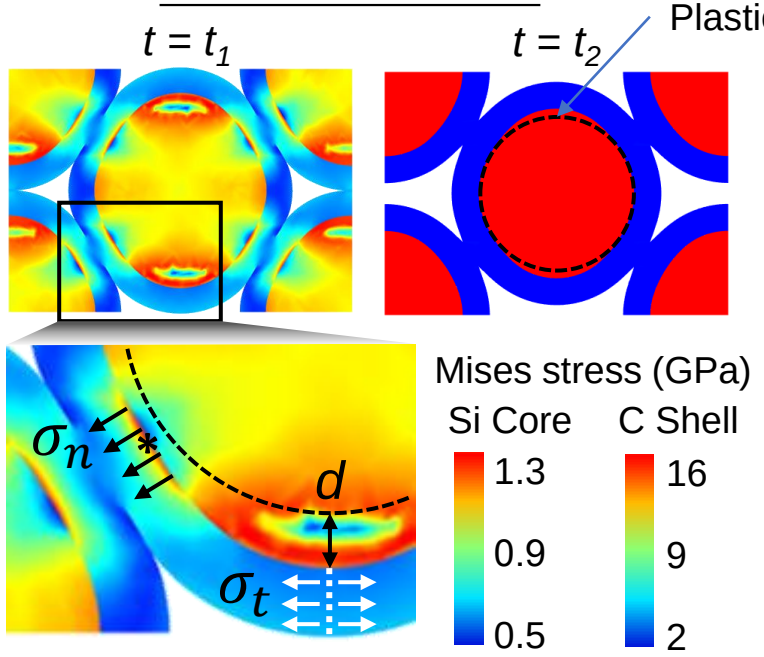
PART II: SI/C CORE-SHELL STRUCTURES

Simulation: Mechanical behavior

- Stress and displacement curve

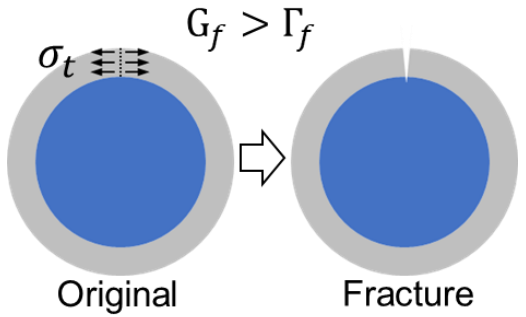


- Stress distribution

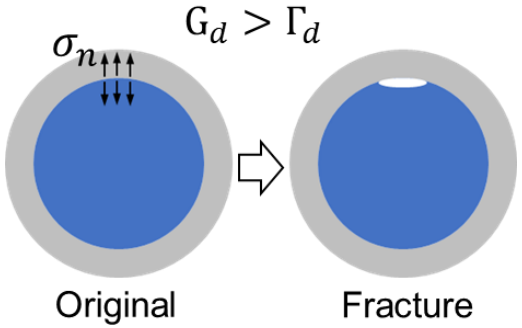


- Failure modes

Shell fracture (lithiation)



Core shell debonding (de-lithiation)



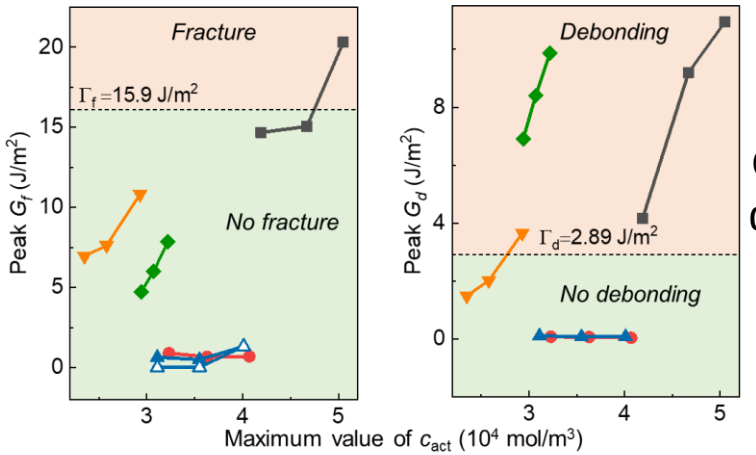
- The normal stress σ_n at the core-shell interface is in compressive stress status and increases during lithiation.
- At the core-shell interface, the maximum normal stress occurs in the contact area of two particles, and the maximum compressive stress is in the center of the C shell

(Gao, et al. *Nano Energy*, 2021)

PART II: SI/C CORE-SHELL STRUCTURES

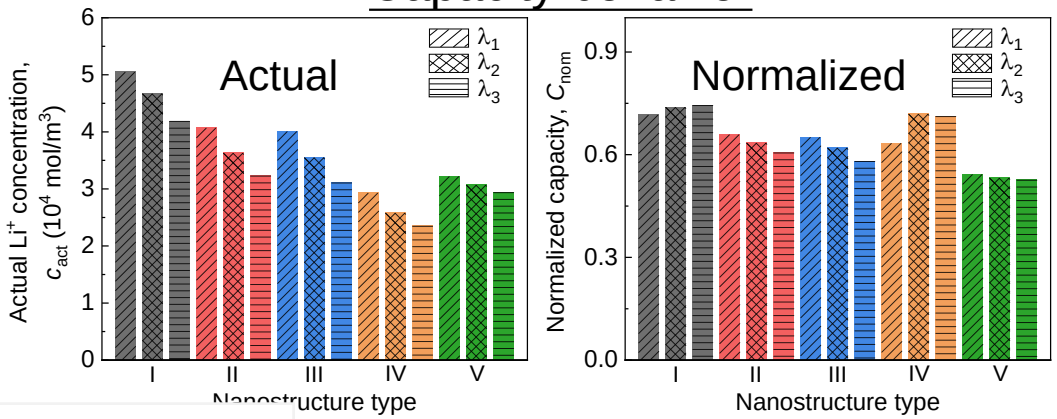
Simulation: Failure, capacity, design

Shell fracture

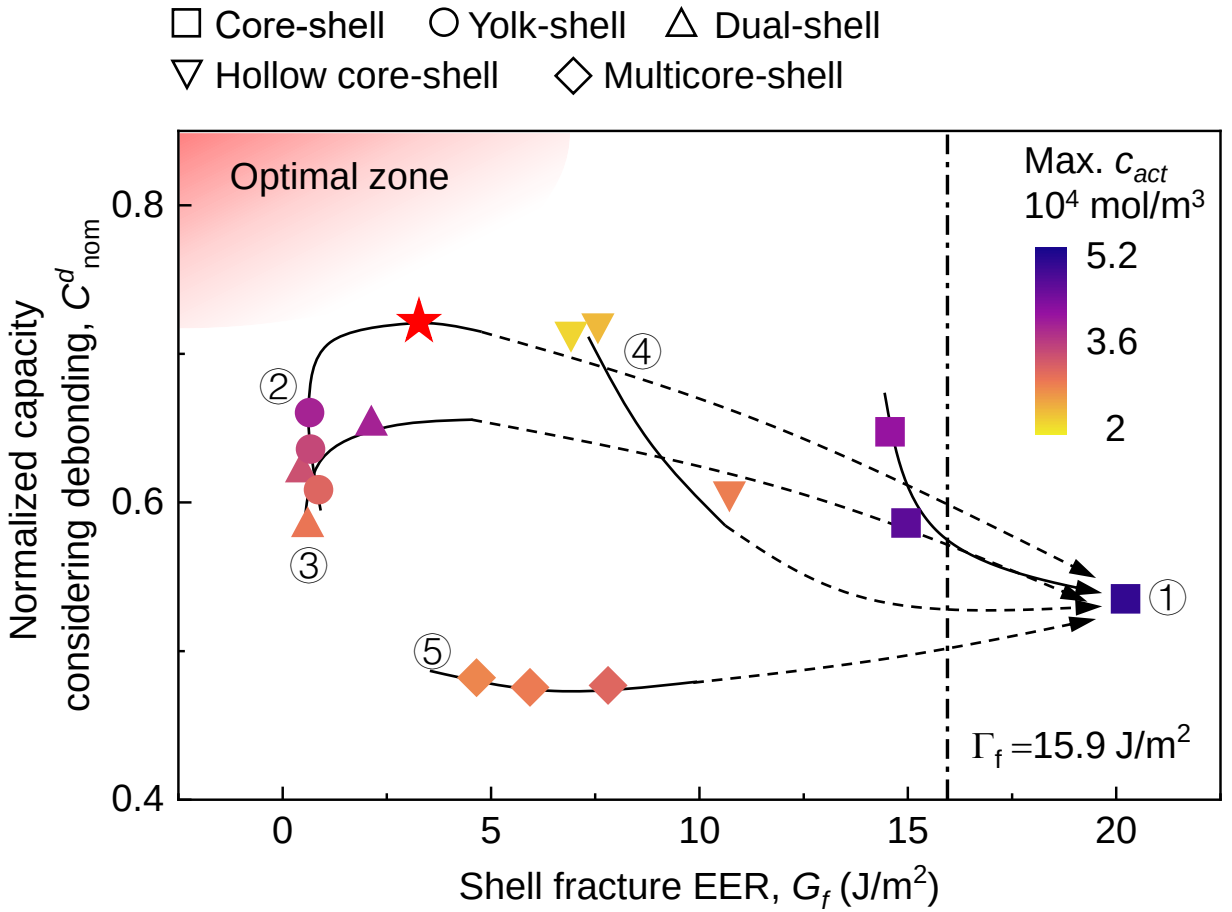


Core-shell debonding

- Capacity behavior



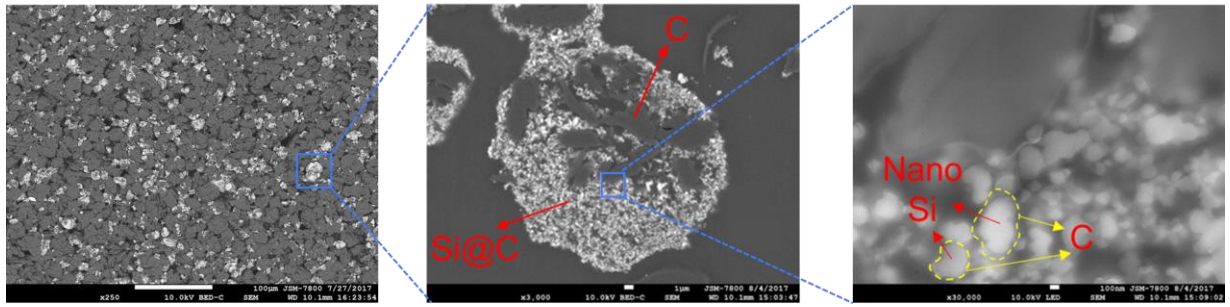
(Gao, et al. *Nano Energy*, 2021)



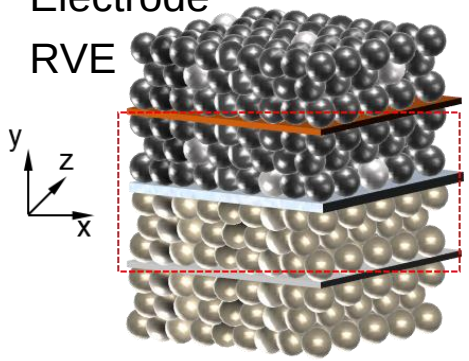
PART III: MULTISCALE-MULTIPHYSICS STUDY

Modeling: Multiphysics coupling strategy

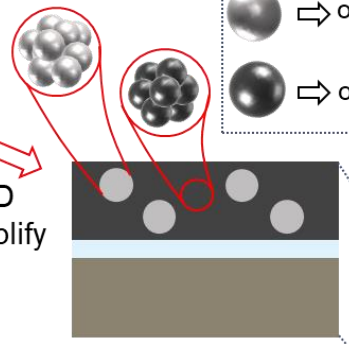
Si/C composite anode



Electrode RVE

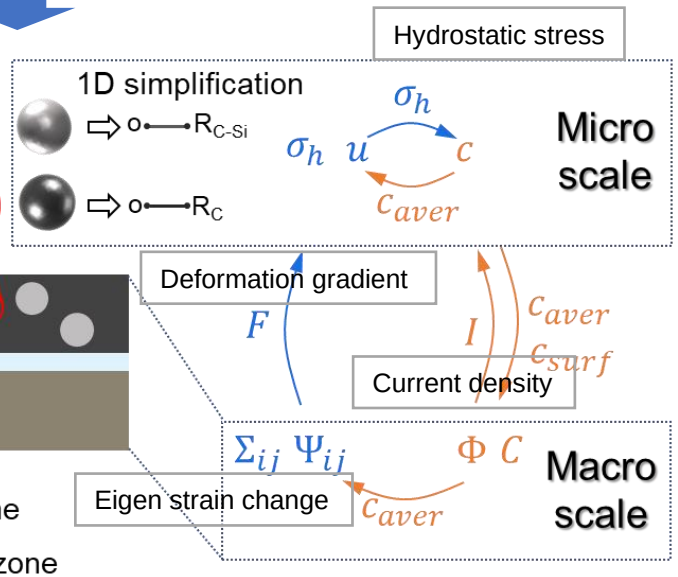


2D simplify



Graphite particle
Si-C composite particle
LCO particle
Current collector Cu
Current collector Al
Separator

C zone
Si-C zone
LCO
Separator



Blue: Mechanical
Orange: Electrochemical

(Gao, et al. *Journal of Power Sources*, 2020)

Governing equations

- Constitutive equation in microscale

$$\sigma_{ij} = 2G\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij} - \Omega_{eff}\Delta c_s \frac{E}{1-2\upsilon}\delta_{ij}$$

- Li diffusion model in microscale

$$\frac{\partial c_s}{\partial t} + \frac{1}{r^2}\frac{\partial r^2 J_s}{\partial r} = 0$$

- Stress-strain model in macroscale

$$\Sigma_{ij} = C_{ijkl}(\Psi_{kl} - \Psi_{eigen}\delta_{kl})$$

- Li flux model in macroscale

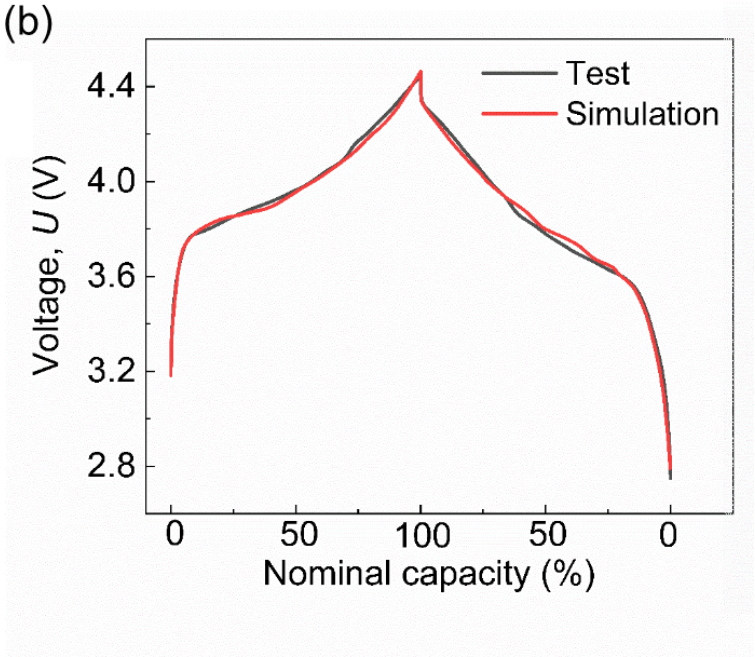
$$\mathbf{I_e} = -\kappa_e^{eff}\left[\nabla\Phi_e - \frac{2RT}{F}\left(1 + \frac{d\ln f_{\pm}}{d\ln C_e}\right)(1-t_+)\nabla\ln C_e\right]$$

$$\varepsilon_e\frac{\partial C_e}{\partial t} = -\nabla\cdot\mathbf{J_e} + \frac{a_s I}{F}$$

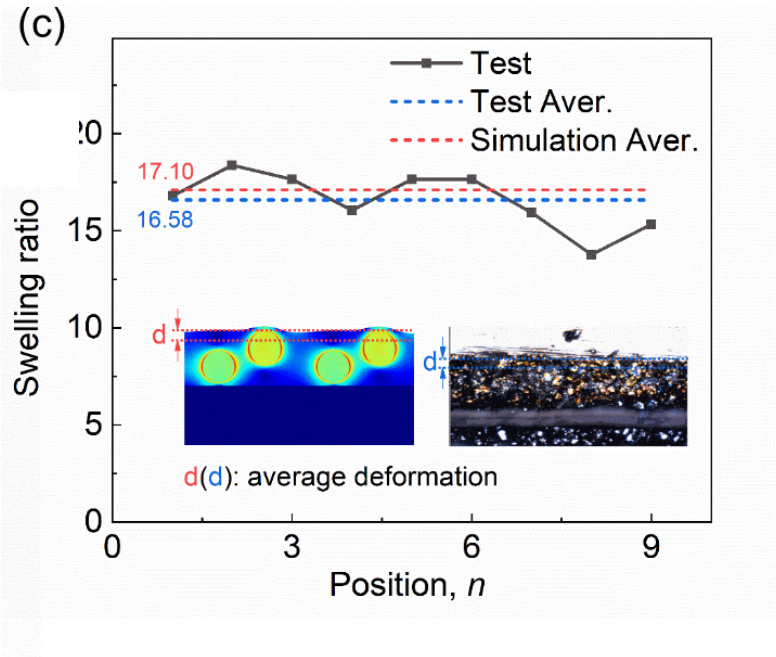
PART III: MULTISCALE-MULTIPHYSICS STUDY

Simulation: Model validation

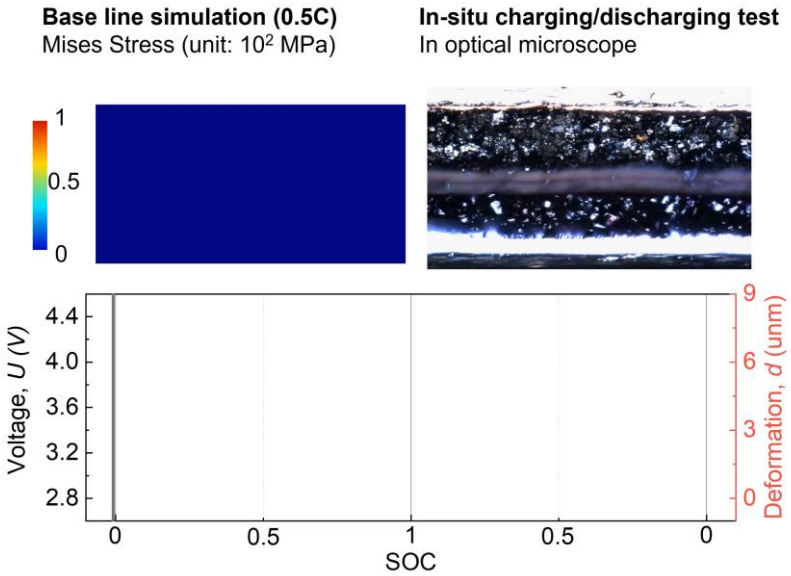
Full-cell voltage



Electrode deformation

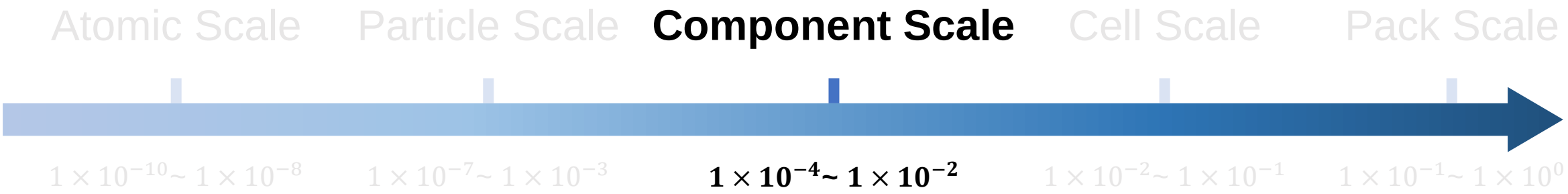


Corresponding video



- Multiscale and Multiphysics coupling model can well predict the voltage and deformation

(Gao, et al. *Journal of Power Sources*, 2020)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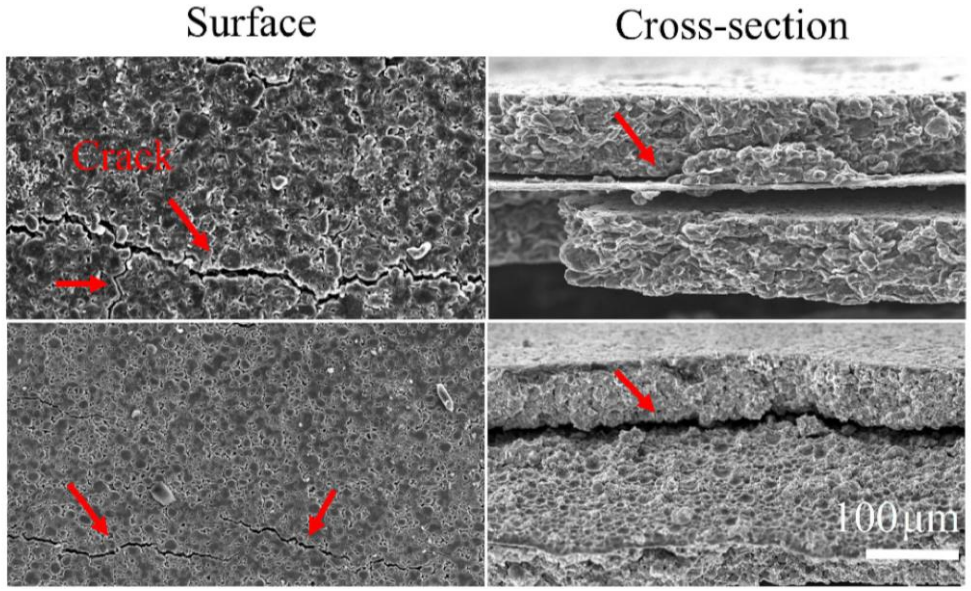
Unit: m

MECHANICAL BEHAVIOR OF ELECTRODE

Experiment: Material test of battery components

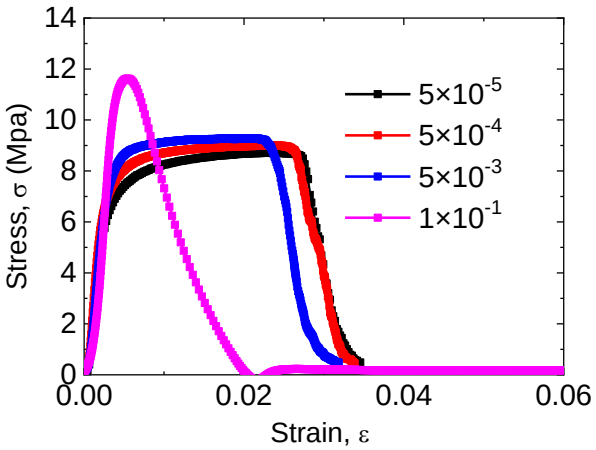
- SEM images after tensile test

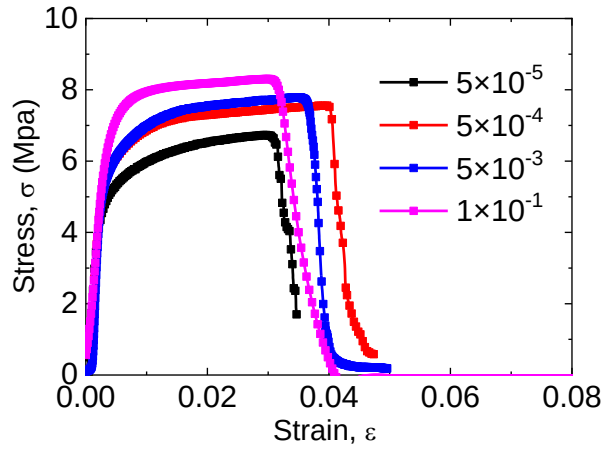


Anode

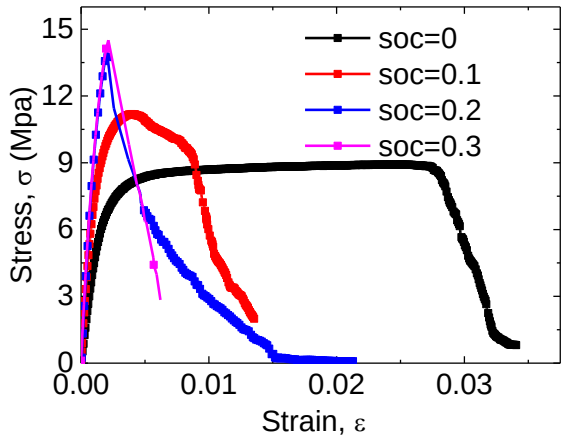
Cathode

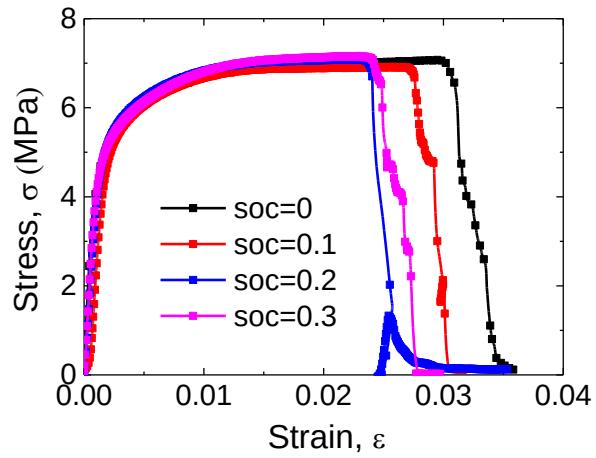
- Strain rate effect





- SOC effect

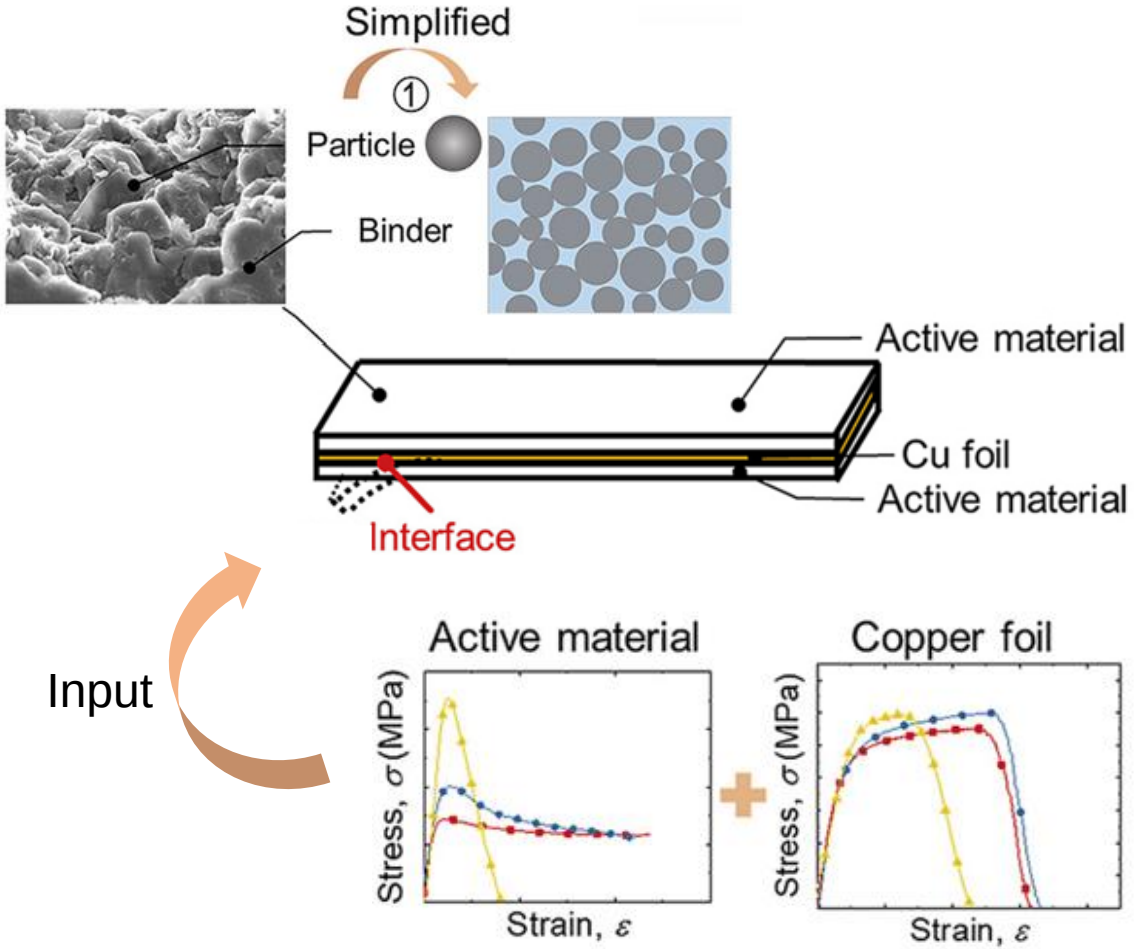




(Wang, et al. *Journal of Power Sources*, 2018)

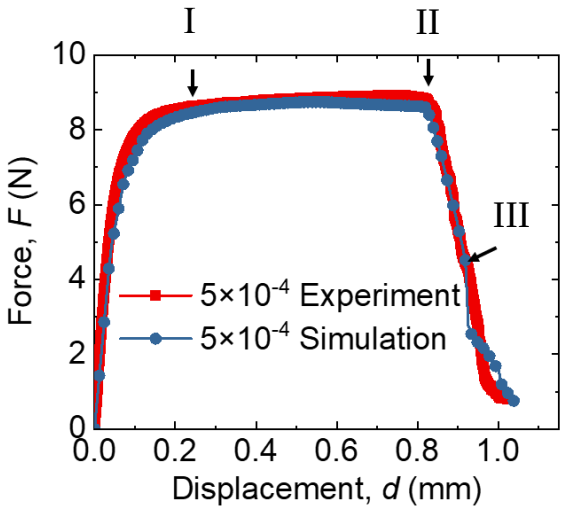
MECHANICAL BEHAVIOR OF ELECTRODE

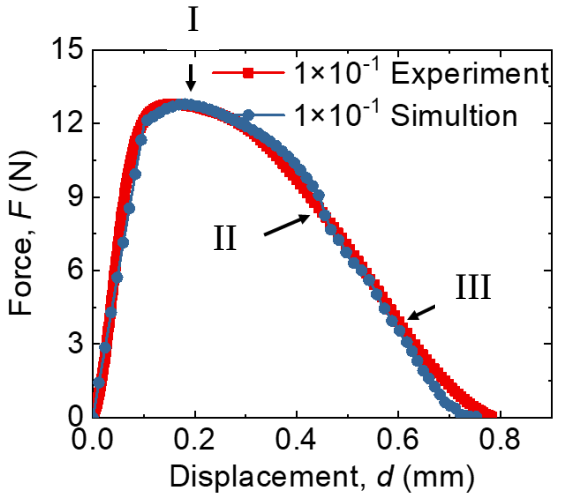
Modeling: Laminate theory and sandwich model

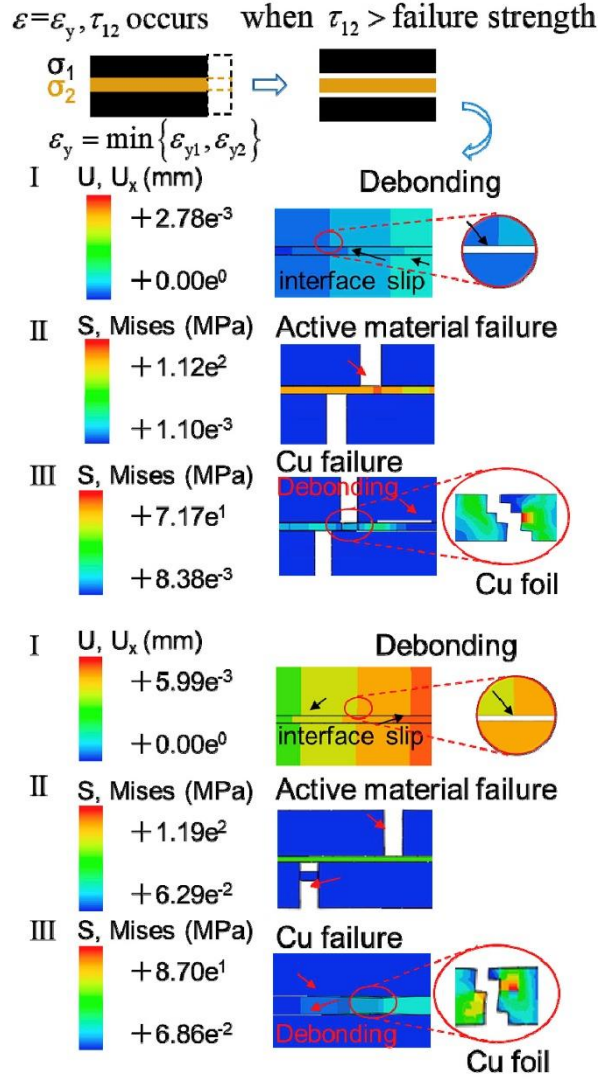


(Wang, et al. *Journal of Power Sources,* 2018)

Simulation: Tension and failure analysis



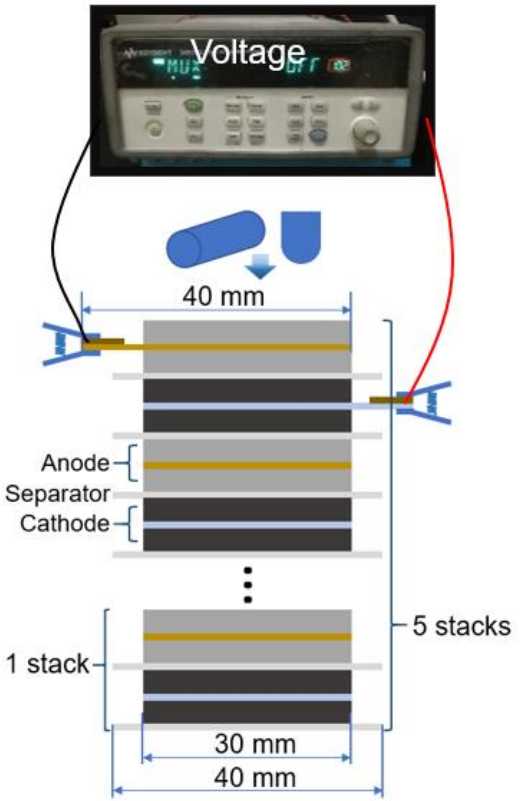




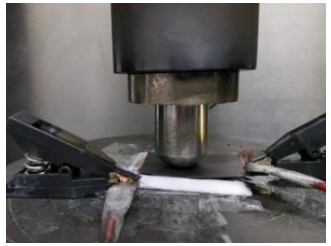
FAILURE BEHAVIOR OF SEPARATOR

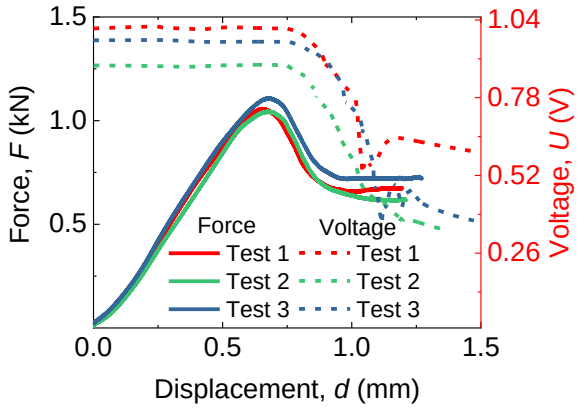
Experiment: Indentation test on anode-separator-cathode stacks

Experiment setup

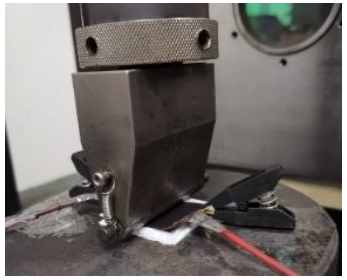


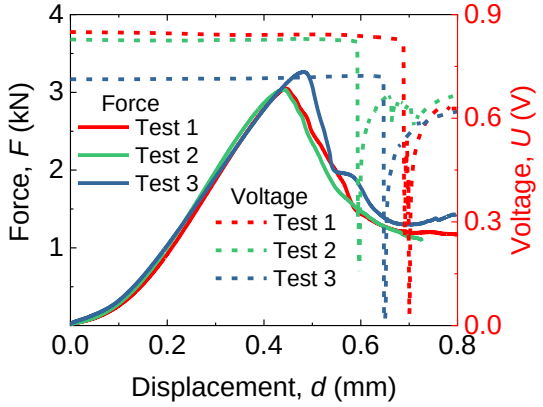
- Sphere indentation



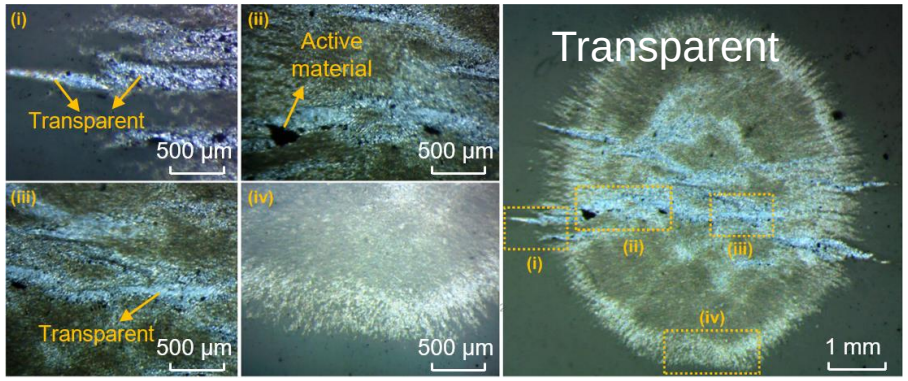


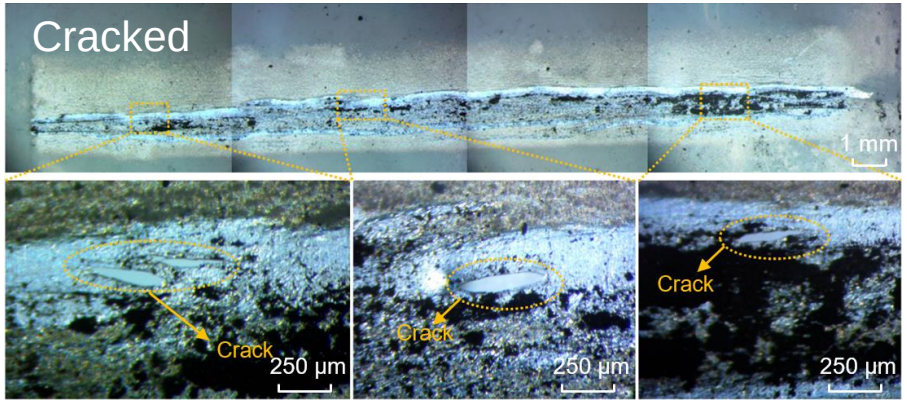
- Cylinder compression





Ex-situ observation of separator morphology





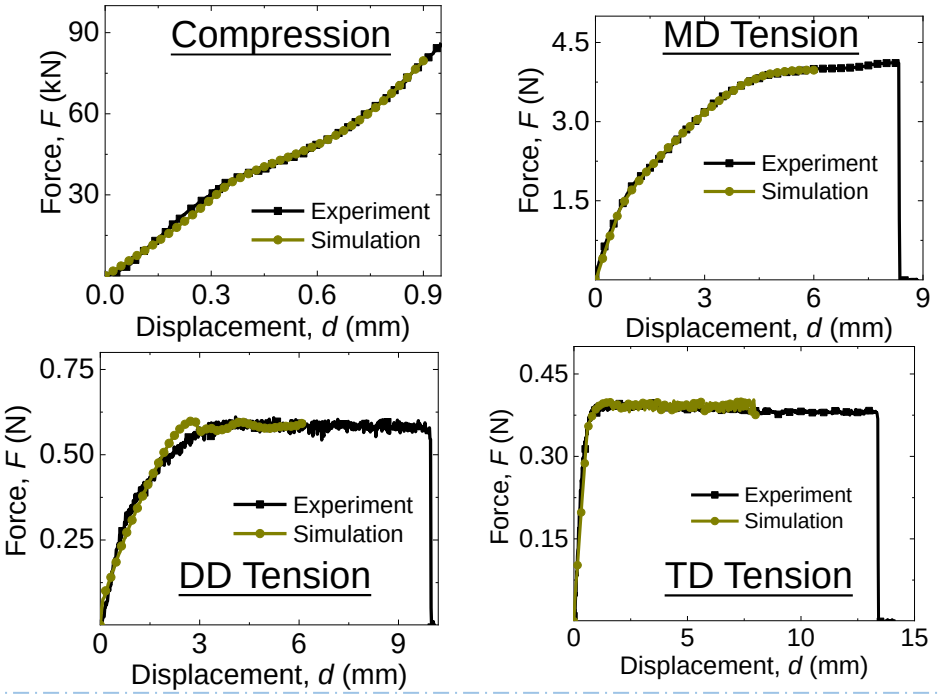
(Yuan, et al. *Journal of Power Sources*, 2020)

Yuan et al., *Journal of Power Sources*, 2020

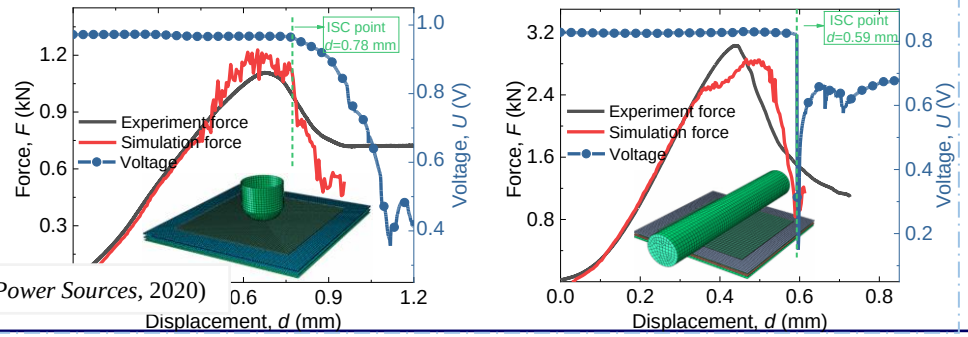
FAILURE BEHAVIOR OF SEPARATOR

Simulation: Separator deformation based short-circuit criteria

Separator anisotropy

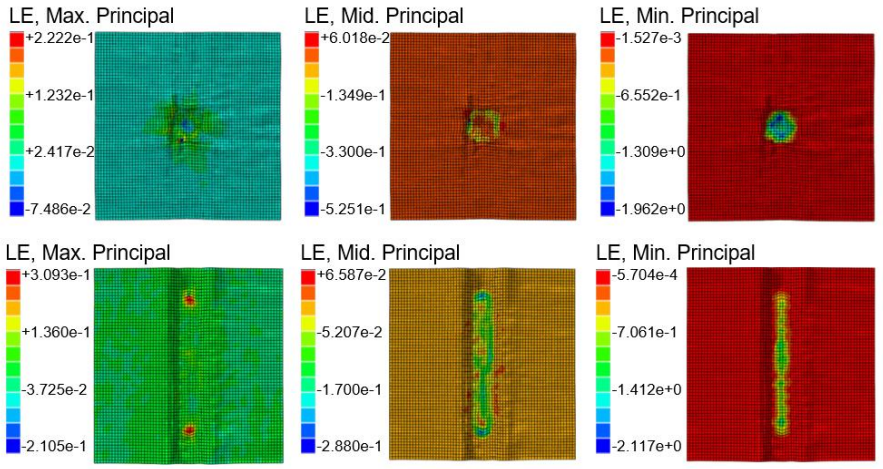


Stack simulation

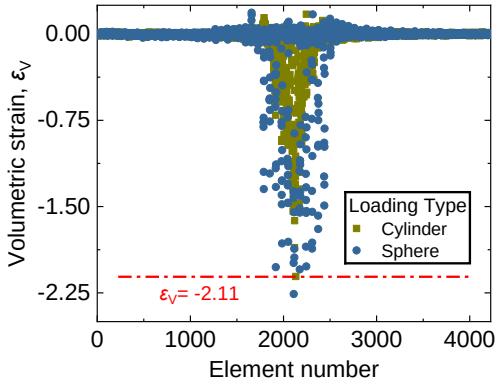


(Yuan, et al. *Journal of Power Sources*, 2020)

Principal strain

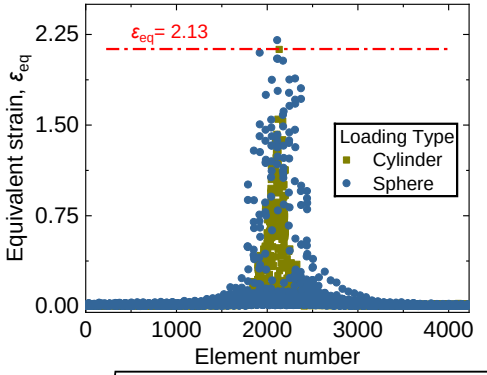


- Volumetric strain criterion

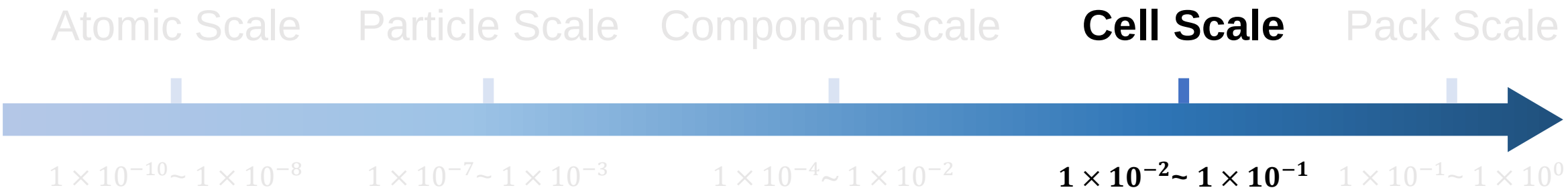


$$\varepsilon_V = J_1 = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$$

- Equivalent strain criterion



$$\varepsilon_{eq} = \sqrt{\frac{1}{2}\left[(\varepsilon_1-\varepsilon_2)^2 + (\varepsilon_2-\varepsilon_3)^2 + (\varepsilon_3-\varepsilon_1)^2\right]}$$

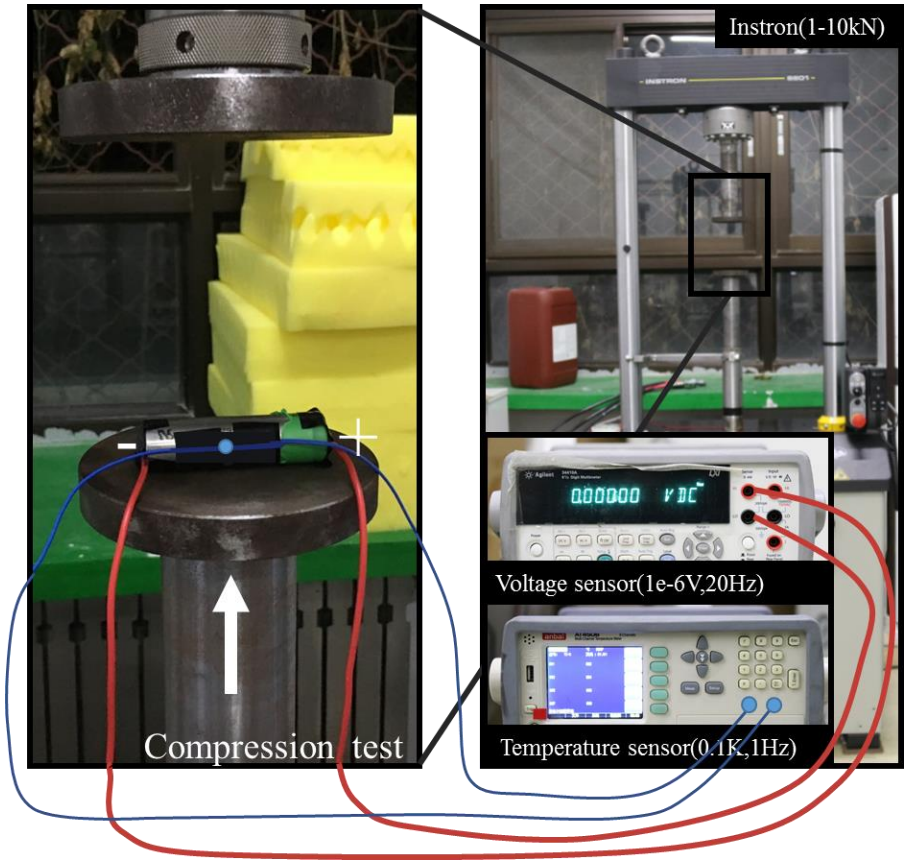

Atomic Scale
Particle Scale
Component Scale
Cell Scale
Pack Scale
$1 \times 10^{-10} \sim 1 \times 10^{-8}$
$1 \times 10^{-7} \sim 1 \times 10^{-3}$
$1 \times 10^{-4} \sim 1 \times 10^{-2}$
$\mathbf{1 \times 10^{-2} \sim 1 \times 10^{-1}}$
$1 \times 10^{-1} \sim 1 \times 10^{0}$

Unit: m

MECHANICAL BEHAVIOR OF STRUCTURE

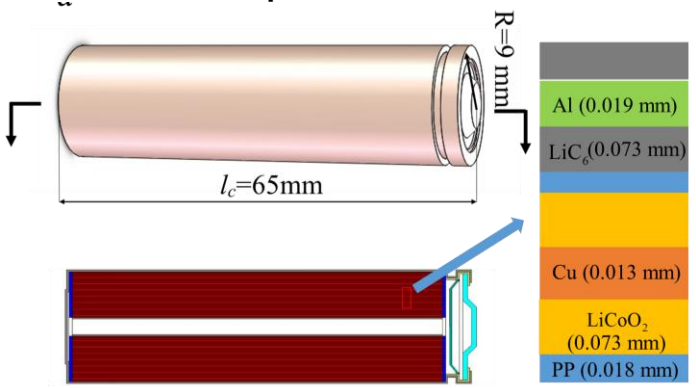
Experiment: Mechanical test of single cell

- Test platform



(Xu et al. *Scientific Reports,* 2016)
(Xu et al. *Experimental Mechanics*, 2018)

- Test samples

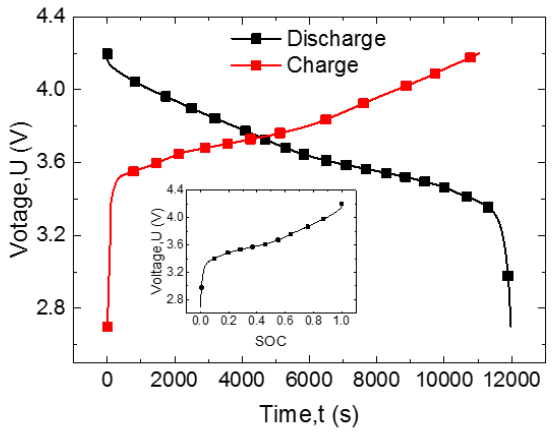


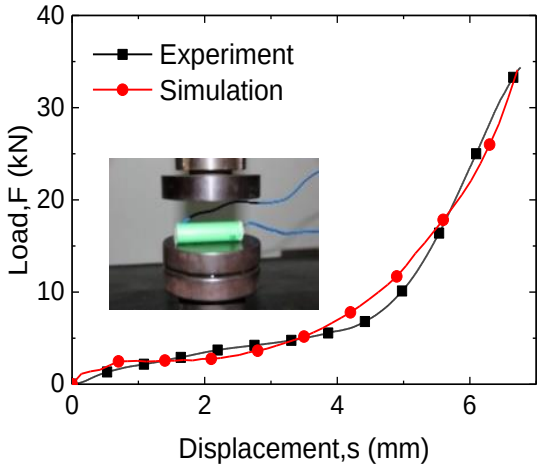
$LiCoO_2$ Battery

$LiFePO_4$ Battery

NCA Battery

- Typical results

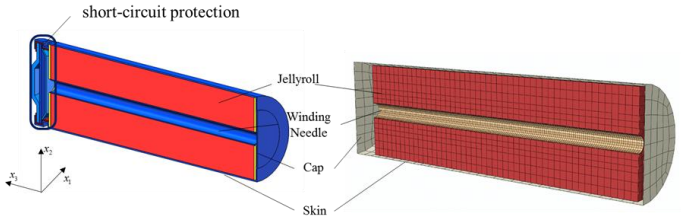




MECHANICAL BEHAVIOR OF STRUCTURE

Modeling: homogenized method and detailed model

Homogenized modeling



Elastic property:

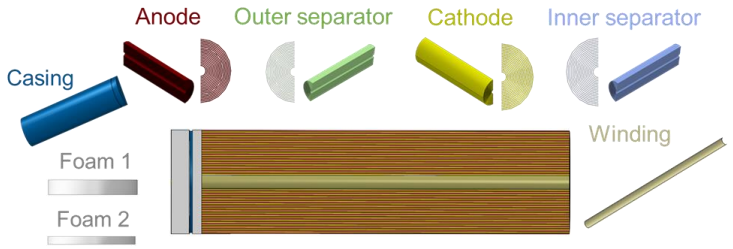
$$\begin{Bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \gamma_{12}\\ \gamma_{23}\\ \gamma_{31}\end{Bmatrix} = \begin{bmatrix} \frac{1}{E_{11}} & -\frac{\nu_{21}}{E_{22}} & -\frac{\nu_{31}}{E_{33}} & 0 & 0 & 0 \\ -\frac{\nu_{12}}{E_{11}} & \frac{1}{E_{22}} & -\frac{\nu_{32}}{E_{33}} & 0 & 0 & 0 \\ -\frac{\nu_{13}}{E_{11}} & -\frac{\nu_{23}}{E_{22}} & \frac{1}{E_{33}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G_{12}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G_{23}} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G_{31}} \end{bmatrix} \begin{Bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \tau_{12}\\ \tau_{23}\\ \tau_{31}\end{Bmatrix}$$

Plastic:

$$\sigma = 930\varepsilon^{3.4} + 0.8$$

$$R = \begin{bmatrix} \frac{\bar{\sigma}_{11}}{\sigma_0} & \frac{\bar{\sigma}_{12}}{\tau_0} & \frac{\bar{\sigma}_{13}}{\tau_0} \\ & \frac{\bar{\sigma}_{22}}{\sigma_0} & \frac{\bar{\sigma}_{23}}{\tau_0} \\ & & \frac{\bar{\sigma}_{33}}{\sigma_0} \end{bmatrix}$$

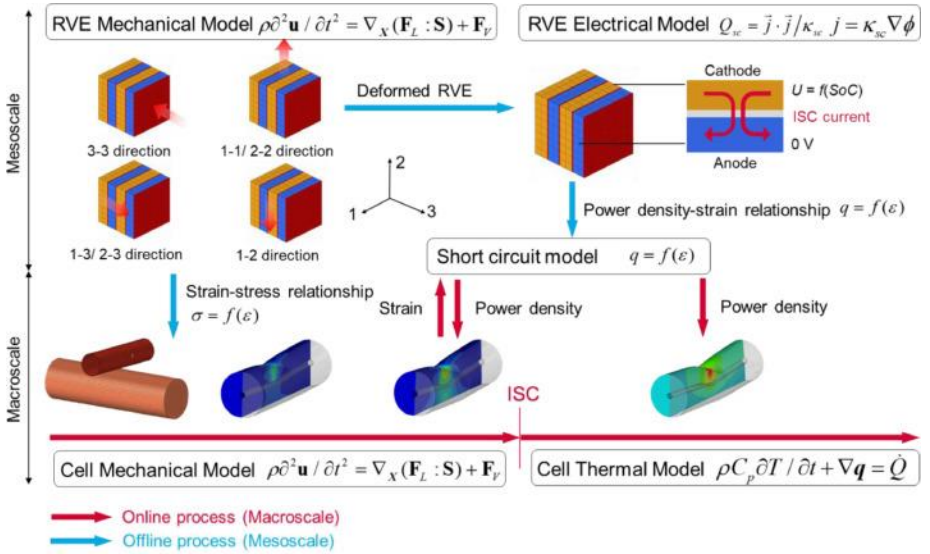
Detailed modeling



mechanical property of each component:

		Density	Modulus	Yield stress	Failure strain
Casing	Steel	7.85e-9	211000	740	η related
Separator	PP/PE	1.2e-9	275	11.39	1
Anode	Cu/Active material	2.27e-9	300	/	/
Cathode	Al/Active material	4.68e-9	720	/	/
Winding	Steel	7.85e-9	100000	2430	/
Foam	/	6.5e3	100	/	/

RVE modeling

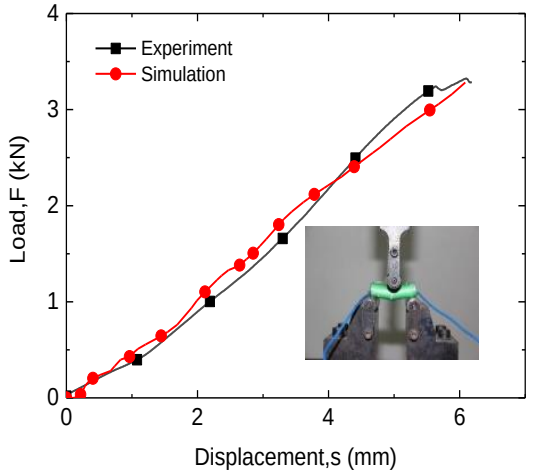


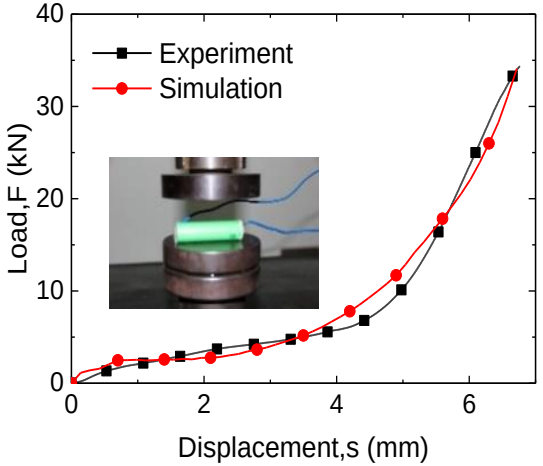
(Liu, et al. *Applied Energy*, 2016)
(Wang et al., *Journal of Power Sources*, 2019)
(Jia et al., *Journal of Energy Storage*, 2021)

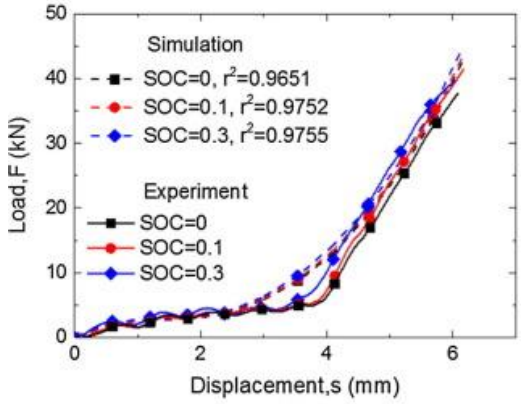
MECHANICAL BEHAVIOR OF STRUCTURE

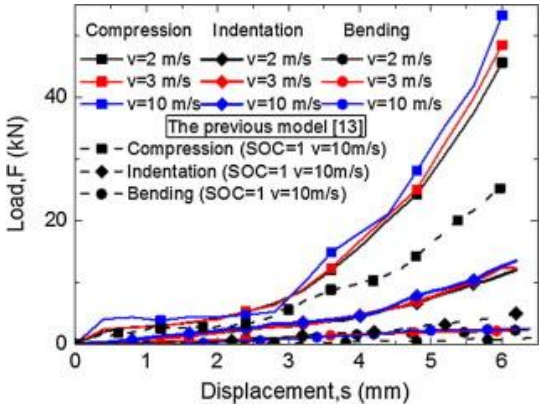
Simulation: various abusive loading conditions

- Simulation results by homogenized model



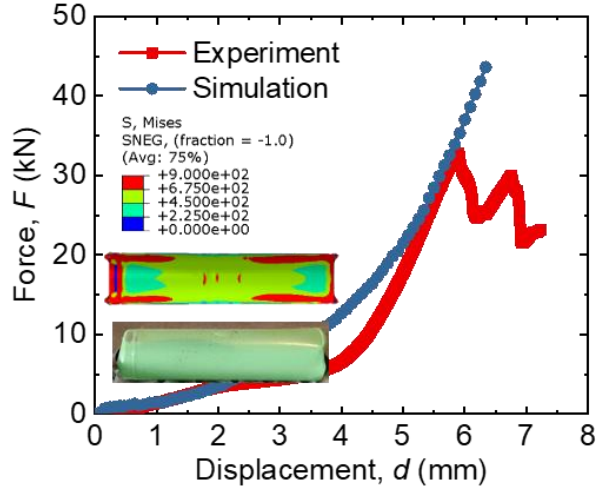


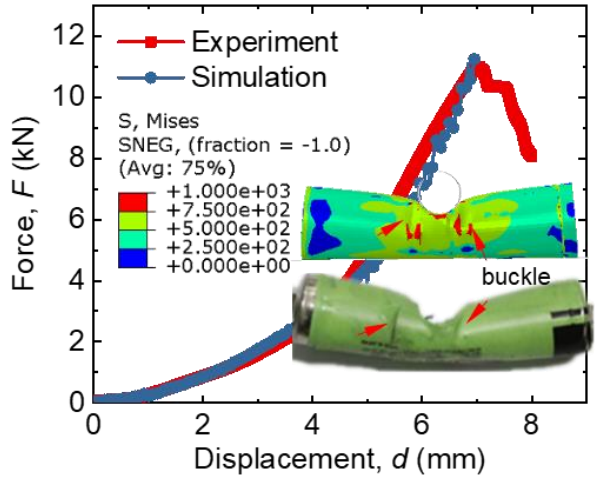


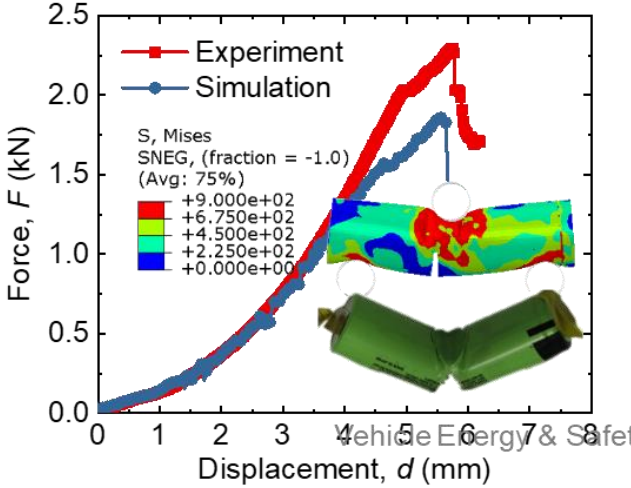


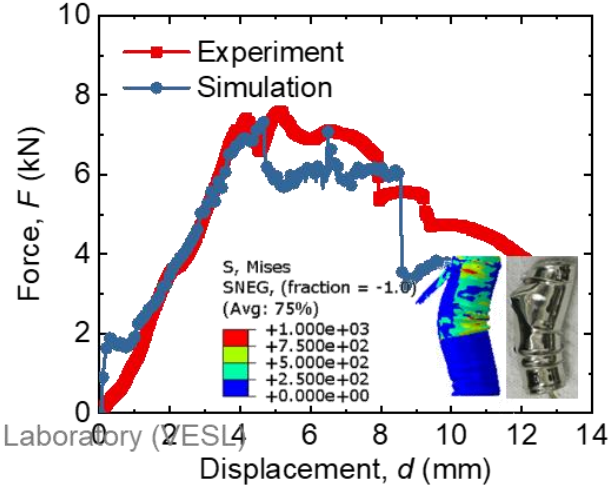
(Liu, et al. *Applied Energy*, 2016)
(Wang et al. *Journal of Power Sources*, 2019)

- Simulation results by detailed model

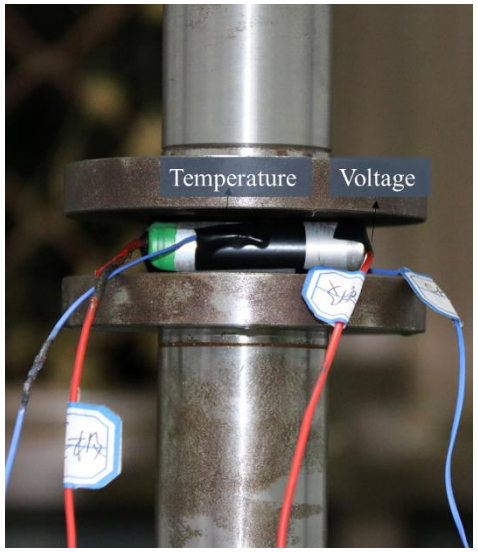








MULTIPHYSICS BEHAVIOR OF LIBS



(Liu, et al. *Electrochimica Acta*, 2017)

Multiphysics modeling strategy

1D battery model

Anode — Separator — Cathode

$$\varepsilon^l \frac{\partial c^l}{\partial t} = -D^l_{eff} \nabla c^l + \frac{i^l t_+}{F}$$

$$i^l = -\kappa^l_{eff} \nabla \phi^l + \frac{2\kappa^l_{eff} R_g T}{F}\left(1 + \frac{\mathrm{d}\ln F}{\mathrm{d}\ln c^l}\right)(1 - t_+)\nabla \ln c^l$$

$U^{1D} = U^{St}$

$A^{1D} i^{1D} = I^{St}$

Short circuit model

Anode — Separator — Cathode

$$\vec{E} = -\vec{\nabla}\phi \qquad \vec{j} = \kappa^{St}\vec{\nabla}\phi$$

$$Q_{St} = \frac{\vec{j}\cdot\vec{j}}{\kappa^{St}}$$

Q_{1D}

$T^{Tm}_a(t) = T^{1D}_a(t)$

Q_{St}

$x_q(t) = x(t)\cdot c(\sigma_1(t) - \sigma_3(t))$

$R^{St}_r = z(1 - S^*_{st})$

Thermal model

$$d_z \rho^{LB} C^{LB}_p \frac{\partial T}{\partial t} + d_z \rho^{LB} C^{LB}_p \upsilon \nabla T + \nabla \cdot d_z q = d_z Q_s$$

Q_{tr}

$T^{Tm}(t) = T^{Tr}(t)$

$T^{Me}(t) = T^{Tm}(t)$

$v^{Me}(t) = v^{Tm}(t)$

Thermal runaway model

$$Q^{sei} = H^{sei} W_c A^{sei} \exp\left[\frac{-E^{sei}_a}{R_g T}\right] c_{sei}$$

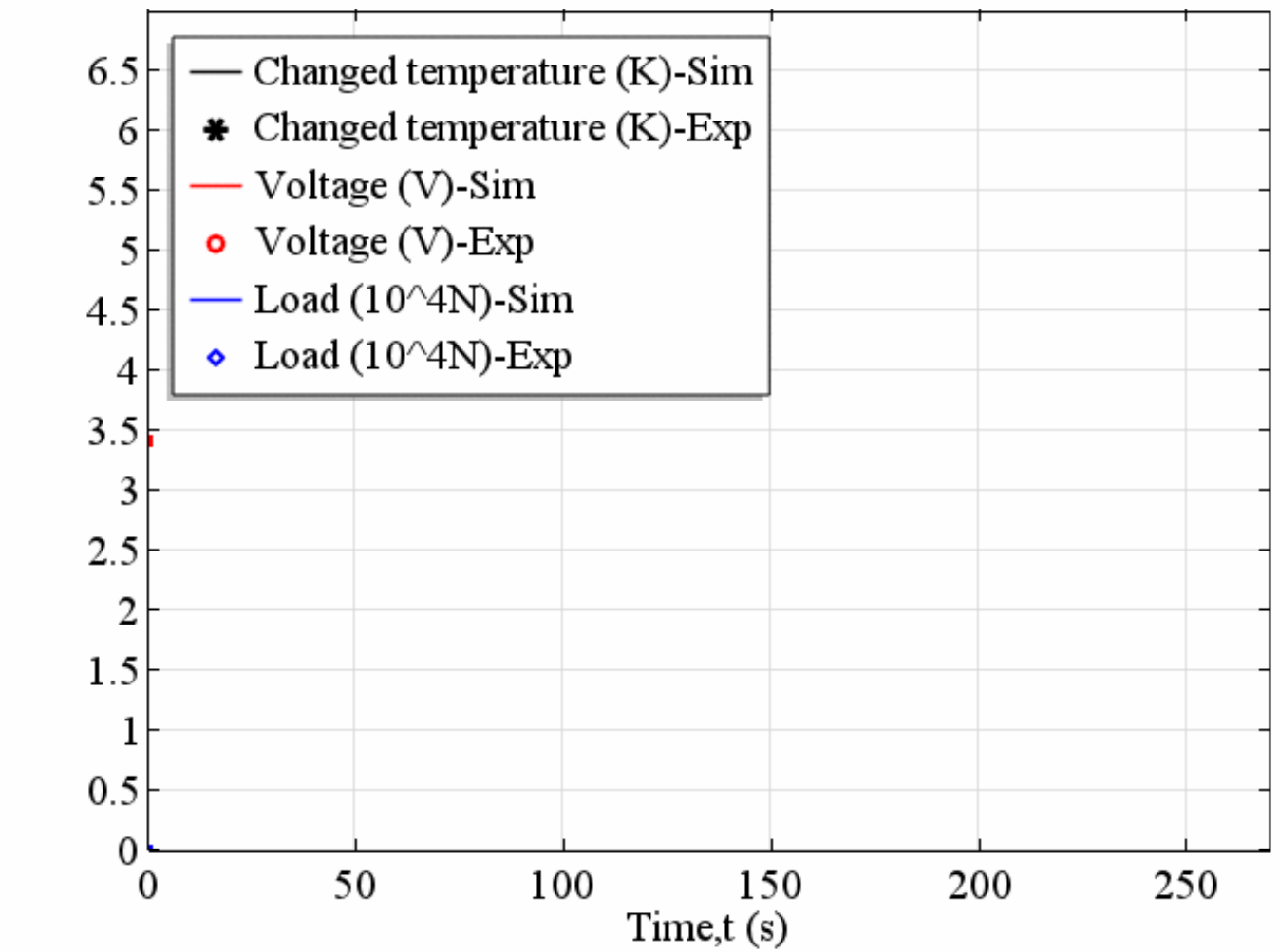
$$\frac{dc_{sei}}{dt} = -A^{sei} \exp\left[\frac{-E^{sei}_a}{R_g T}\right] c_{sei}$$

Mechanical model

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla_X (F_L S) + F_V$$

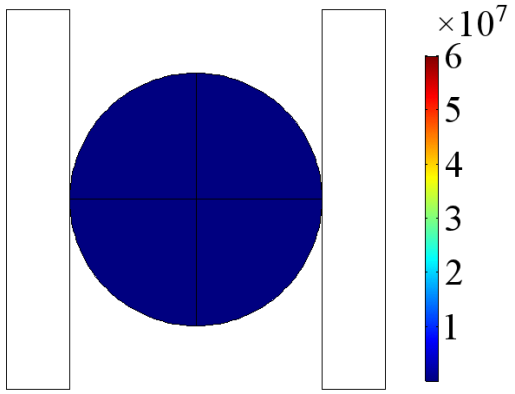
Force — Elastic-plastic model — Fixed

MULTIPHYSICS BEHAVIOR OF LIBS

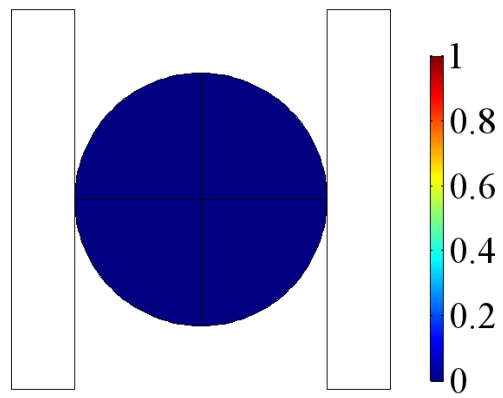


(Liu, et al. *Electrochimica Acta,* 2017)

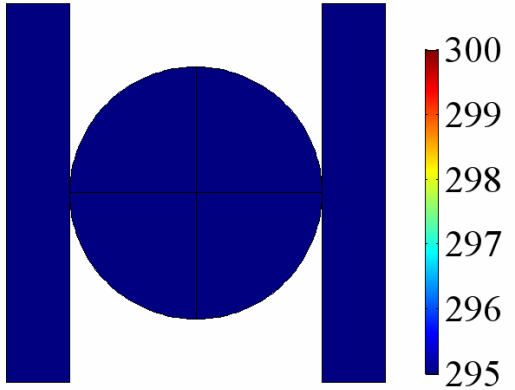
Tresca stress (Pa)



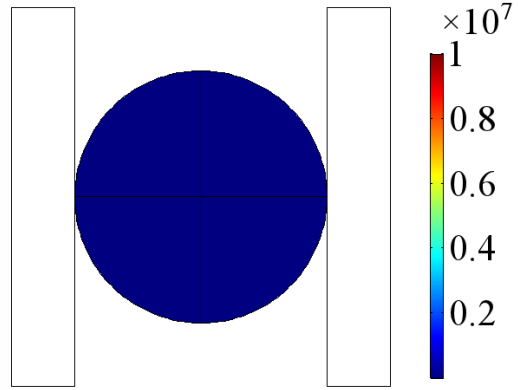
Short circuit position



Temperature (K)

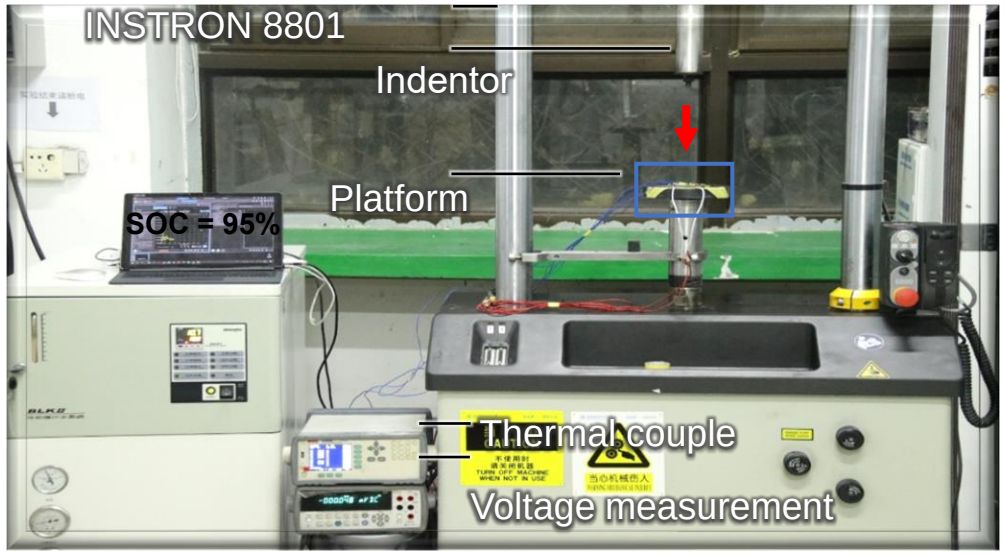


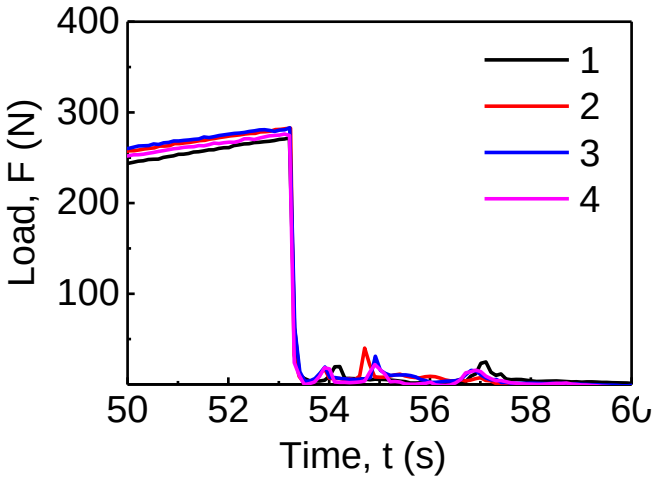
Thermal runaway heat

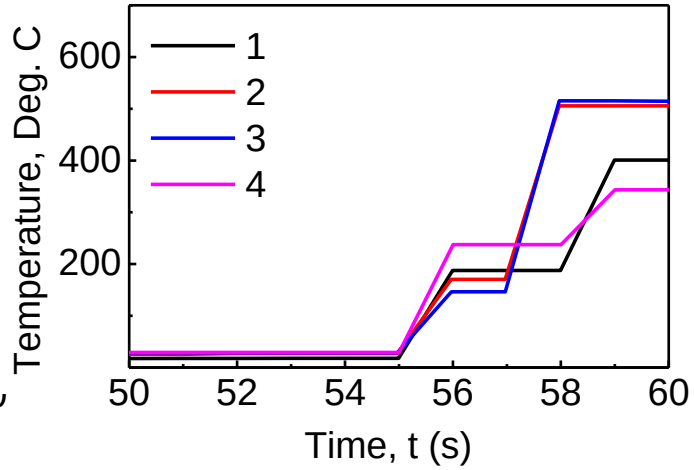


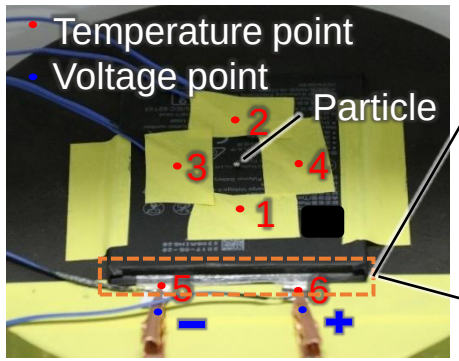
ISC EVOLUTION

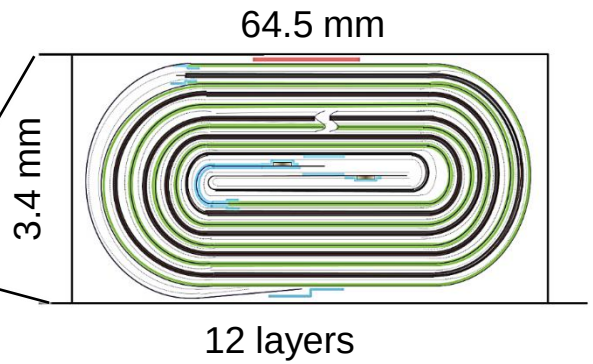
Experiment: *In-situ* particle indentation of a cell

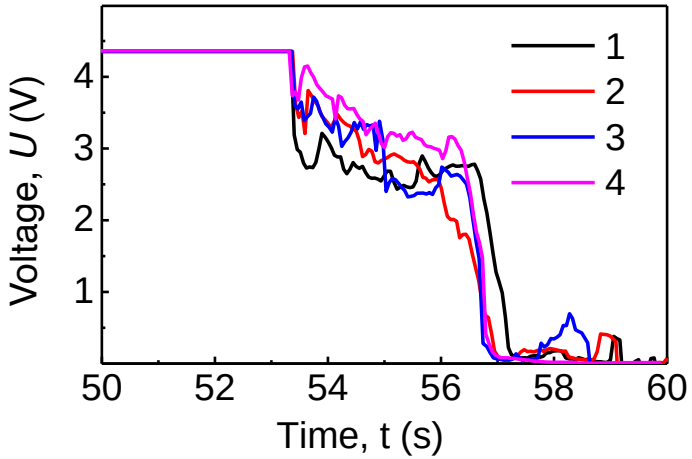












Comparing force/voltage/thermal

Highly repeatable experiment

(Liu and Jia et al. *Journal of Materials Chemistry A*, 2018)

ISC EVOLUTION

Multiphysics model → Prediction of mechanical, electrochemical & thermal behavior after short-circuit

Mechanical model

$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \nabla_x (F_L S) + \mathrm{F}_V$$

Thermal runaway model

$$\frac{dc^{sei}}{dt} = -A^{sei} \exp[\frac{-E_a^{sei}}{R_g T}] c_{sei}$$

Deformation

Heat

Temperature

Stress status

Heat model

$$\rho C_p (\frac{\partial T}{\partial t} + u_{trans} \cdot \nabla T) + \nabla (q + q_r) = Q$$

Temperature

Heat

Temperature

Heat

Short circuit model

$$j = \kappa^{St} \nabla \phi \qquad R_{st} = \frac{1}{\kappa^{St}}$$

Current

Voltage

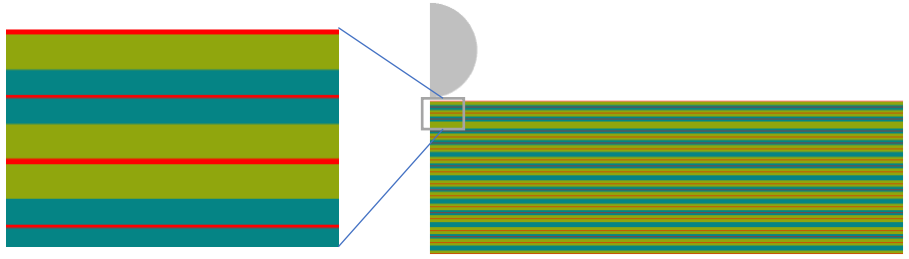
Battery model

$$i_{cell} = \frac{\Delta \phi}{R_{sol}} \qquad \frac{\partial c_s}{\partial t} = \nabla \cdot (-D_s \nabla c_s)$$

$$E_{cell} = \phi_s^{pos} - \phi_s^{neg} \qquad Q_{h,cell} = Q_{h,pos} + Q_{h,sol}$$

(Liu and Jia et al. *Journal of Materials Chemistry A*, 2018)

Detailed components



Separator and current collector melting

Melting

$$\frac{dc_{sep}}{dt} = -A^{sep} \exp[\frac{-E_a^{sep}}{R_g T}] c_{sep}$$

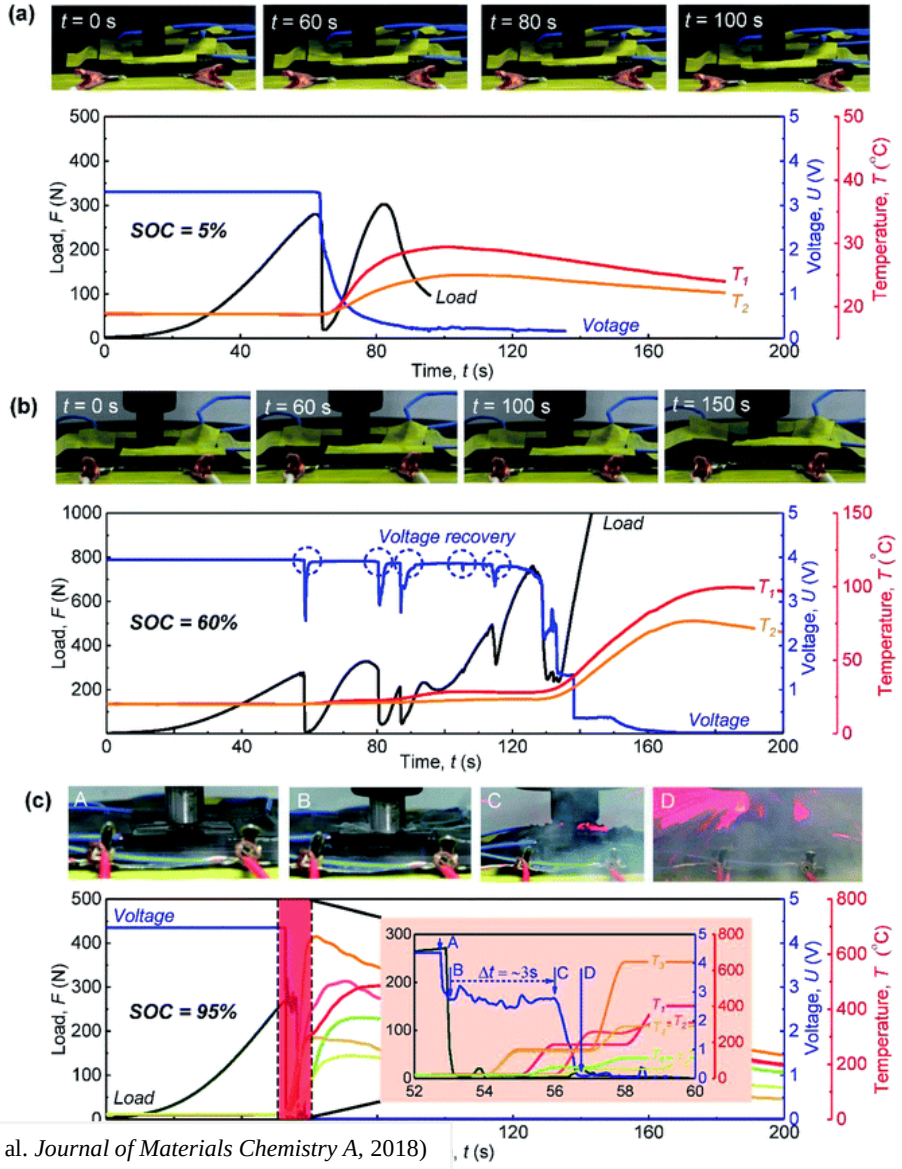
$$\frac{dc_{cc}}{dt} = -A^{cc} \exp[\frac{-E_a^{cc}}{R_g T}] c_{cc}$$

Resistance change

$$\kappa^{cc} = \kappa_0^{cc} c_{cc} + \kappa_e^{cc}$$

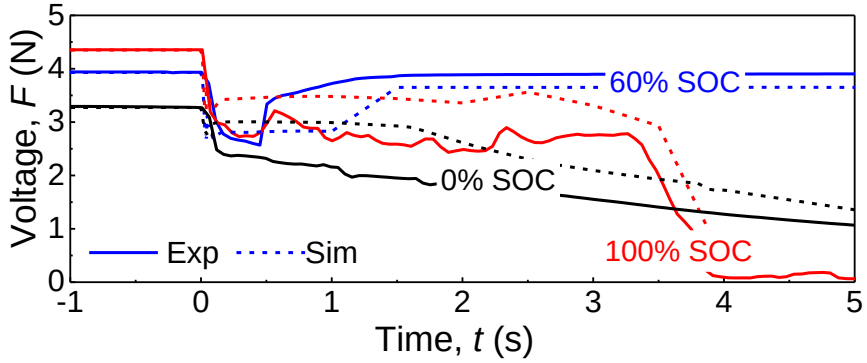
$$\kappa^{sep} = \kappa_e^{sep} * (1 - c_{sep}) + \kappa_0^{sep}$$

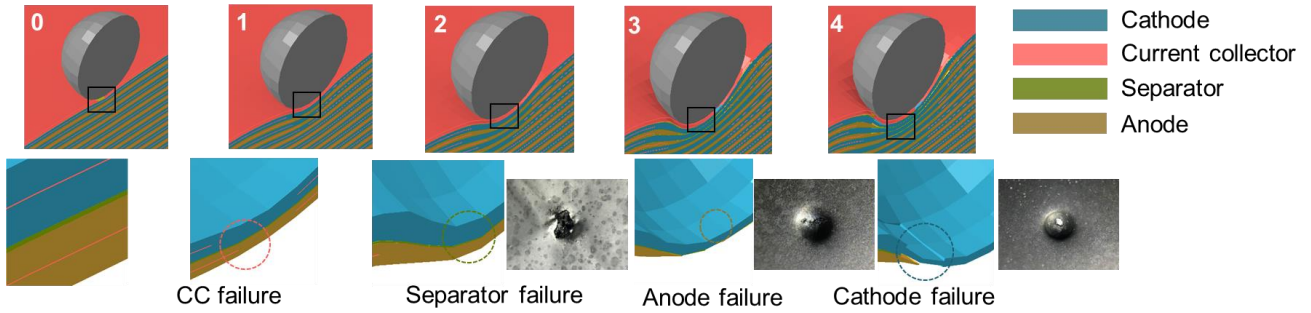
ISC EVOLUTION

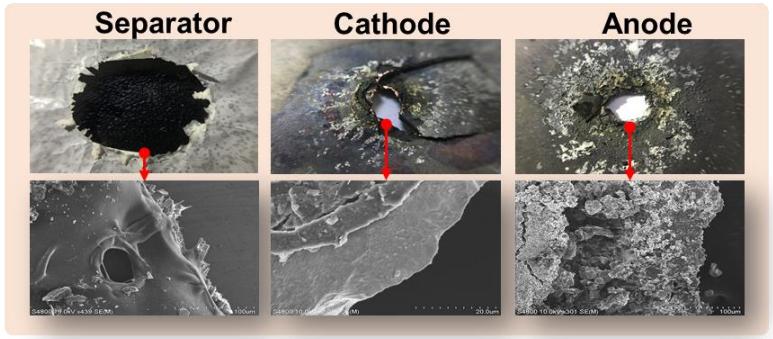


(Liu and Jia et al. *Journal of Materials Chemistry A*, 2018)

Computation: Internal short circuit (ISC) analysis





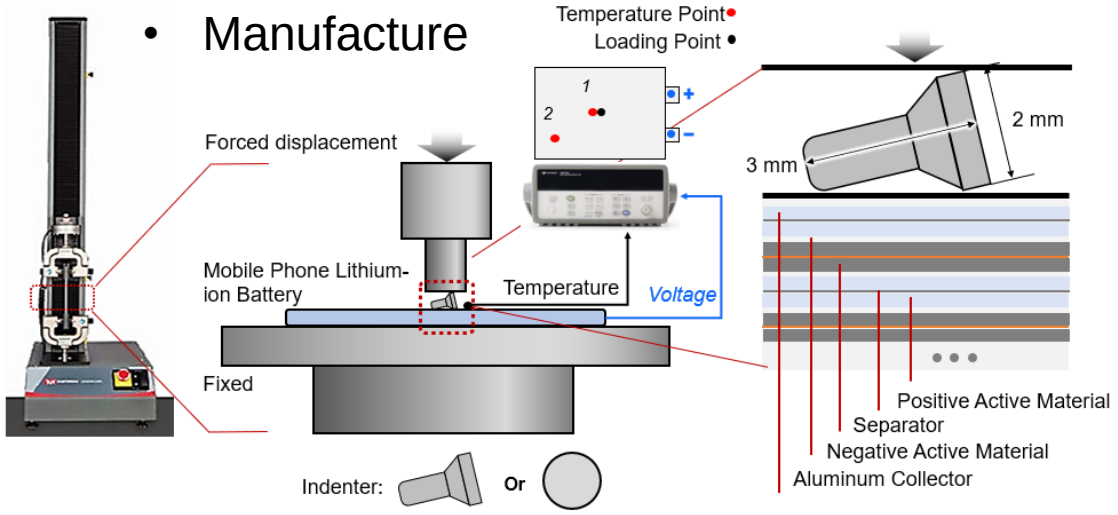


Indications from computational model

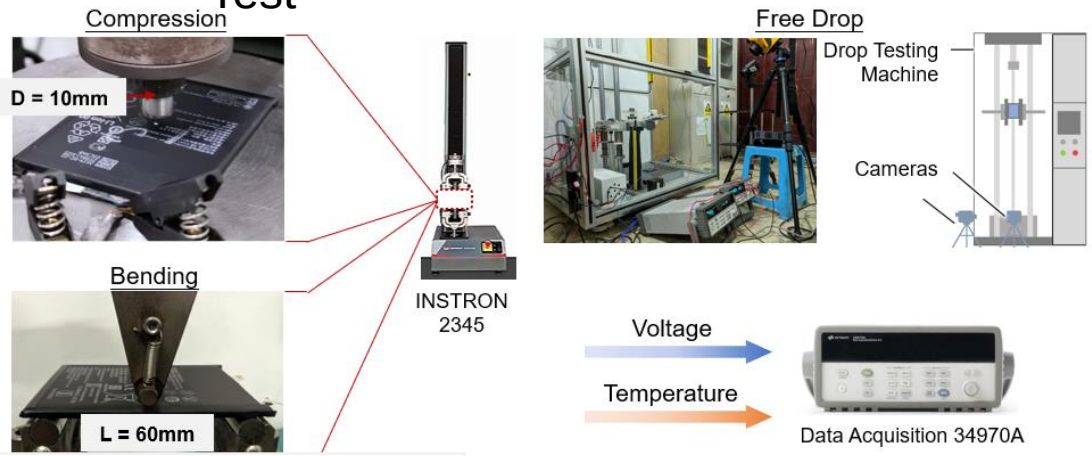
SAFETY EVALUATION OF DEFECTIVE BATTERY

Experiment: Manufacture/test of defective battery

- Manufacture



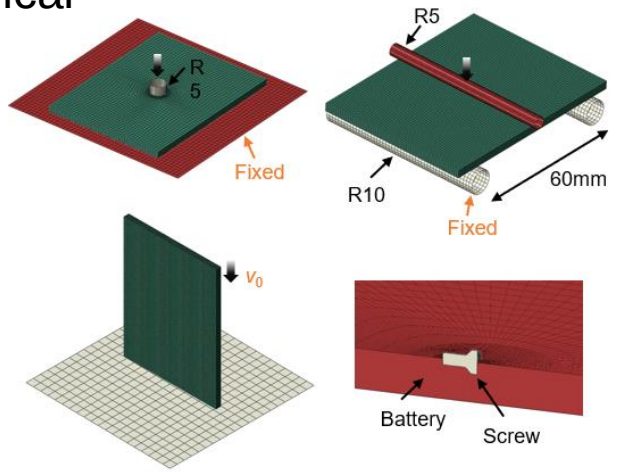
- Test



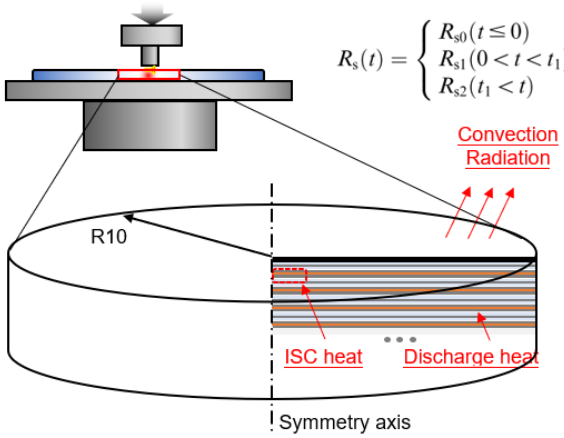
(Jia et al. *Journal of Materials Chemistry A*, 2020)

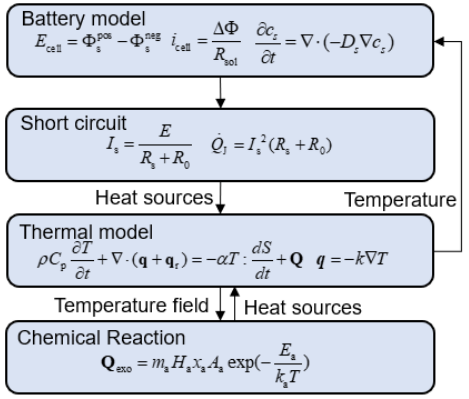
Modeling: Mechanical & multiphysics models

- Mechanical



- Multiphysics

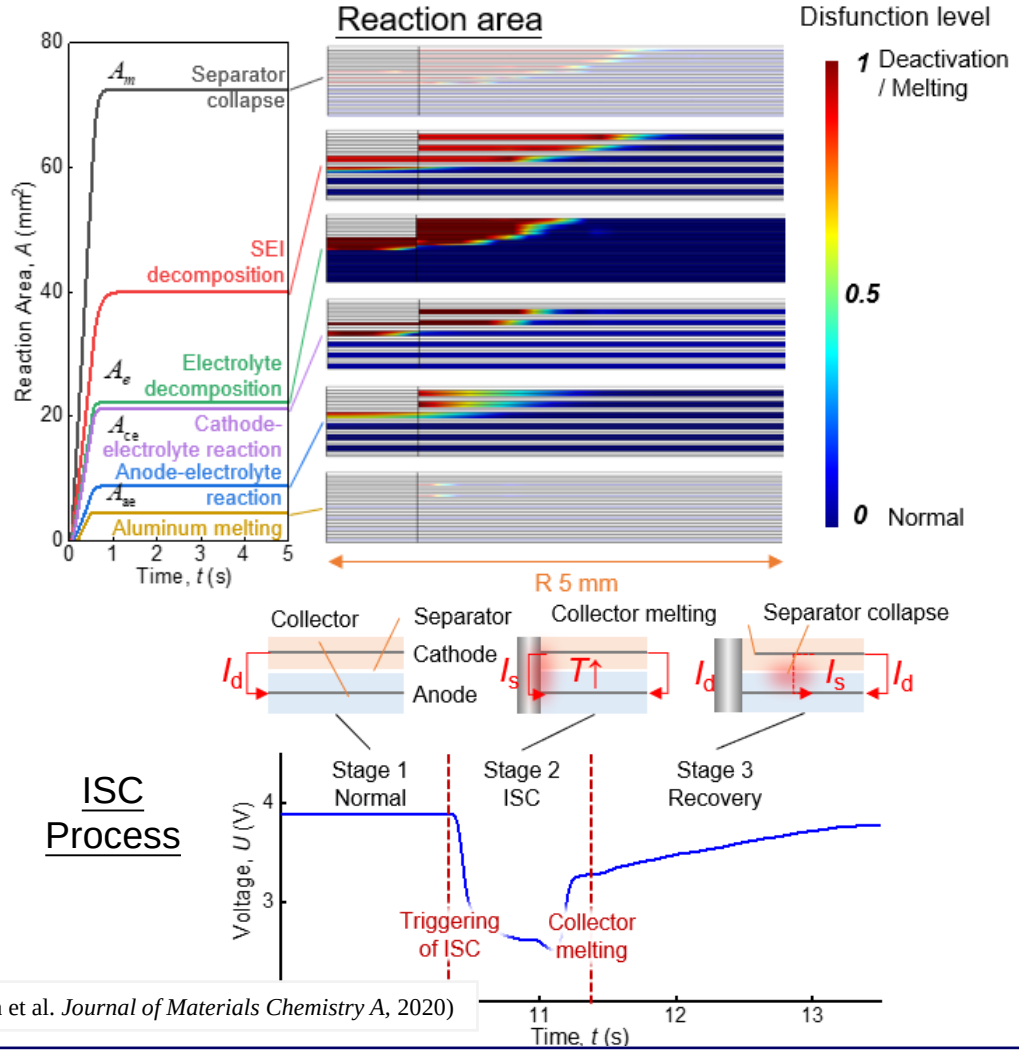




SAFETY EVALUATION OF DEFECTIVE BATTERY

Simulation: Risk evaluation

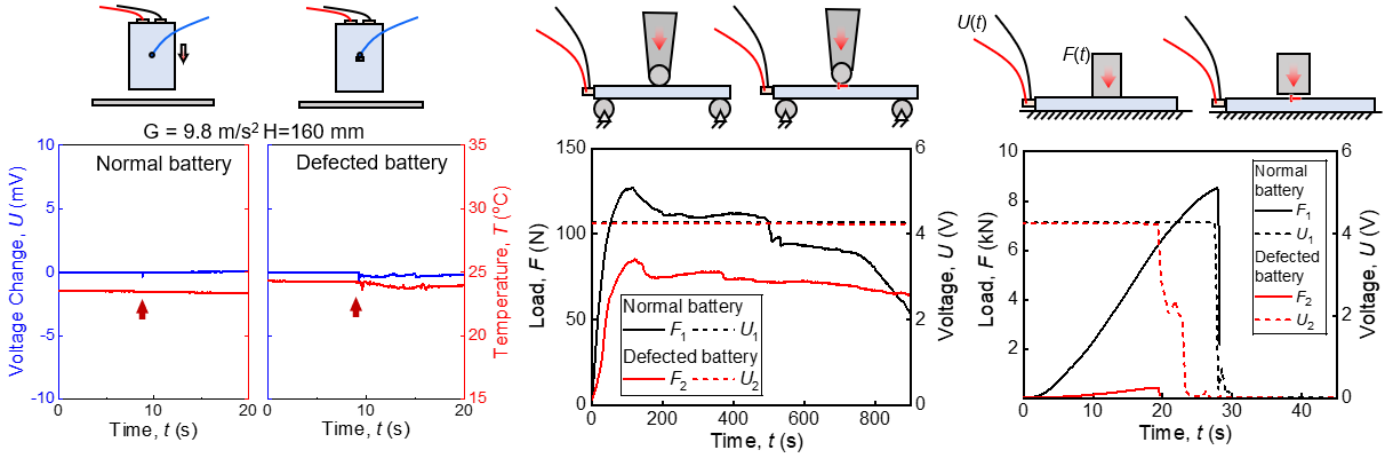
- Mechanisms (defection introduction process)



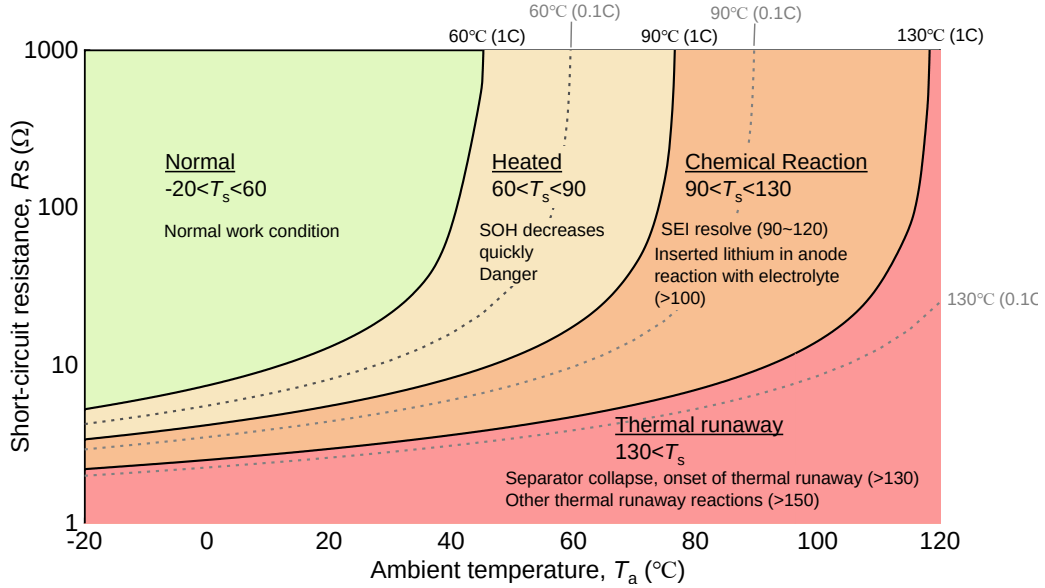
ISC Process

(Jia et al. *Journal of Materials Chemistry A*, 2020)

- Mechanical safety evaluation



- Electrochemical-thermal safety evaluation

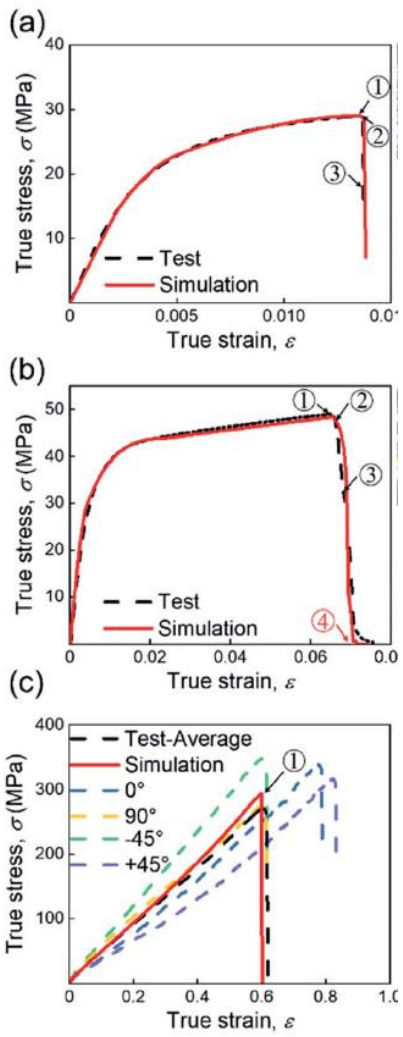


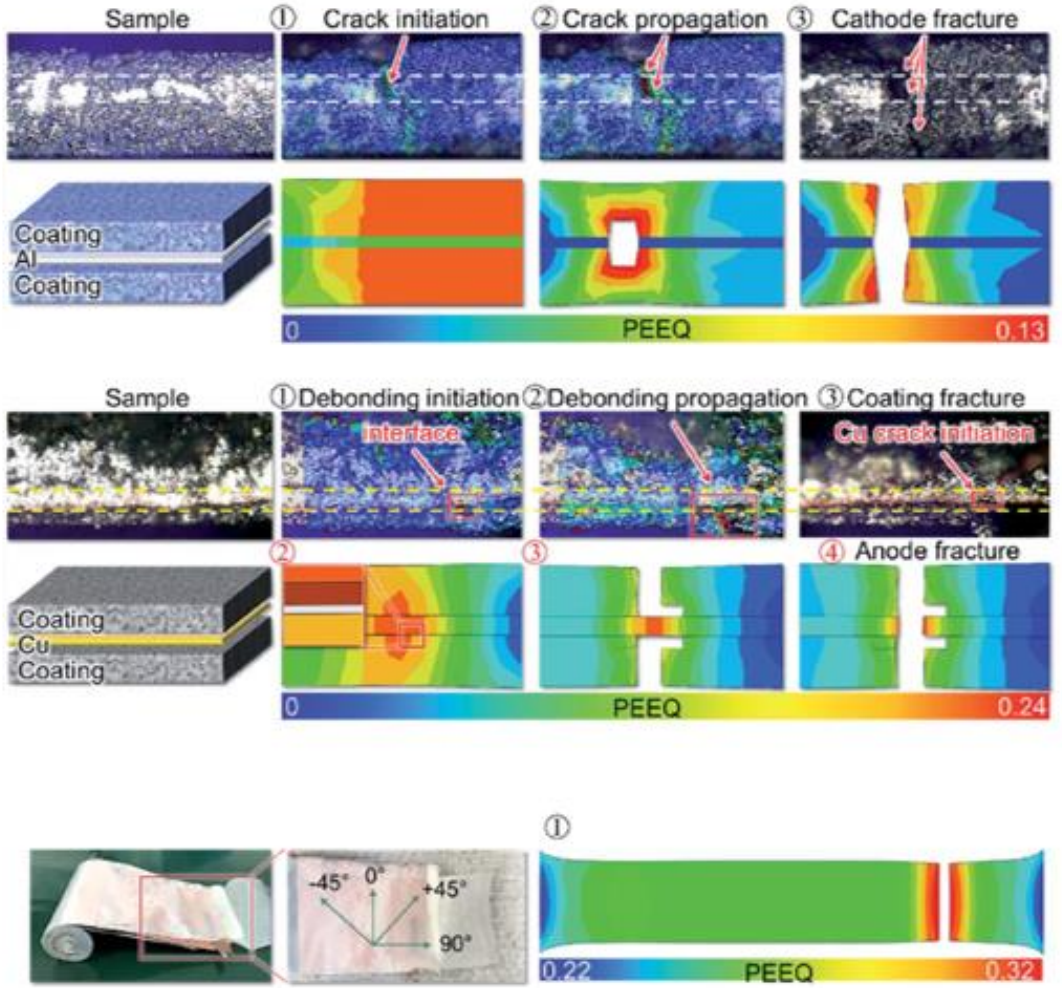
STRESS-DRIVEN SHORT-CIRCUITS

Experiment & Simulation: Mechanical behavior characterization of components

❑ In-plane tension

- Cathode
- Anode
- Separator





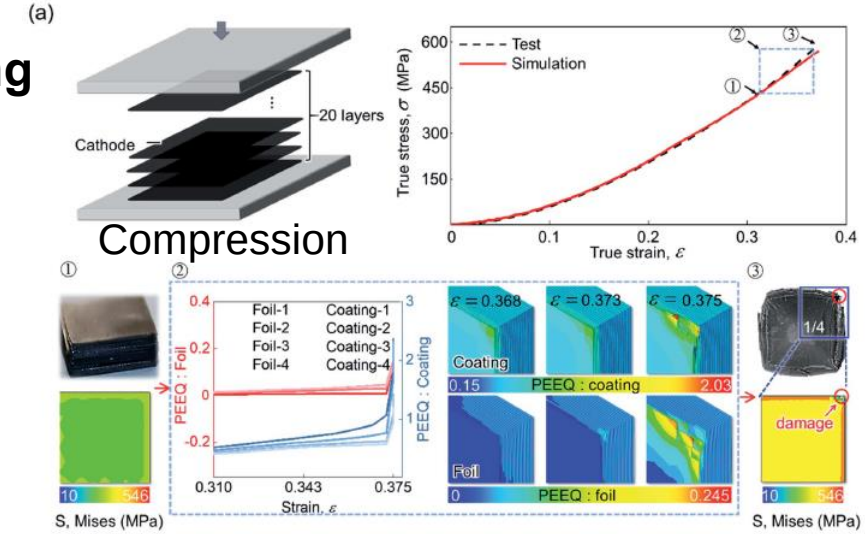
(Liu & Duan et al. *Journal of Materials Chemistry A*, 2021)

STRESS-DRIVEN SHORT-CIRCUITS

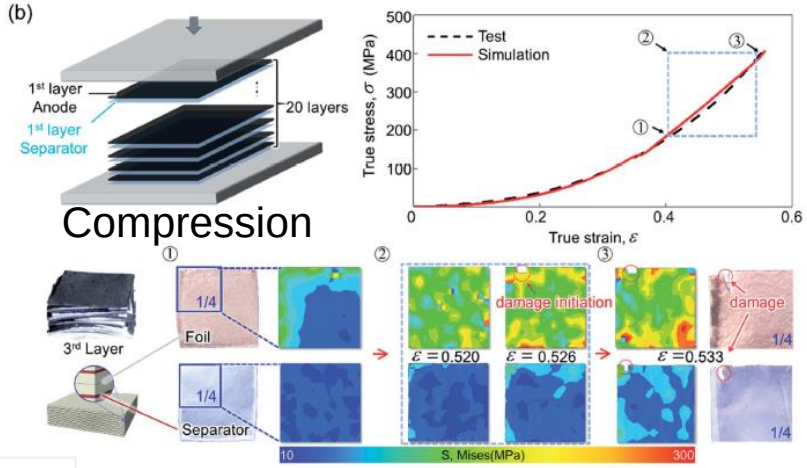
Experiment & Simulation: Mechanical behavior characterization of components

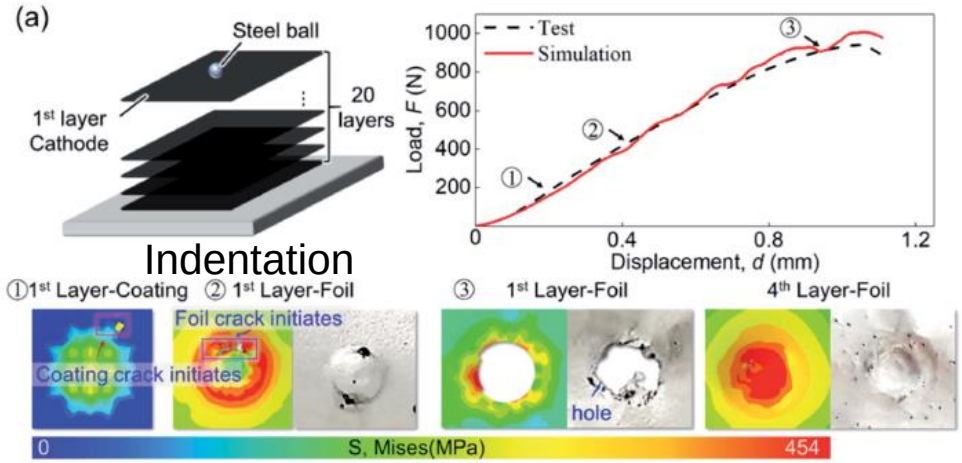
❑ Out-of-plane loading

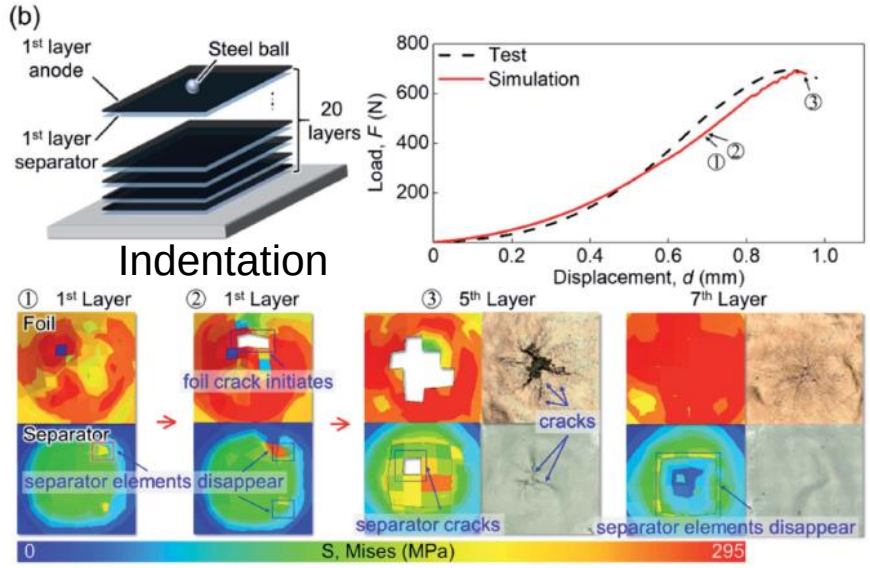
- Cathode



- Anode + separator





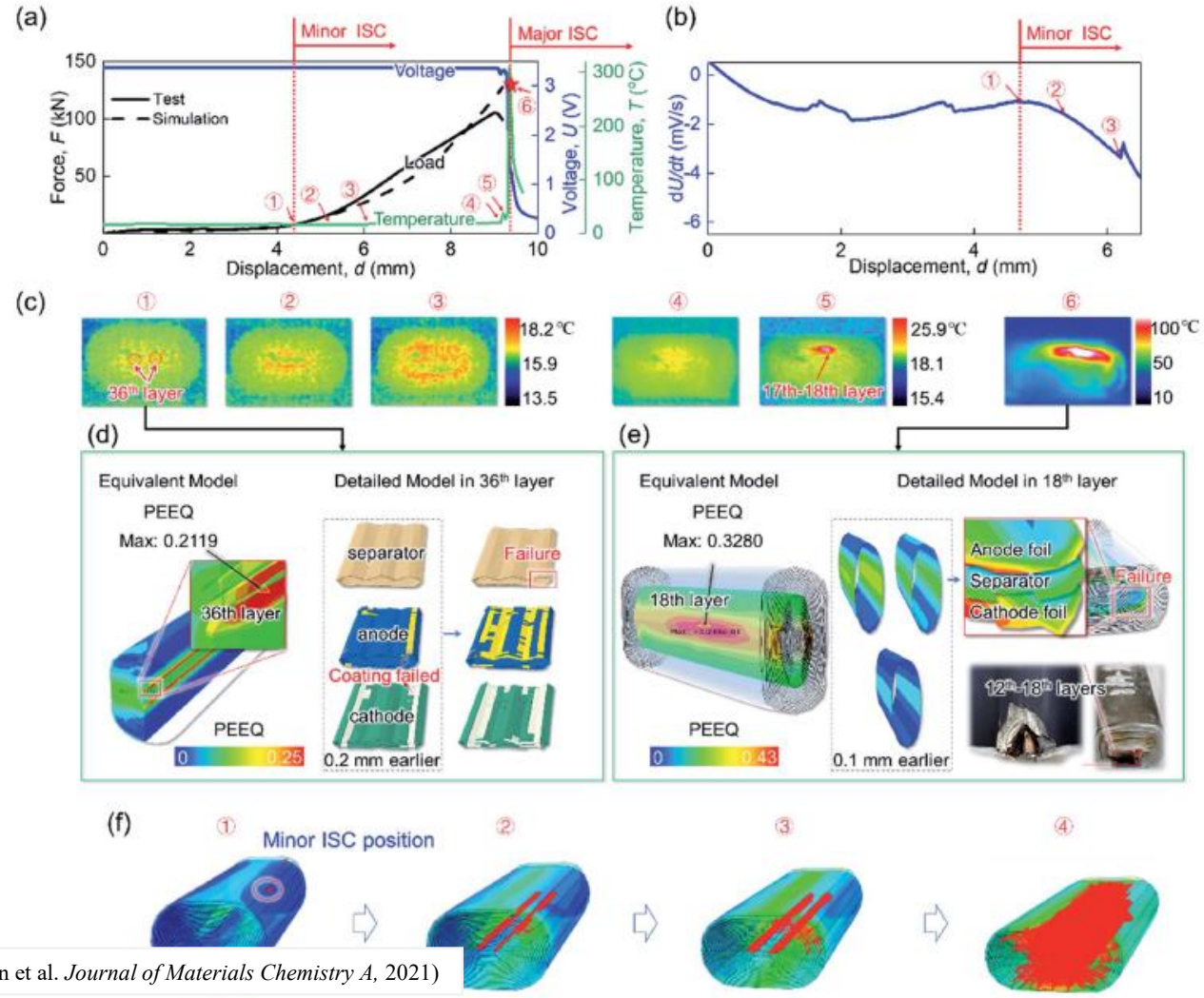


(Liu & Duan et al. *Journal of Materials Chemistry A,* 2021)

STRESS-DRIVEN SHORT-CIRCUITS

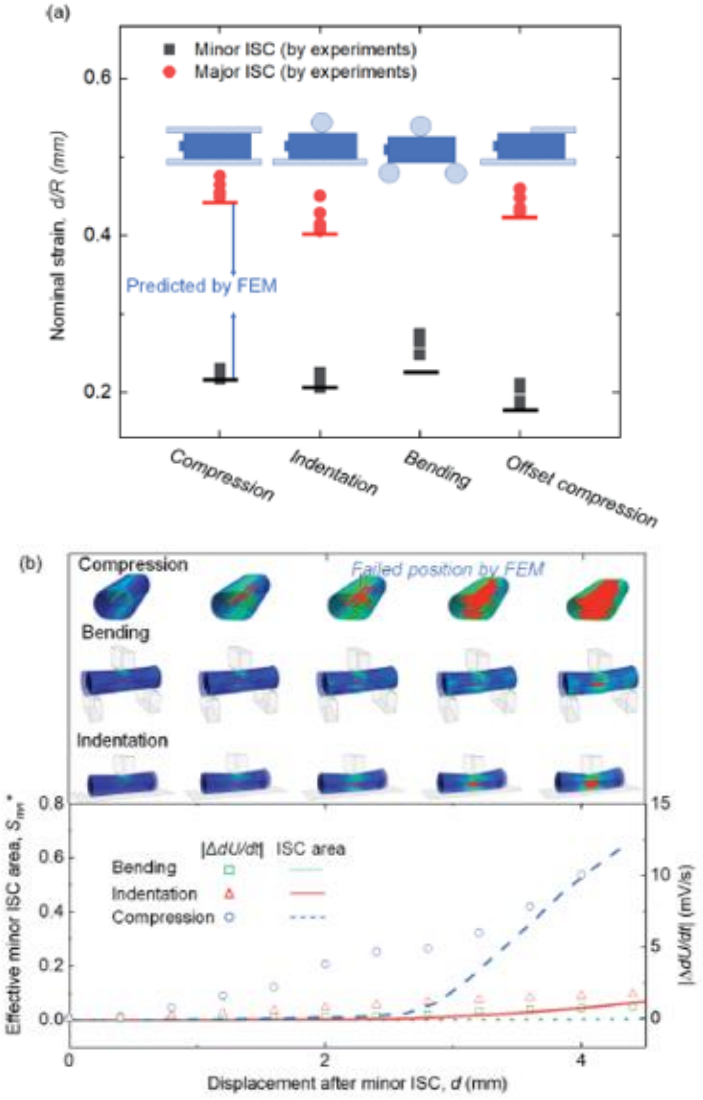
Experiment & Simulation: Short-circuit behavior and criteria

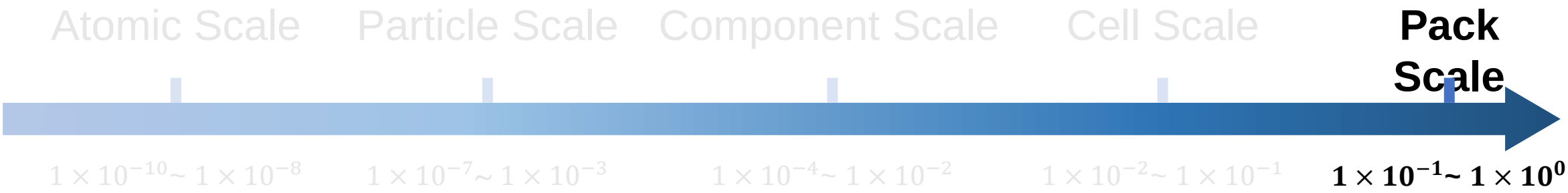
- Short-circuit behavior



(Liu & Duan et al. *Journal of Materials Chemistry A,* 2021)

- PEEQ based short-circuit criteria

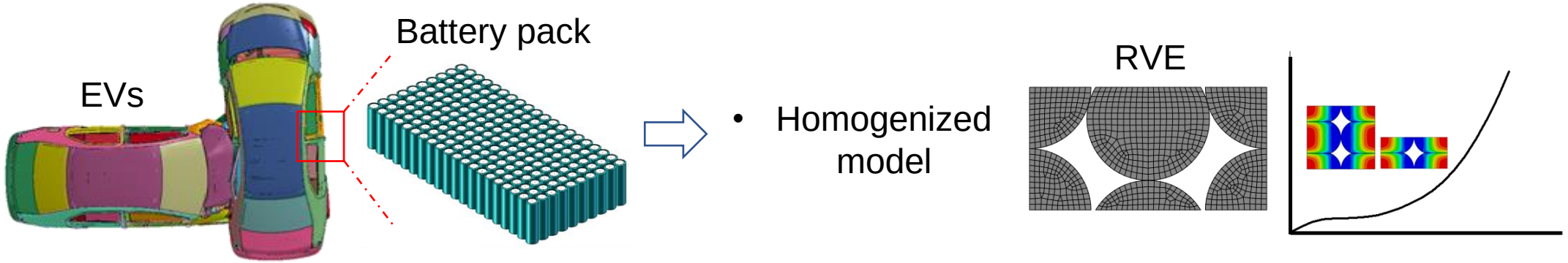



Atomic Scale
Particle Scale
Component Scale
Cell Scale
Pack Scale
$1 \times 10^{-10} \sim 1 \times 10^{-8}$
$1 \times 10^{-7} \sim 1 \times 10^{-3}$
$1 \times 10^{-4} \sim 1 \times 10^{-2}$
$1 \times 10^{-2} \sim 1 \times 10^{-1}$
$\mathbf{1 \times 10^{-1} \sim 1 \times 10^{0}}$

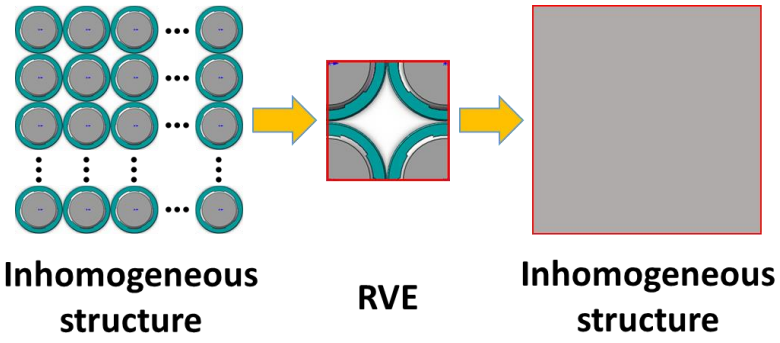
Unit: m

HOMOGENIZATION OF BATTERY PACK

Modeling: homogenized methodology

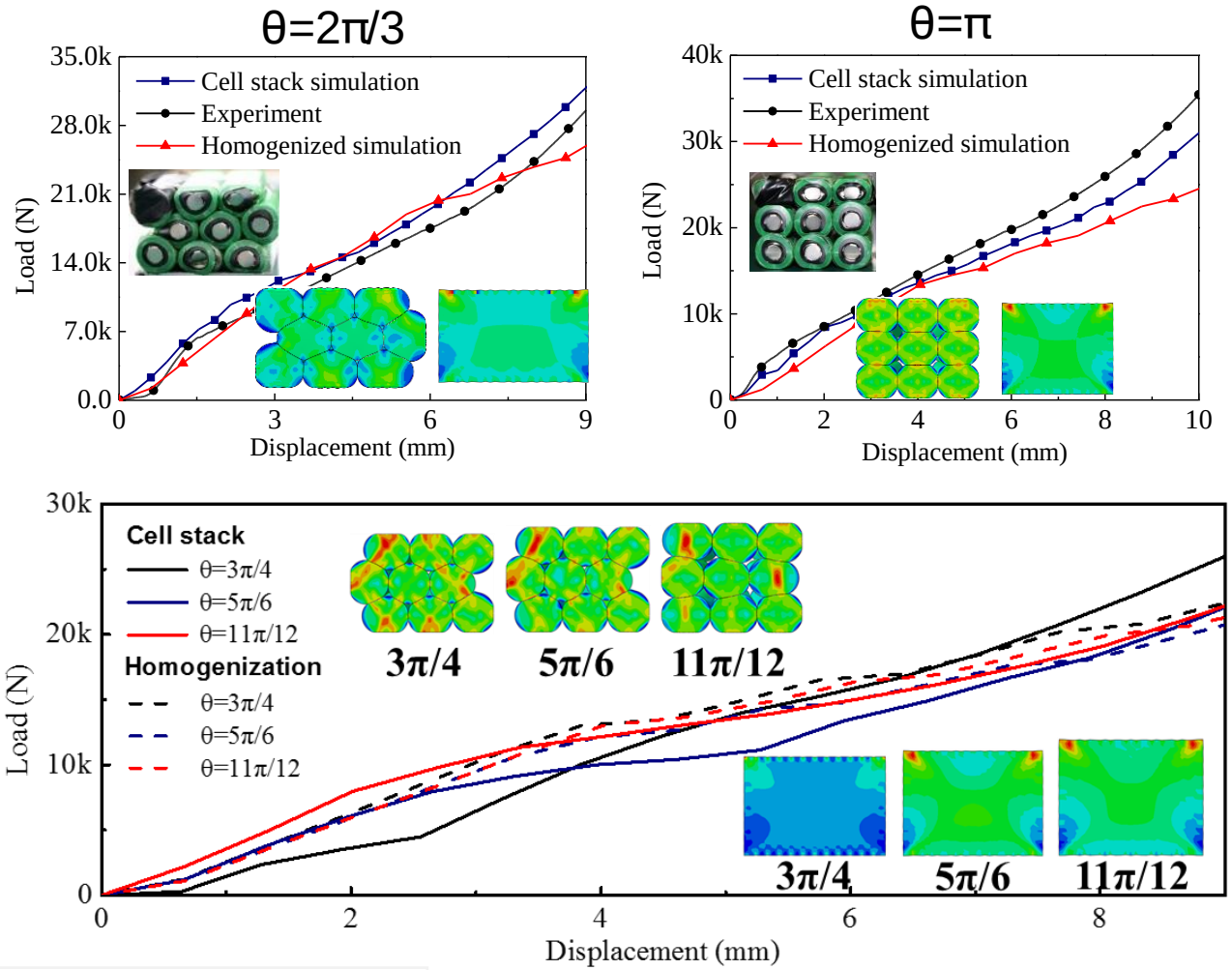


Battery pack → RVE (Representative Volume Element) module with periodic boundary conditions → RVE module compression simulation → Stress-strain data → Equivalent model for battery pack

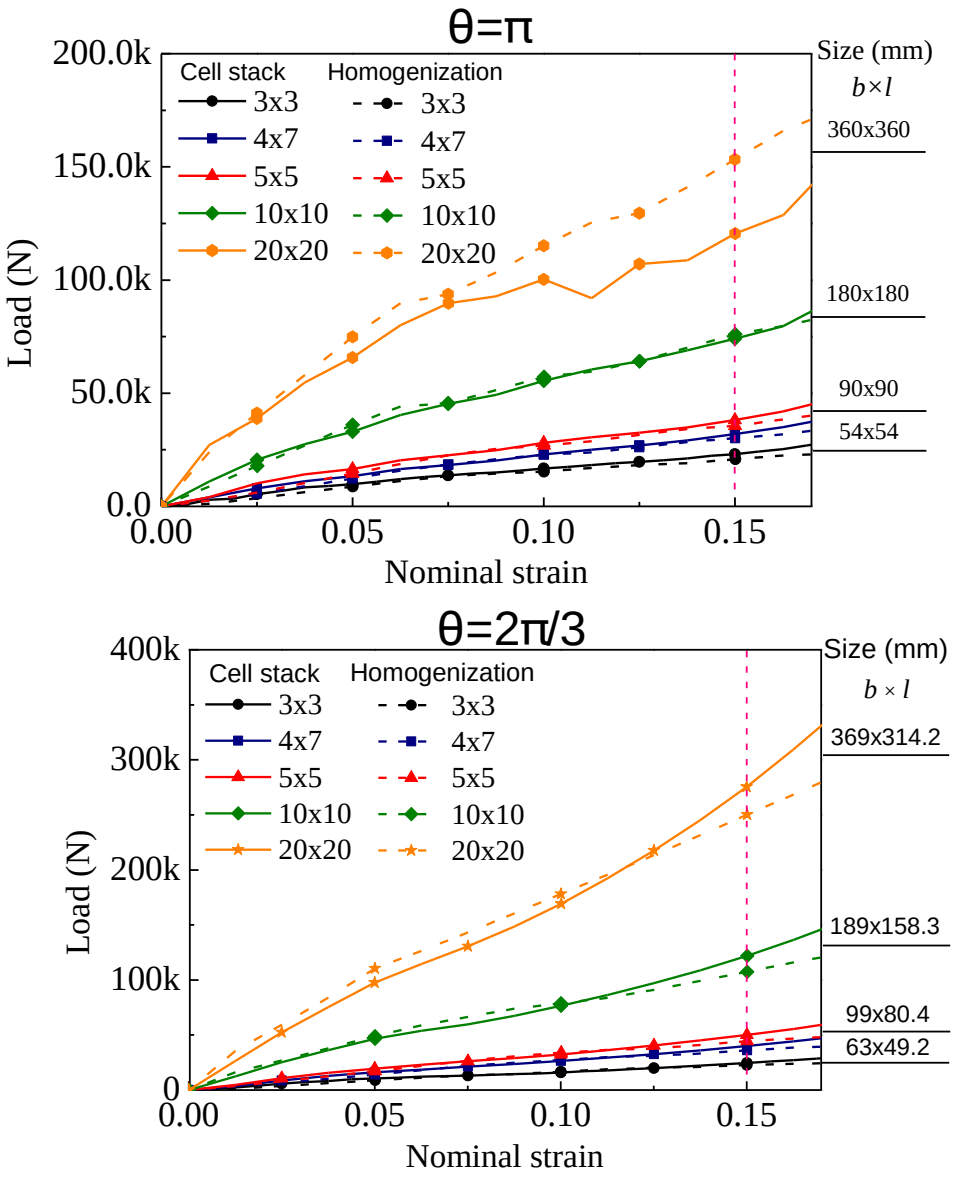


HOMOGENIZATION OF BATTERY PACK

Simulation: various packing modes in small sacle

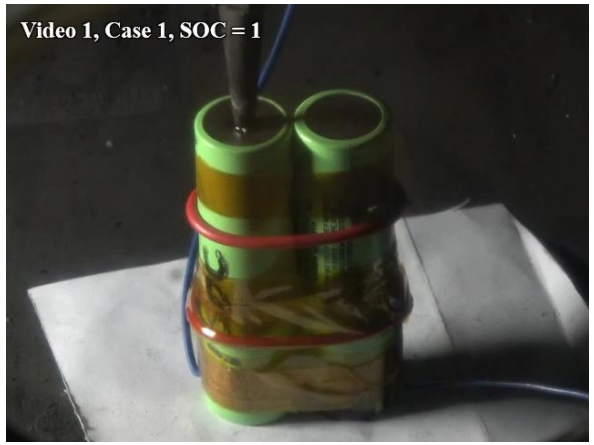


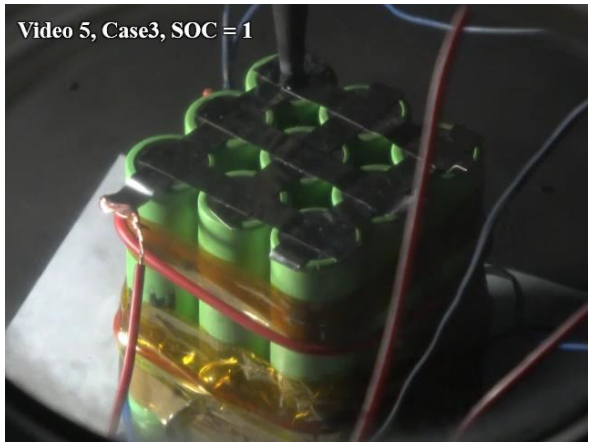
(Liu et al. *Engineering Failure Analysis*, 2018)

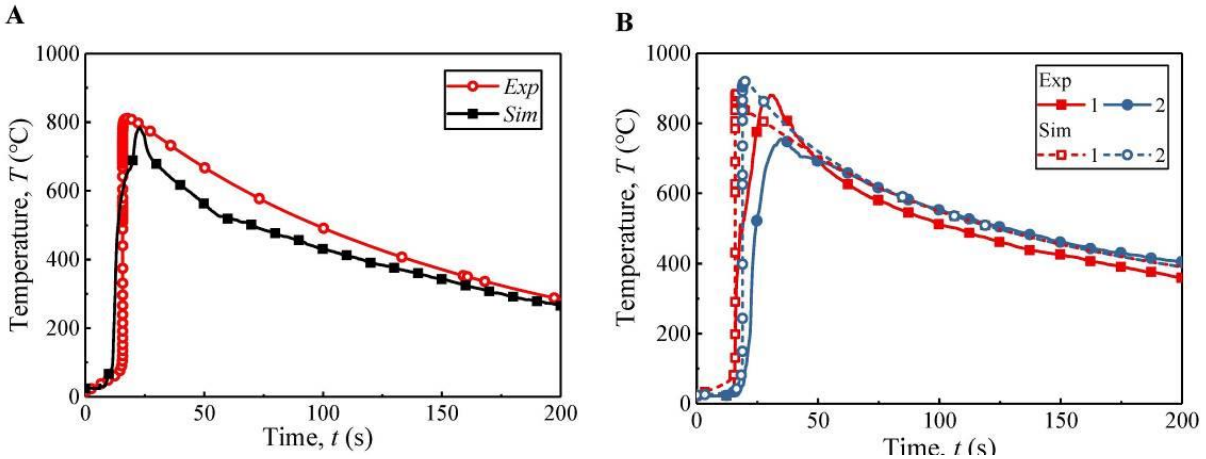


THERMAL RUNAWAY PROPAGATION

Experiment: penetration caused thermal runaway (TR)

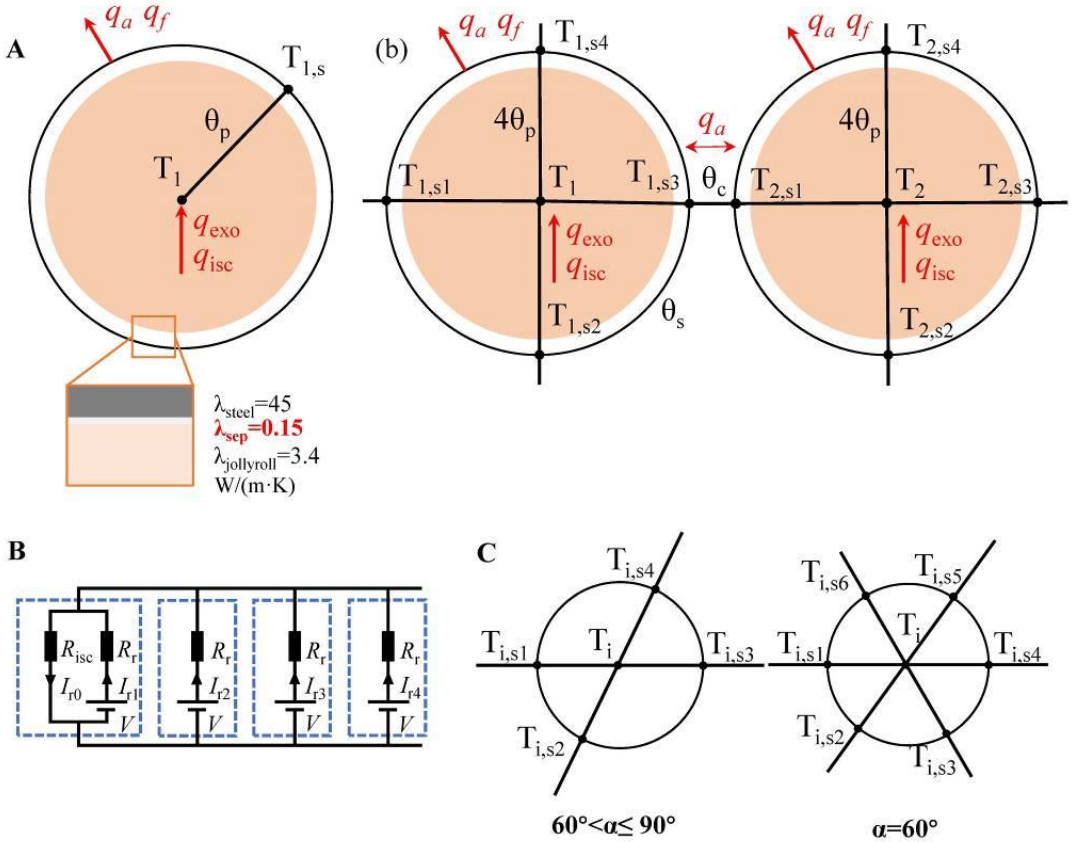






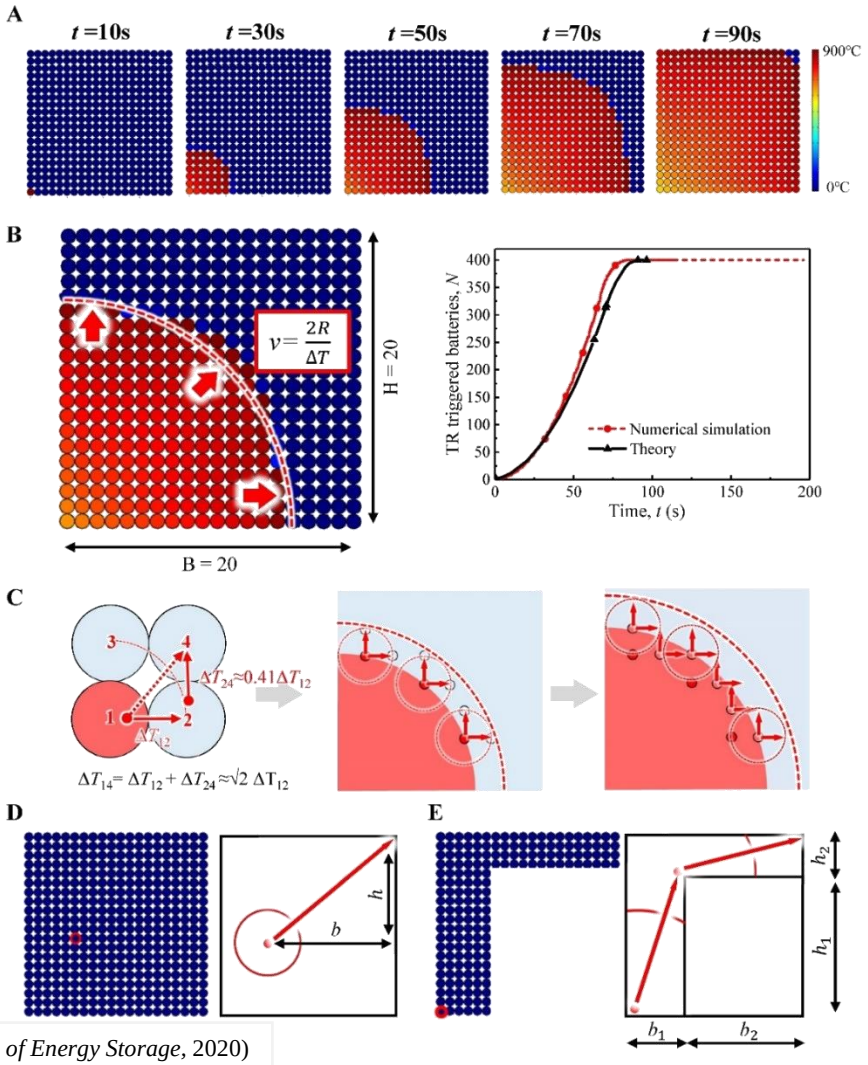
(Jia et al. *Journal of Energy Storage*, 2020)

Modeling: TR propagation model

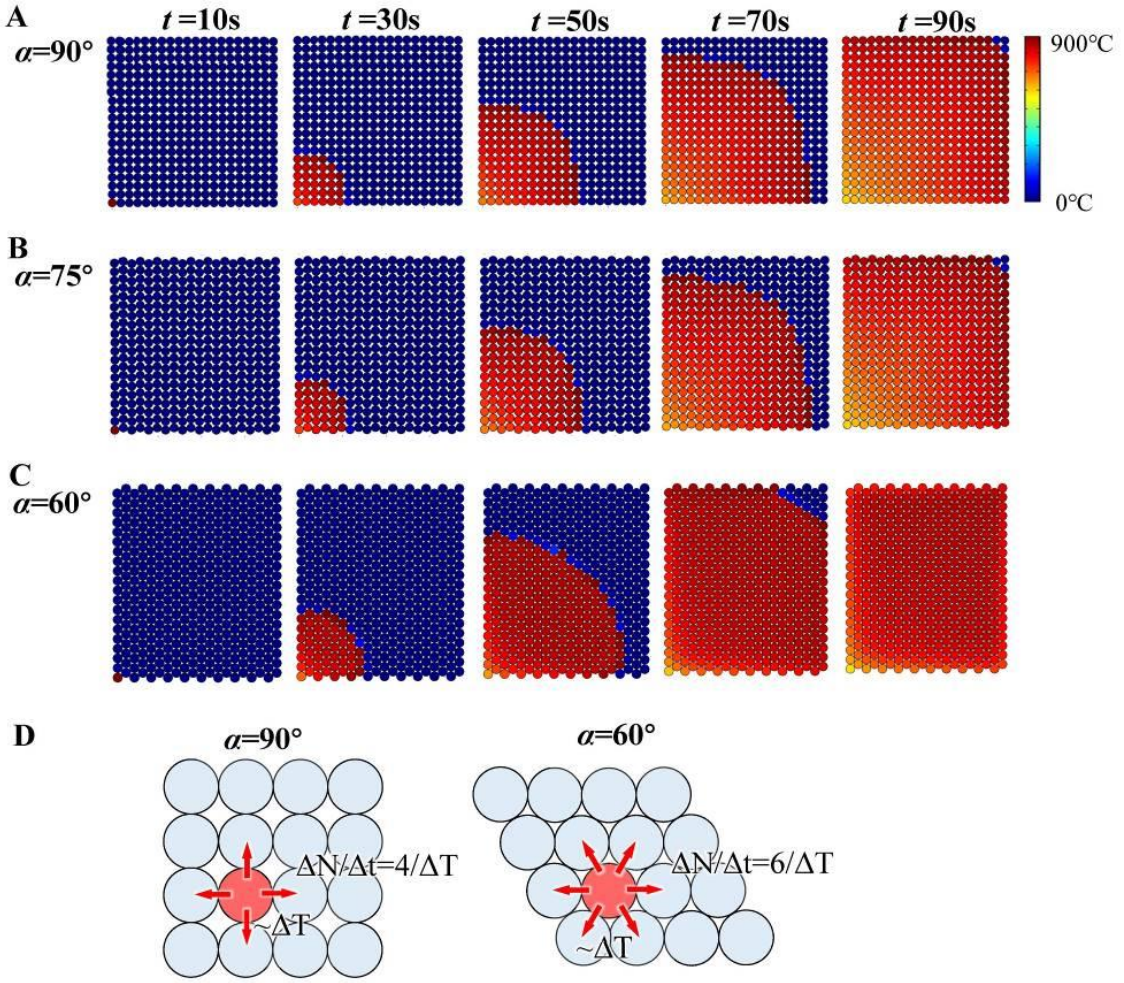


THERMAL RUNAWAY PROPAGATION

Simulation: TR propagation in various stacking modes



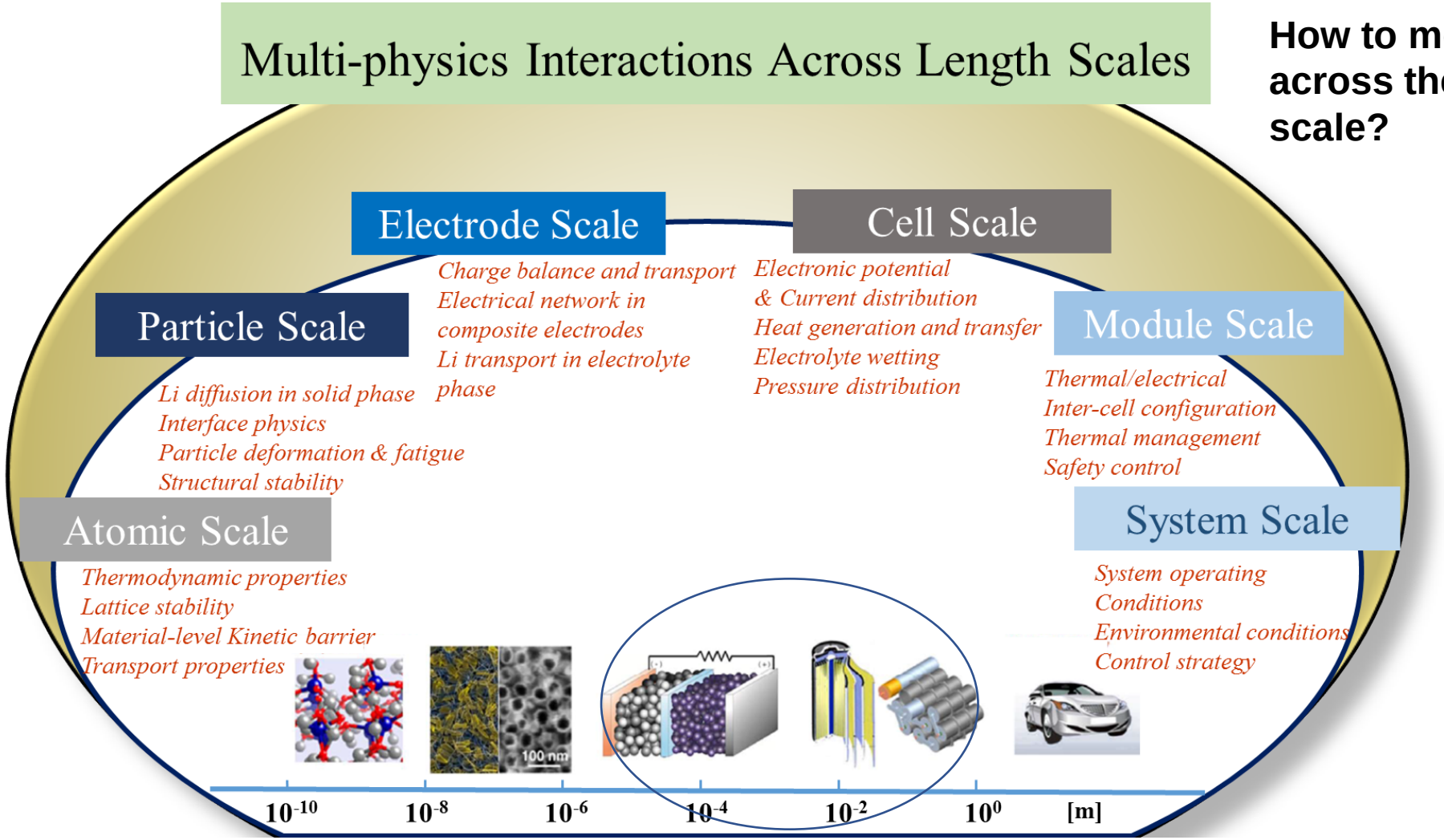
(Jia et al. *Journal of Energy Storage*, 2020)



OUTLOOK

Lithium-ion battery safety research

- Physics
- Electro-chemistry
- Mechanics



How to model across the scale?

(Abada et al. *Journal of Power Sources,* 2016)

THANK

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Email: jun.xu@uncc.edu

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Thank you for your time.

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jun.xu@uncc.edu

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Email: NFP.BatterySafety@ul.org