Understanding Battery Safety and Durability Issues from Physics-Informed Data-Driven Modeling

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BACKGROUND

My neighbor Tonny asked: What not buy an electric car?

Range Anxiety?

Higher energy density → *Larger pack*

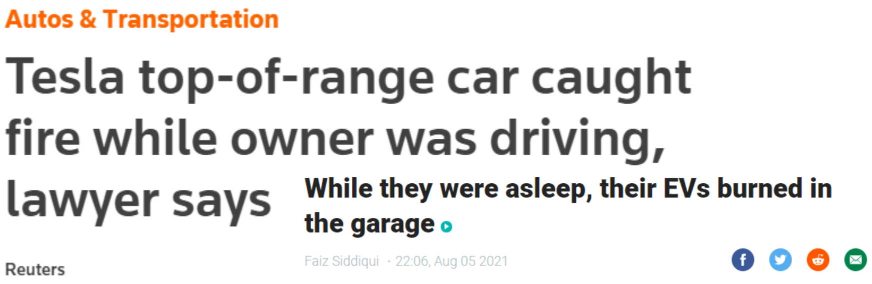
e.g., Lucid Air: 600 mi

Charging time?

Larger charging current →

e.g., Tesla: super fast charging, 80% in 40 mins

Safety!


Autos & Transportation

Tesla top-of-range car caught fire while owner was driving, lawyer says

Reuters

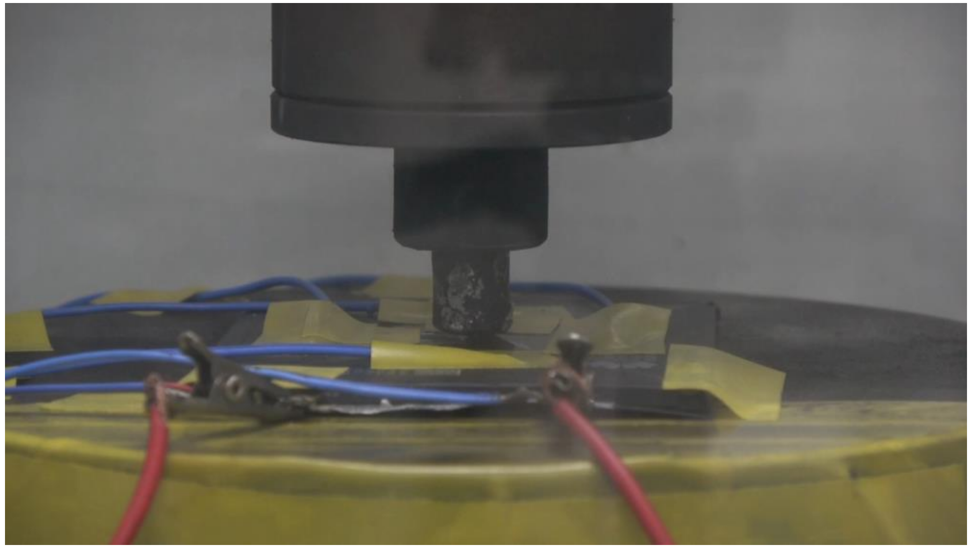
While they were asleep, their EVs burned in the garage

Faiz Siddiqui · 22:06, Aug 05 2021

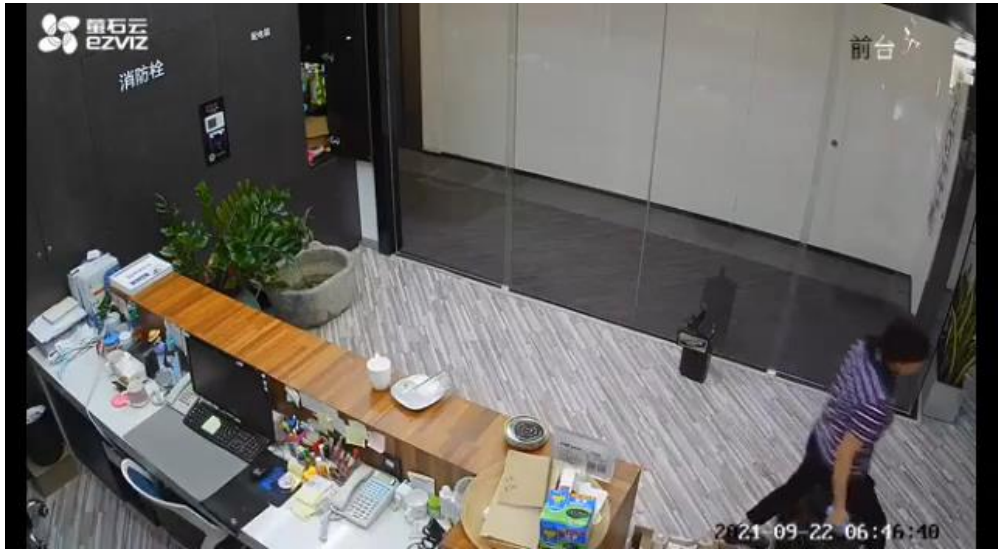
→ Limited progress..

BACKGROUND

Short-term Safety



Long-term Safety



External Triggers: Short-term Safety

Internal Triggers: Long-term Safety

(ISC) Internal Short Circuit → (TR) Thermal Runaway → Fire/Explosion

Temp.↑→Gas→Pressure ↑

Energy Storage Materials, 2020

FIRST TRY ON MODELING

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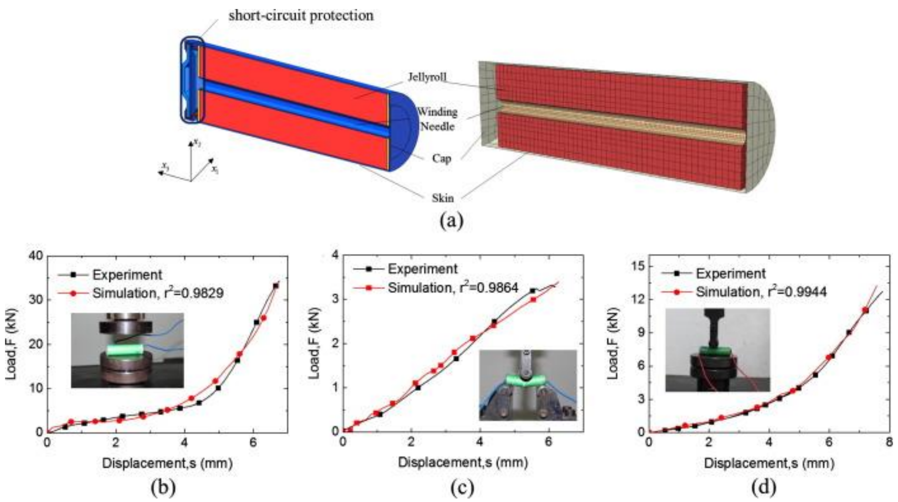
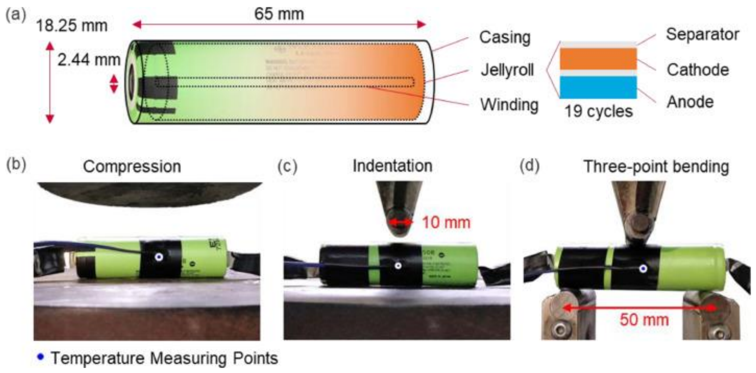
Homogeneous Modeling

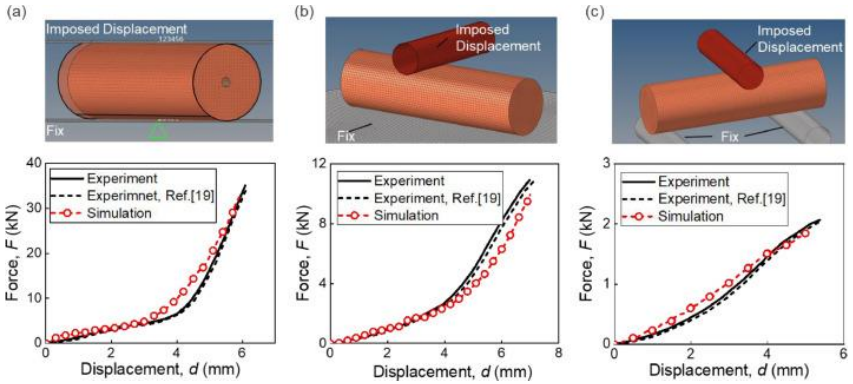
considering compression-tension anisotropicity

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

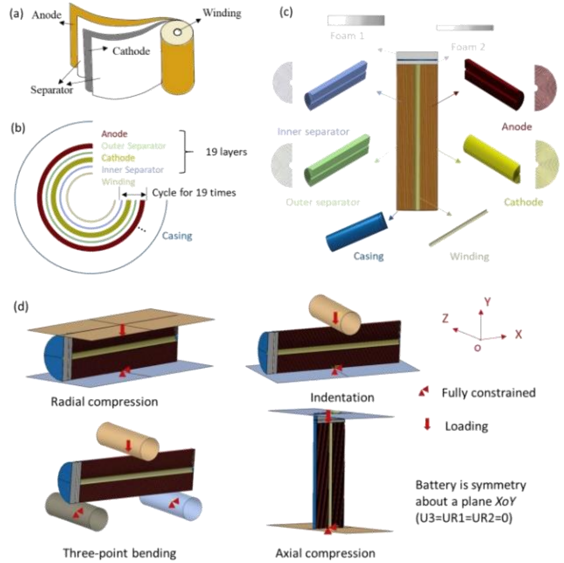


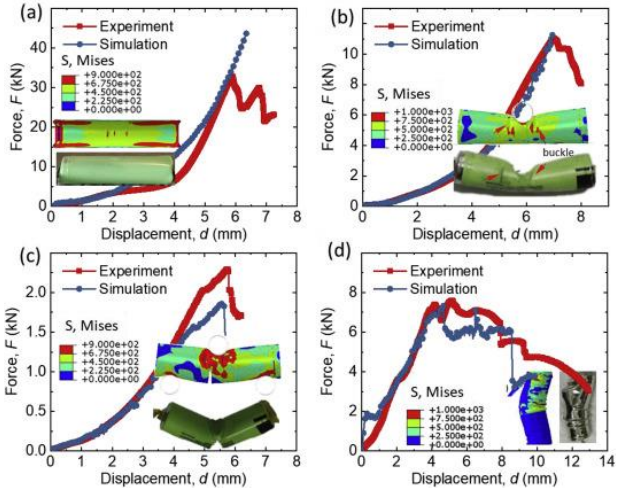
RVE Modeling





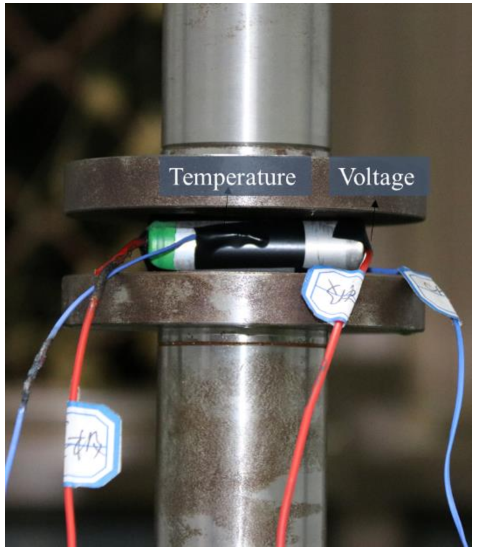
Detailed Modeling





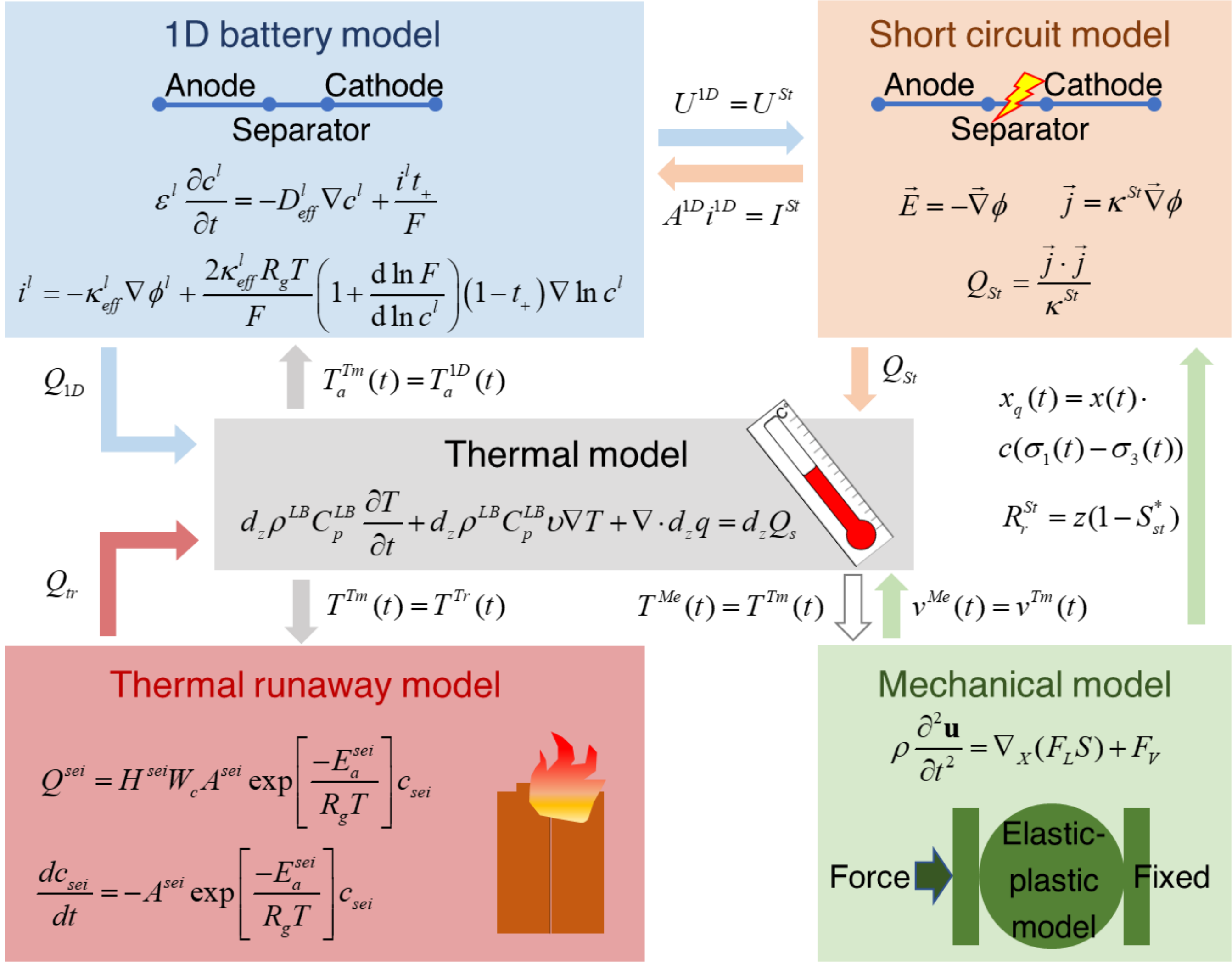
Applied Energy, 2016
J. Energy Storage, 2021
J. Power Sources, 2018

FIRST MULTIPHYSICS MODELING



Electrochimica Acta, 2017

Multiphysics modeling strategy



FIRST MULTIPHYSICS MODELING

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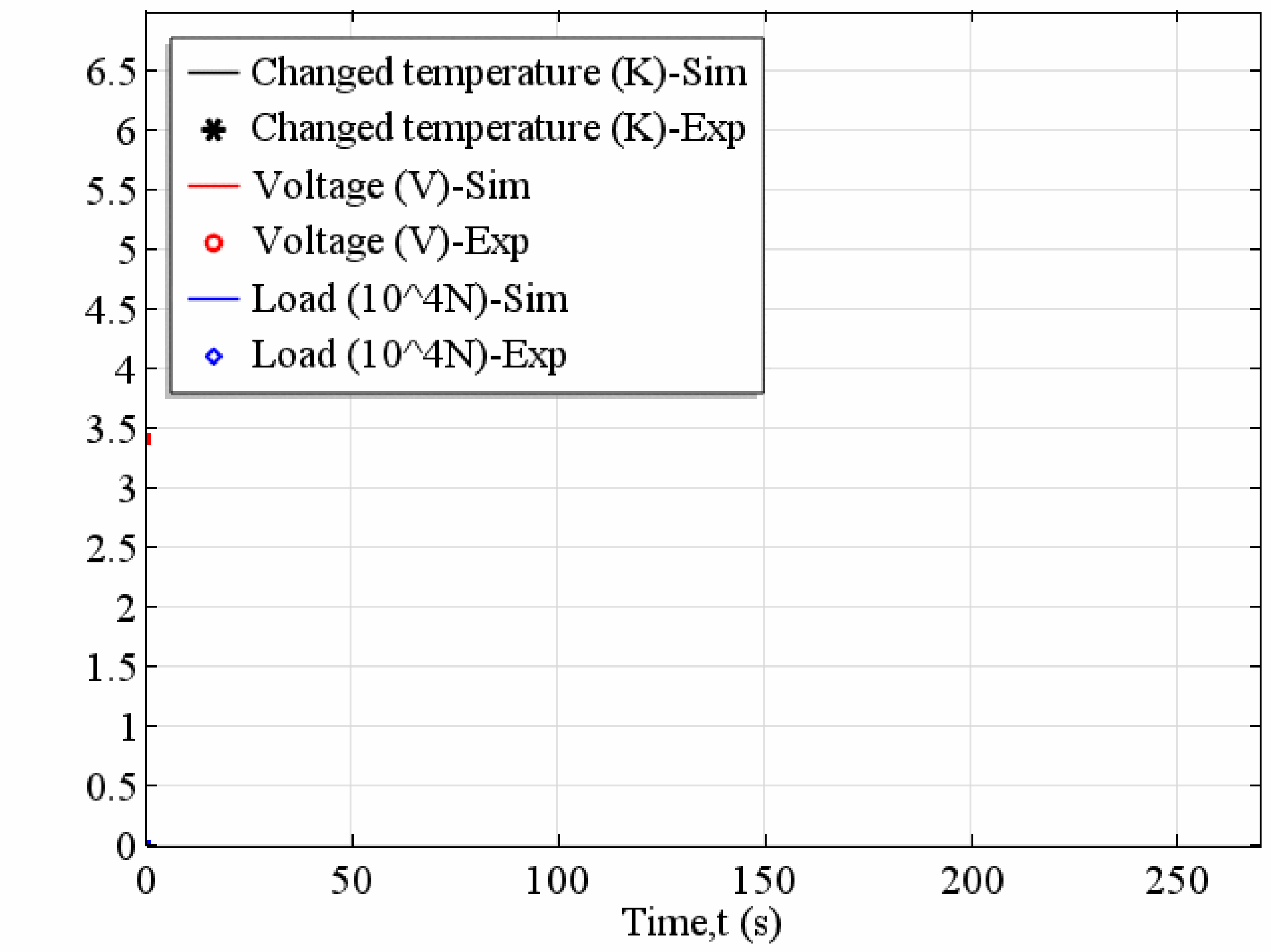

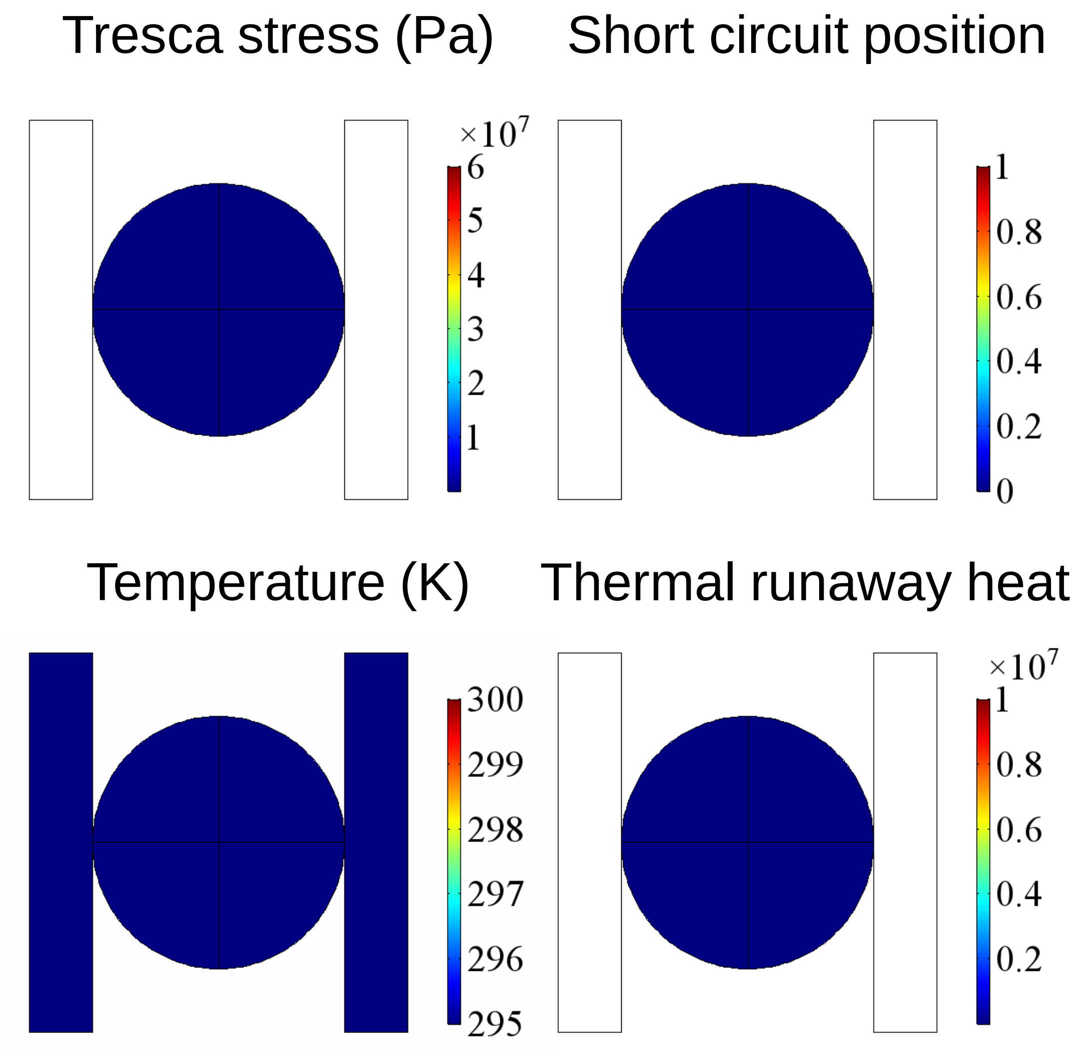

Electrochimica Acta, 2017

FURTHER REFINEMENT

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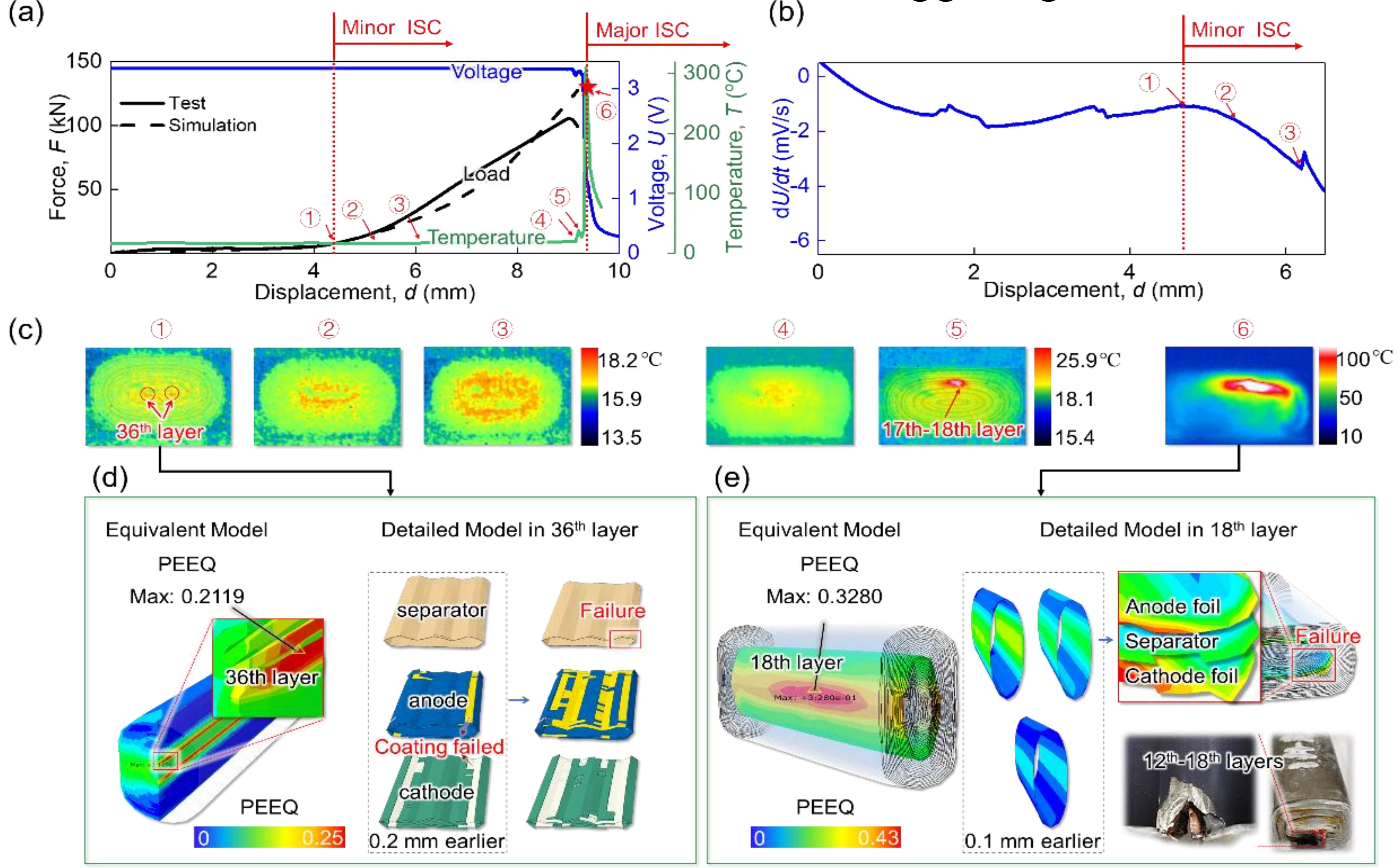
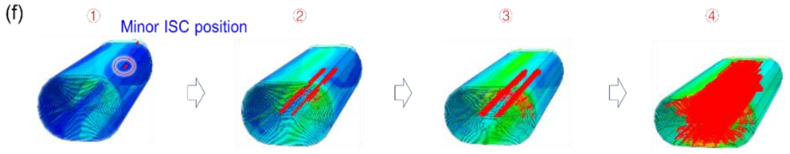
ISC triggering process can be investigated based on a detailed model

Indentation → ISC triggering: Minor ISC → Major ISC



Minor ISC
- Absolute voltage drop ~1 mV
- dU/dt starts to decrease
- Significant voltage recovery/steady

Major ISC
- Absolute voltage drop>0.1V
- No significant voltage recovery



J. Mater. Chem. A, 2021

A BRIEF SUMMARY

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Three milestone events

- Triggering of ISC → • Evolution of ISC → • Triggering of TR

Physics-based models

Mechanical model

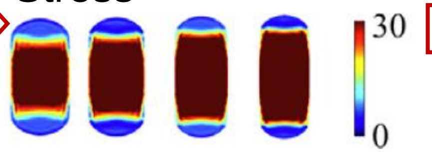
Stress

Triggering criteria

- ❑ Experimental data
- ❑ Theoretical model
- ❑ Relatively inaccurate

Multiphysics model

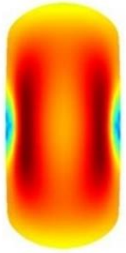
Stress



FE Calculation

- ❑ Accurate
- ❑ Low efficiency

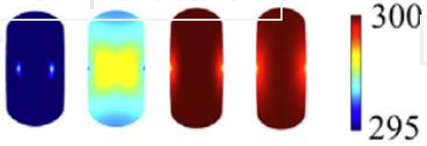
Finial consequences
Thermal runaway or not?



ML criteria

- ❑ Accurate
- ❑ Universality

Temperature



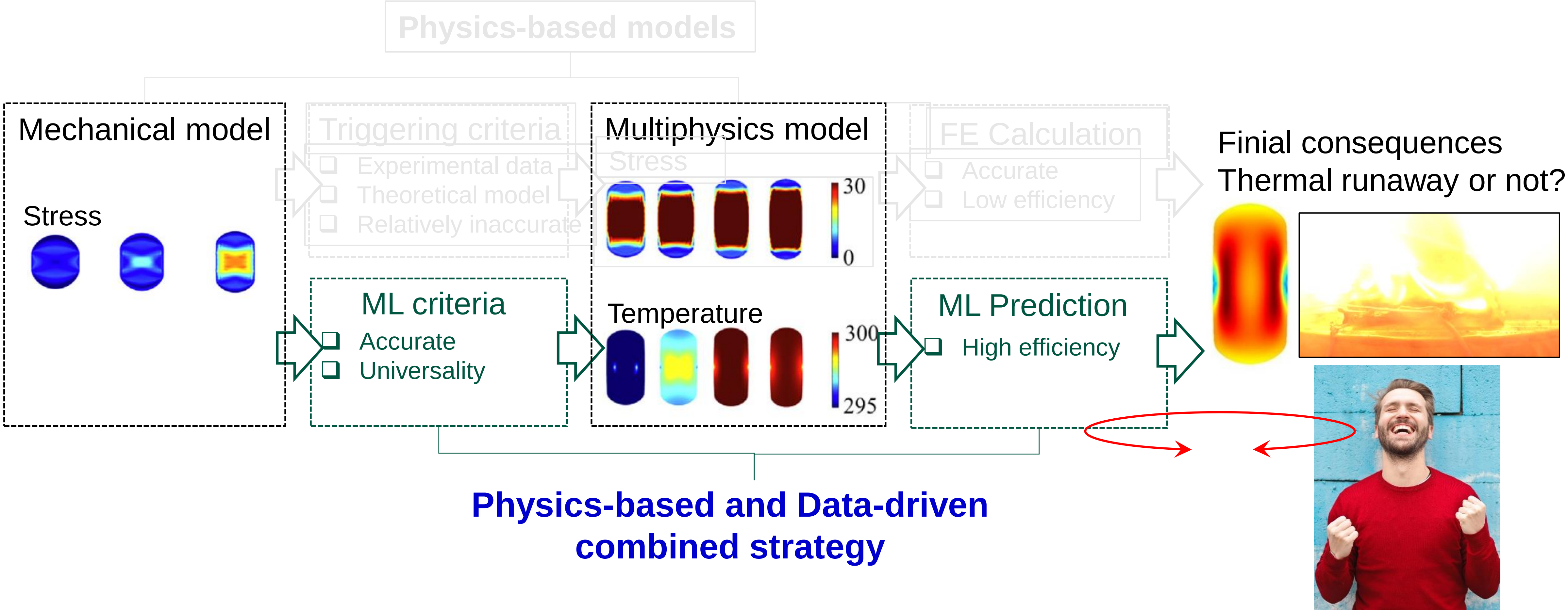
ML Prediction

- ❑ High efficiency

Physics-based and Data-driven combined strategy

A BRIEF SUMMARY

- Triggering of ISC → • Evolution of ISC → • Triggering of TR



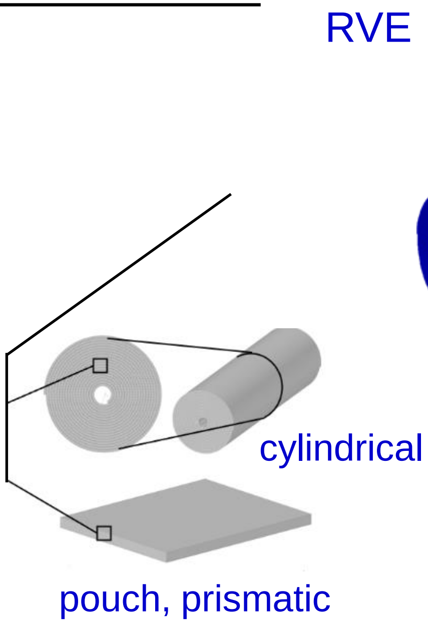
Data generation: computational results

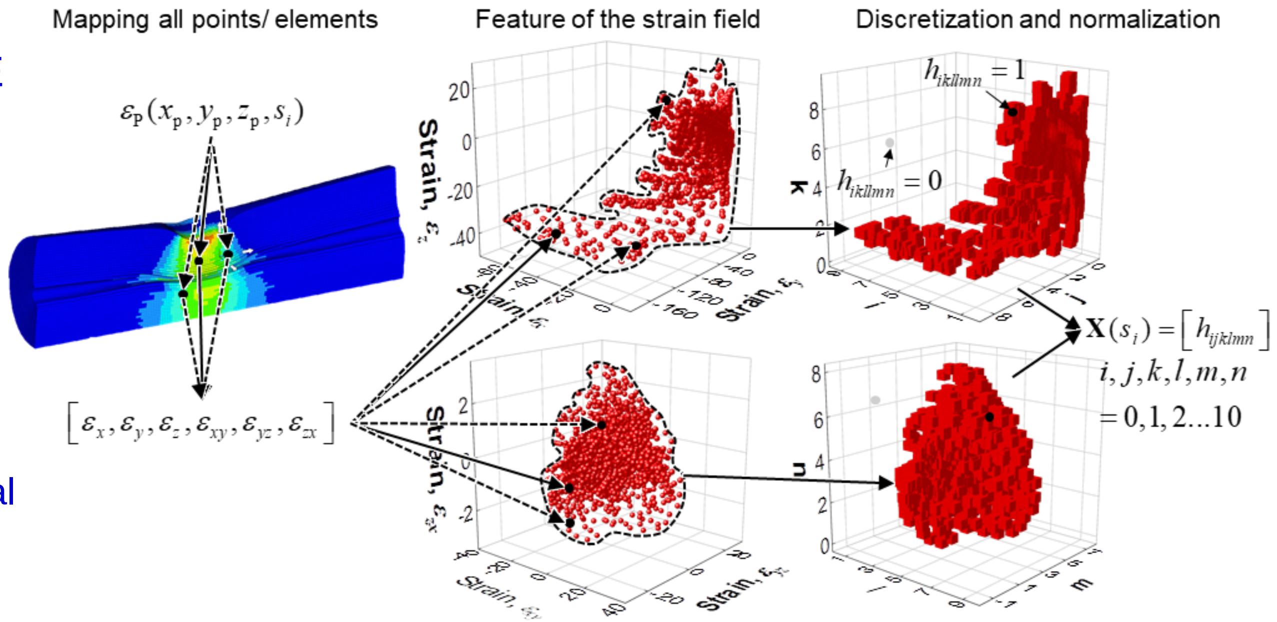
Step 1: Dataset creating

X: Strain tensor

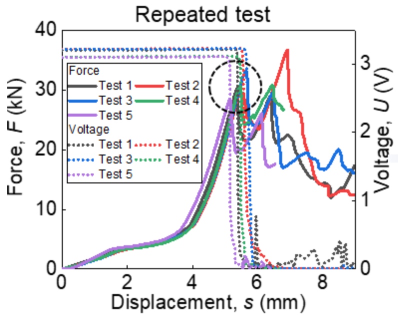
(1) Experiment
(2) Numerical simulation

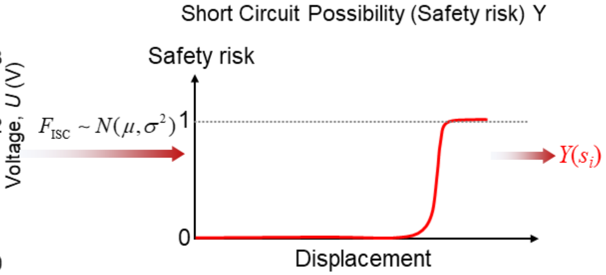
Strain tensor field $\varepsilon_{ij}(x, y, z)$

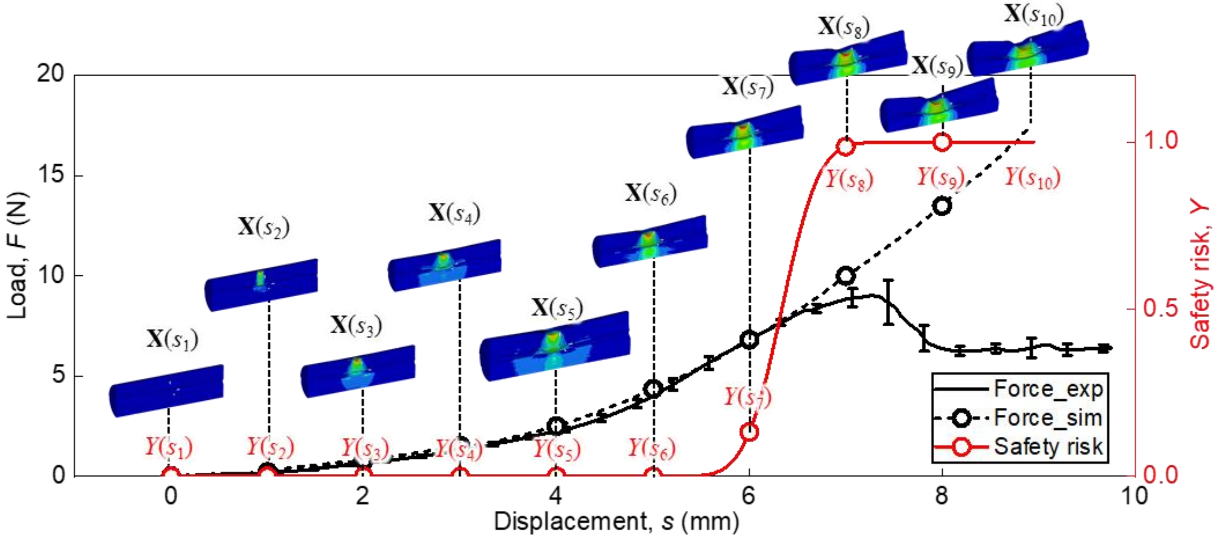




Y: Safety risk



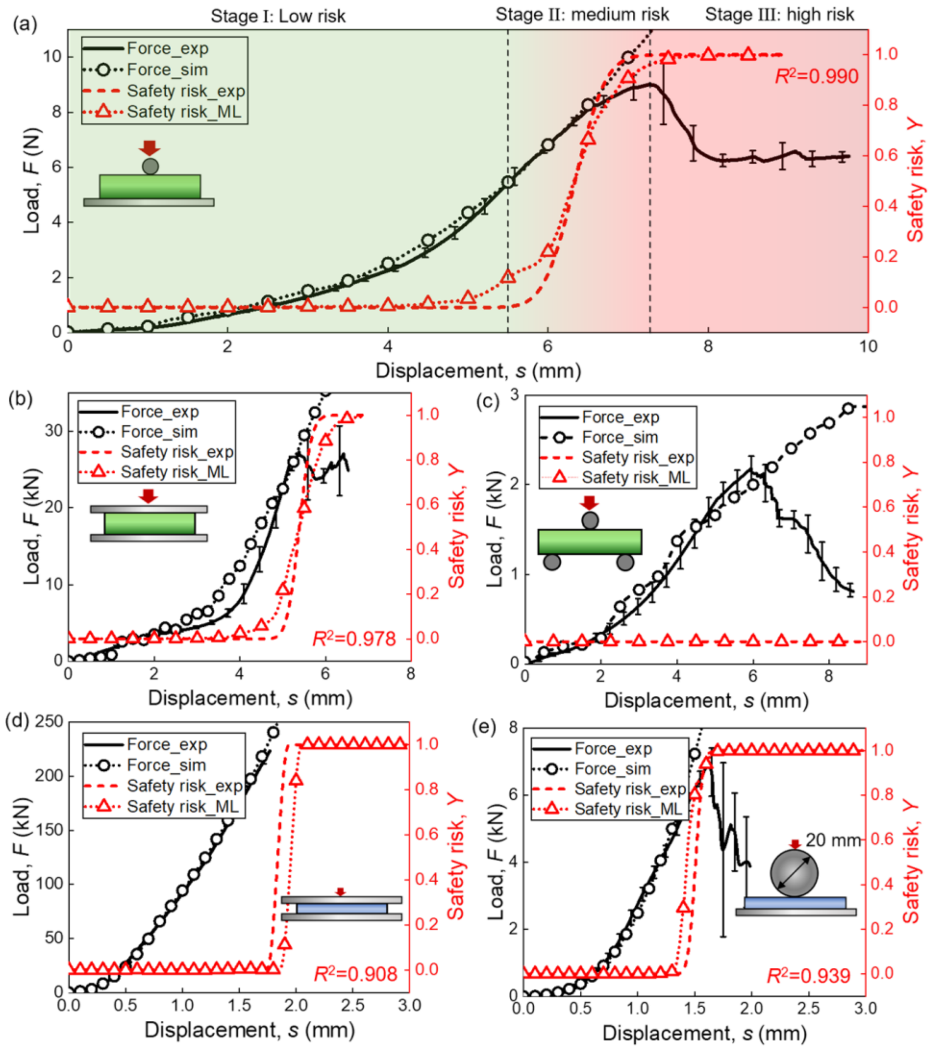




Adv. Energy Mater., 2021

MODEL PREDICTION

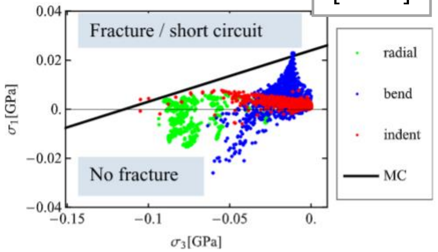
Data-driven prediction results



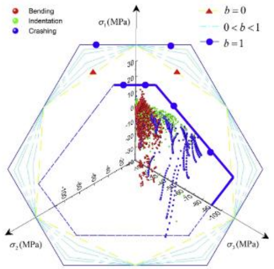
Adv. Energy Mater., 2021

[2] Greve et al. *Journal of Power Sources*, 2012
[3] Xu et al. *Engineering Failure Analysis*, 2015

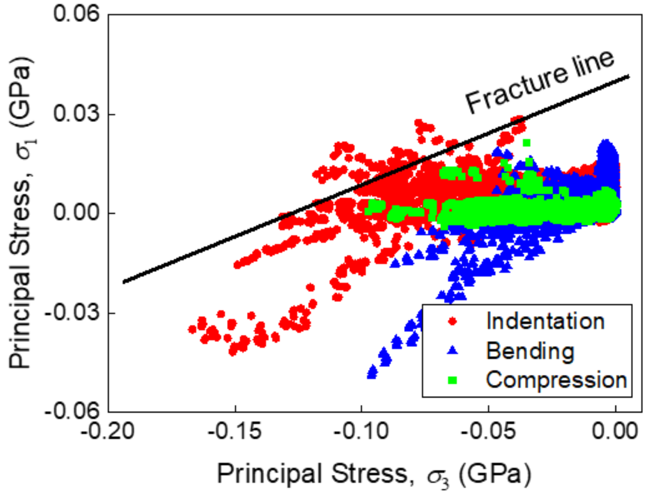
[Ref.1]

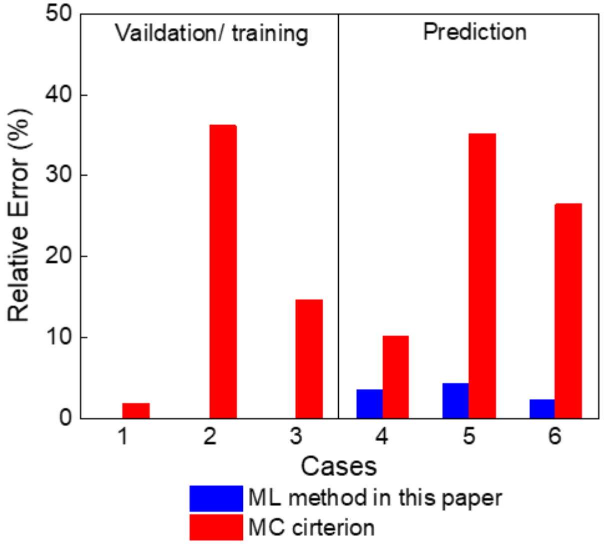


[Ref.2]



A common intrinsic problem: ISC criteria is pre-set and patterned



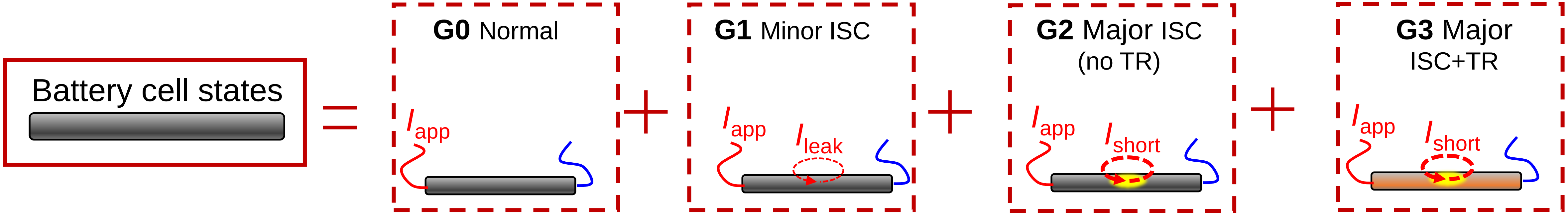


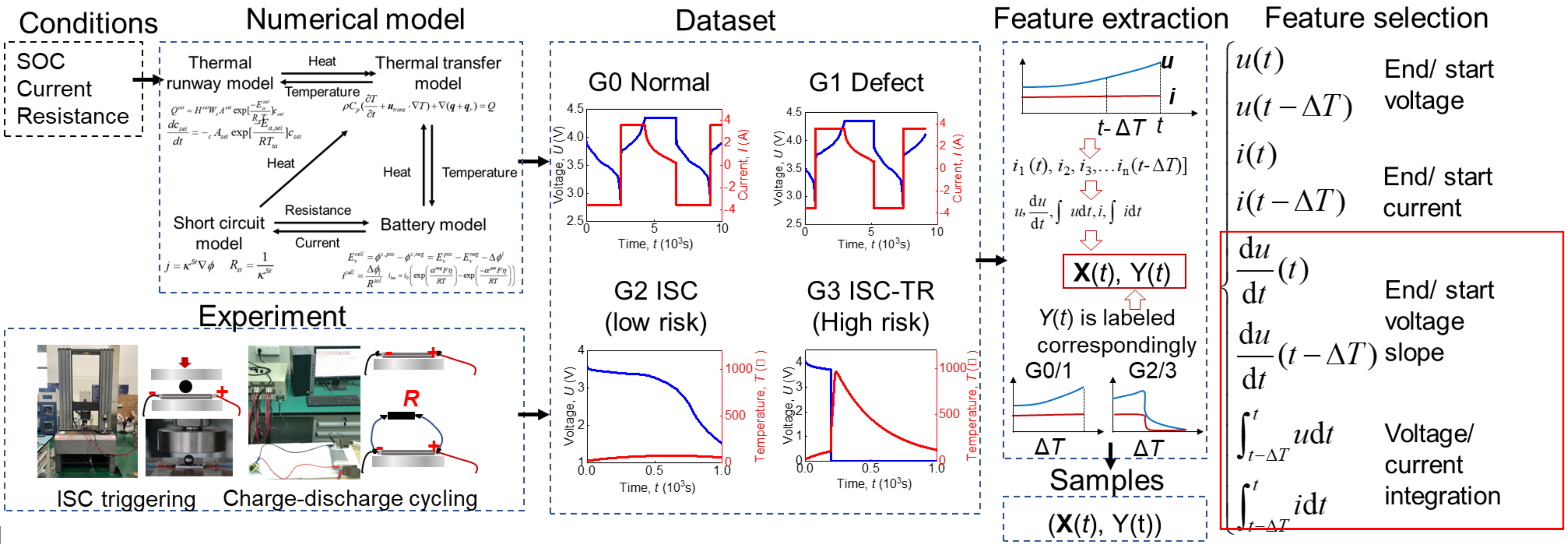
Comparison between the SVR predictor and the Mohr-Coulomb failure criterion

- MC: 2.6%-36.2% (validation sets)
  10.1%-35.2% (prediction sets)
- ML: 0% (training sets)
  2.5%-4.3% (prediction sets)

HOW CAN WE TELL?

Data-driven classification





J. Power Sources, 2022

CLASSIFICATION RESULTS

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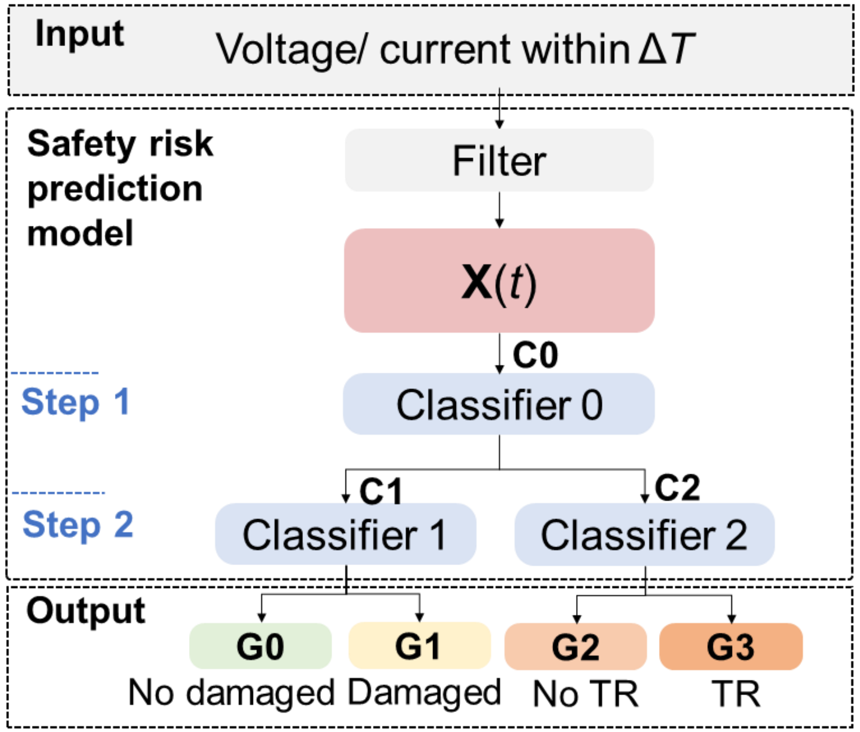
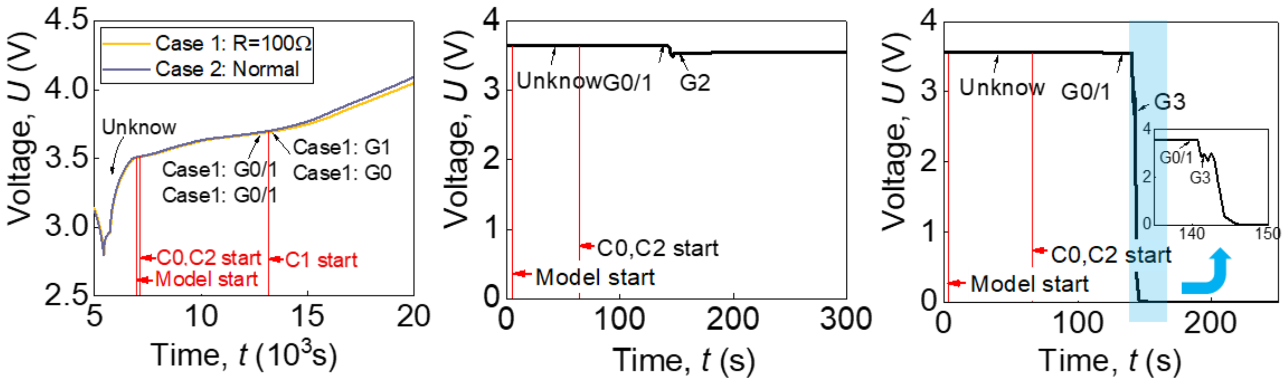
Data driven safety risk prediction



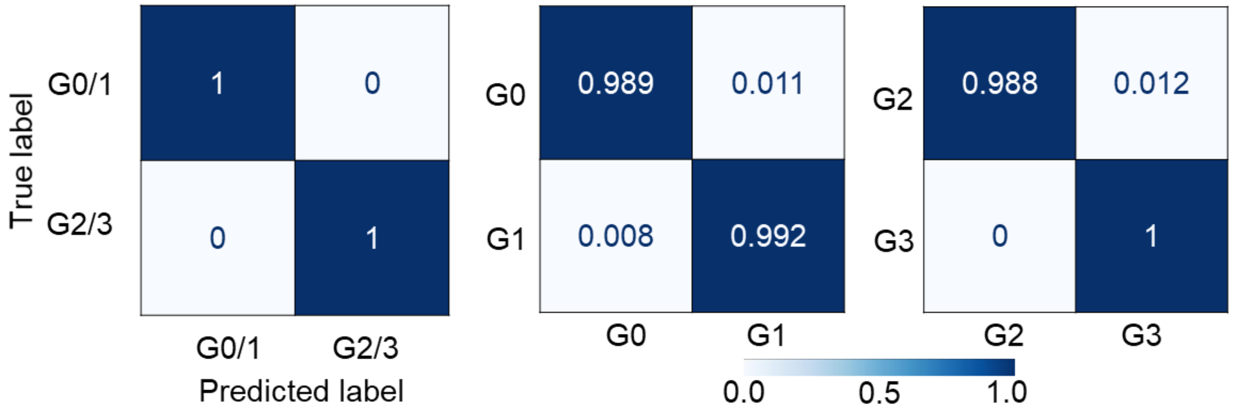
- 293,990, 46,600, and 180,768 samples were generated and used in the training of C0, C1, and C2,
- 10 % of the samples will be used as test samples, 5 randomly splitting.

Prediction process



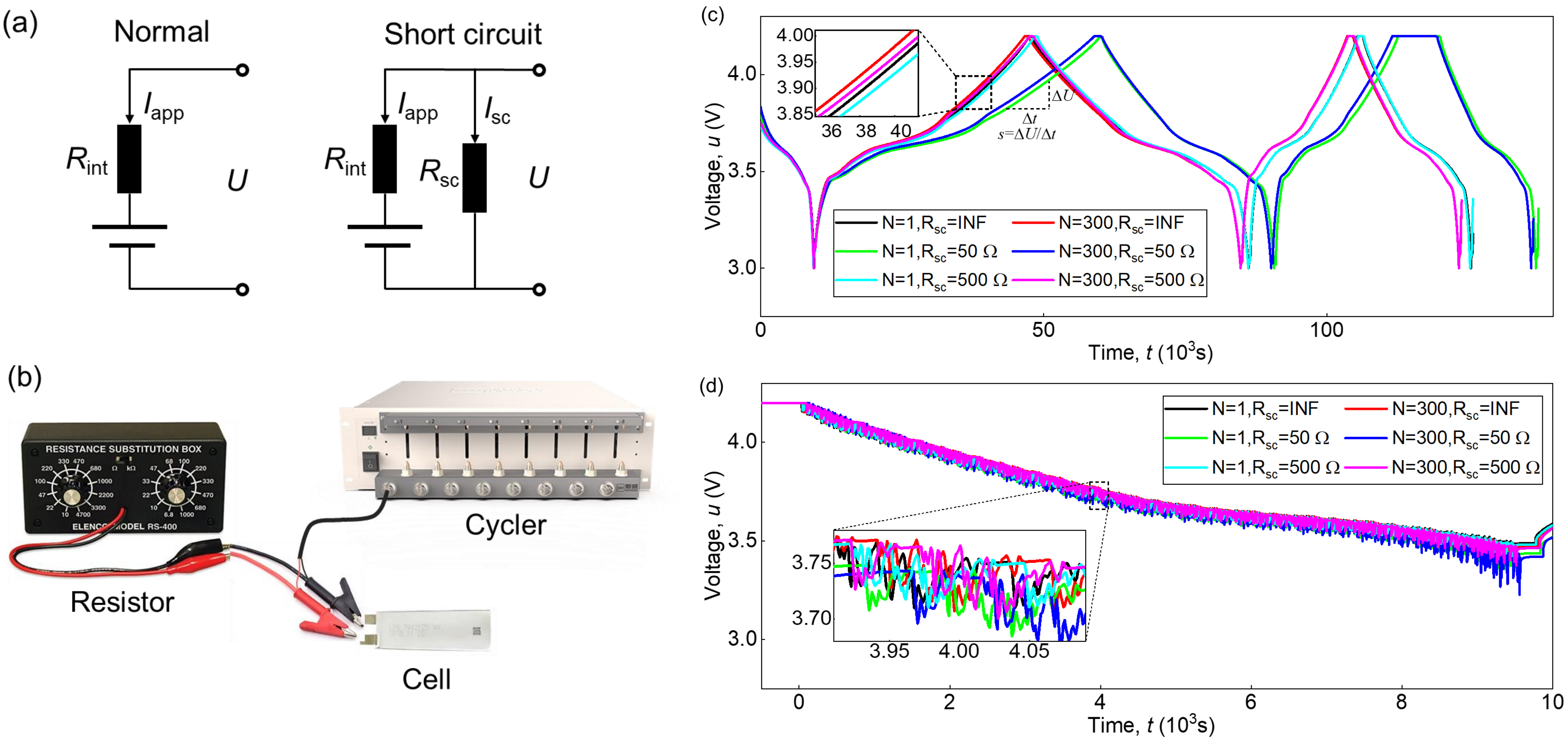
Defective cell detection | ISC prediction (no TR) | ISC prediction (TR)

Confusion matrix



J. Power Sources, 2022

SHORT-CIRCUIT RESISTENCE



J. Energy Chemistry, 2023

SHORT-CIRCUIT RESISTENCE

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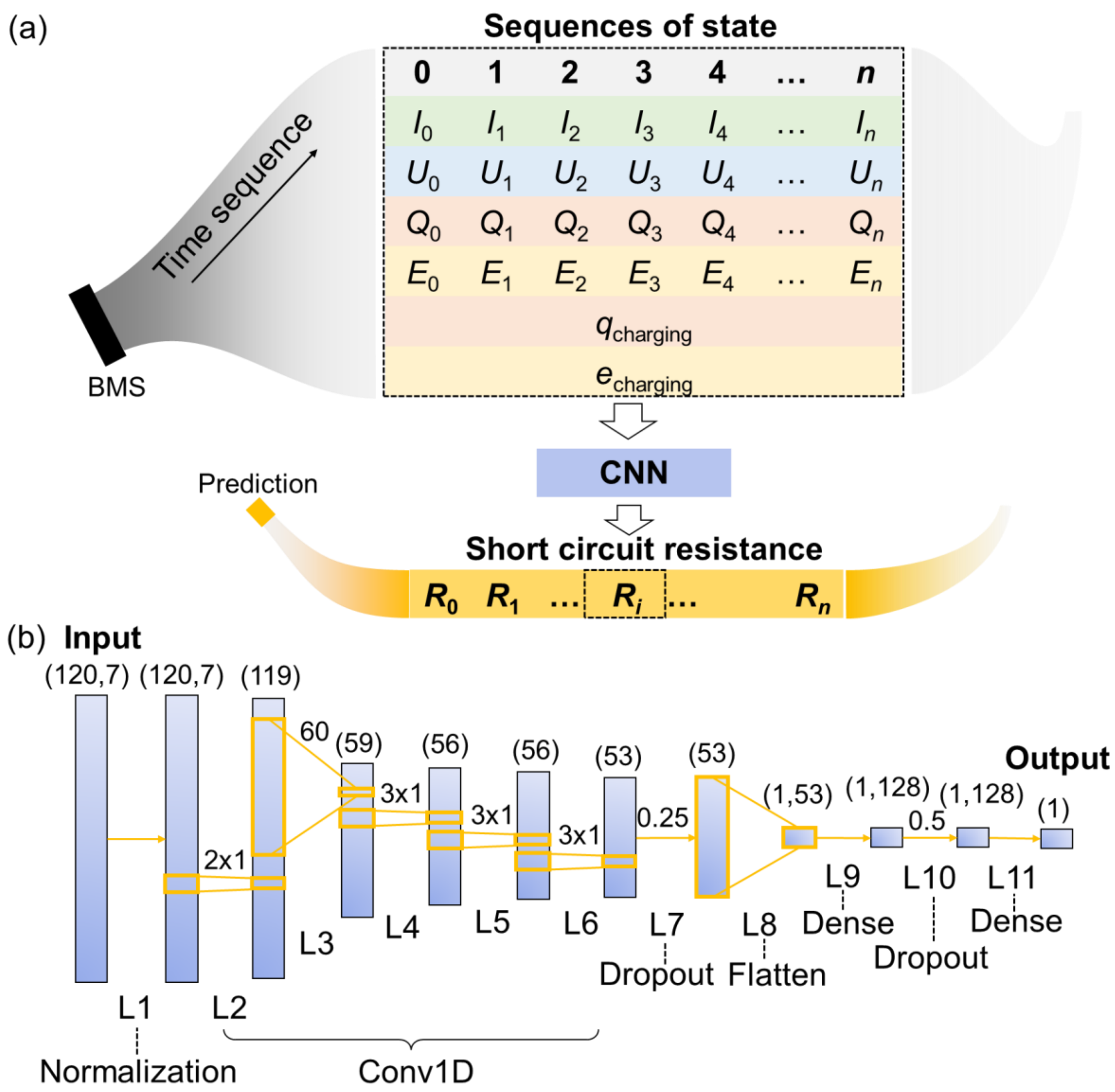

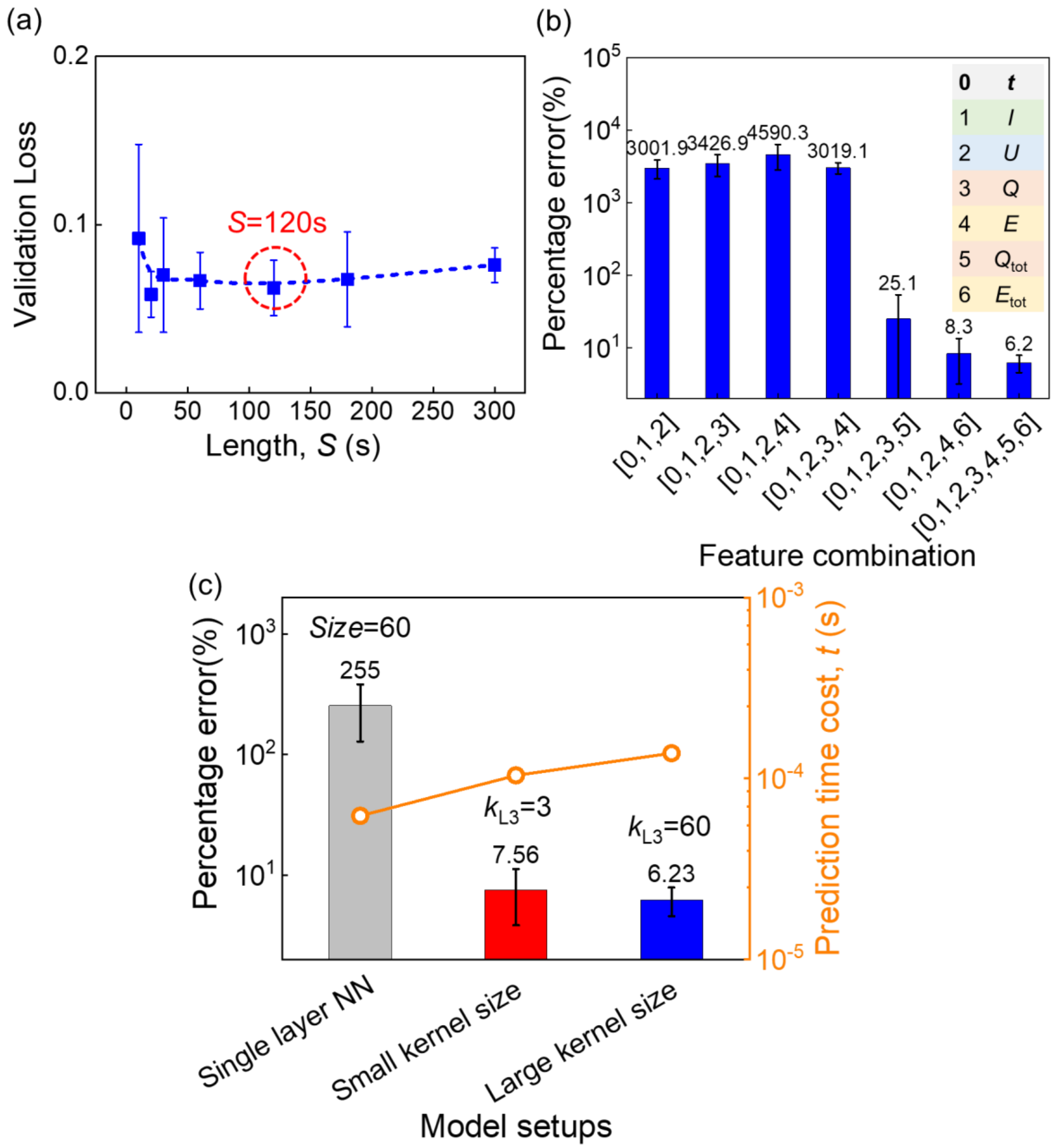

J. Energy Chemistry, 2023

TECHNICAL TAKEAWAYS

- Battery safety and durability is a highly complicated problem
- Data-driven has demonstrated the strong capability to solve complex system problem
  - Predict safety risk
  - Classify safety status
  - Predict the short circuit resistance (determinant factor)

What is next?

GRAND CHALLENGES

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Battery Safety & Durability ➡ Battery Design, Manufacturing, etc.

Data ⟷ **Model**

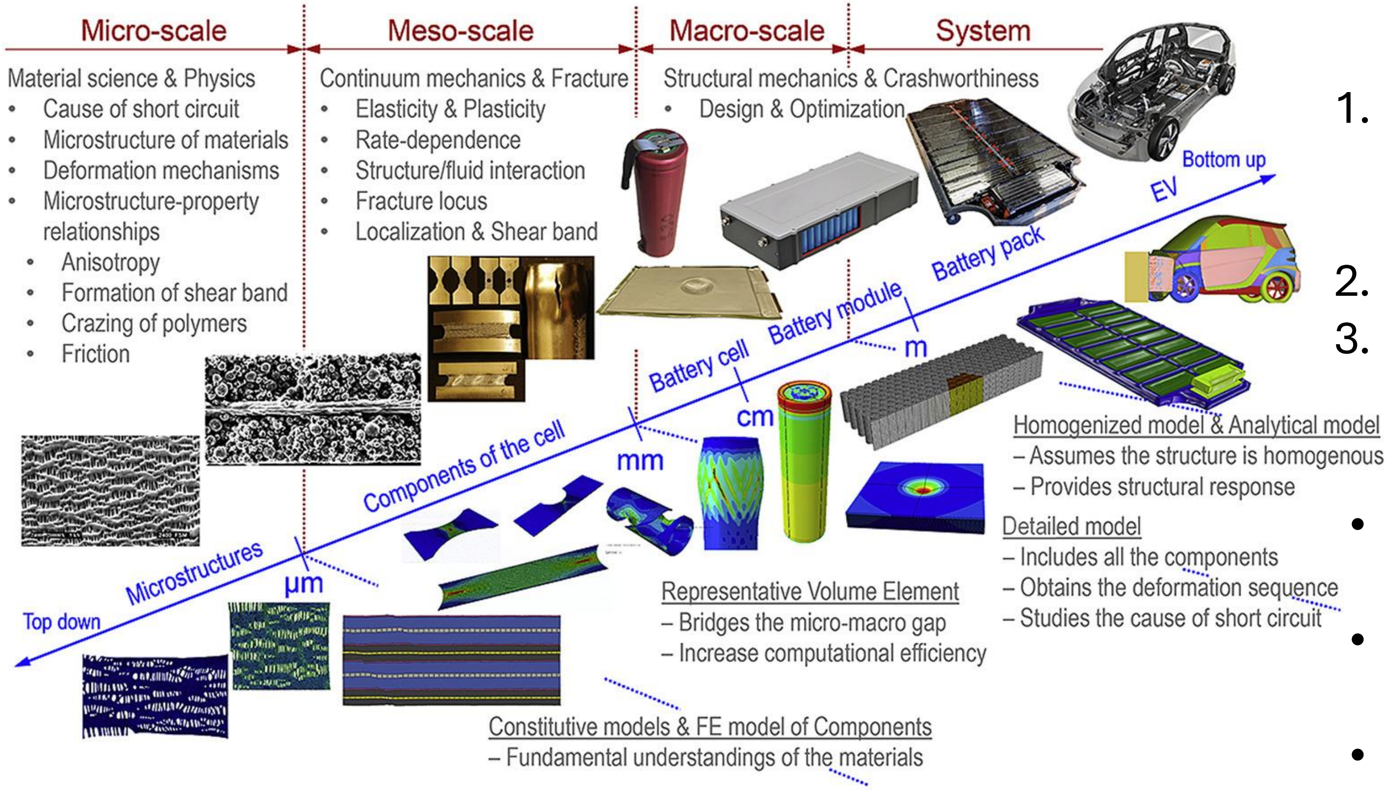
Model-driven Description and Prognostic

Data

1. Controlled lab tests
2. Field data
3. Model data

Challenges

- Inconsistent testing methodologies
- Data missing, noise, sampling frequency, accuracy …



Model

1. Physics-based model
   1) Single physics
   2) Multi physics
2. Control/Empirical model
3. Data-driven model

Challenges

- Complexity vs. Efficiency
- Physical insights vs. Data fitting
- Lengthscale

[1] Zhu et al., *J. Power Sources*, 2018

GRAND OPPORTUNITIES

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- Establish testing methodology for battery safety and durability
  - Work with FM Global

- Establish shared database
  - Work with some universities and companies

- Room for improvement
  - Develop fast, safe, low-cost testing/characterization
  - Dive deep into fundamental mechanism and develop new physics-based models
  - Deal with multiscale descriptions
  - For ML
    - How to deal with insufficient data or missing data
    - How to deeply interact data-driven and physics
    - How to use ML in testing and characterization
    - How to use LLM in collecting data and feed them into the database?
    - …

THANKS

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Dr. Donal Finegan (NREL)

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