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ADVANCED SIMULATION MODEL FOR BATTERY MANUFACTURING USING EDEM AND ROMAI

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Introduction to EDEM

Jungkil Shim / Altair Korea

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OUTLINE OF EDEM

Particles around us

Natural

Artificial

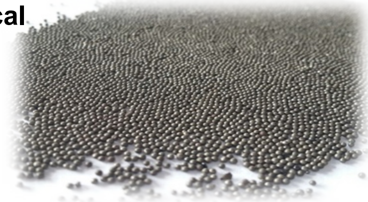
Agriculture

Mineral

Food

Ground

Mechanical



Pharmaceutical

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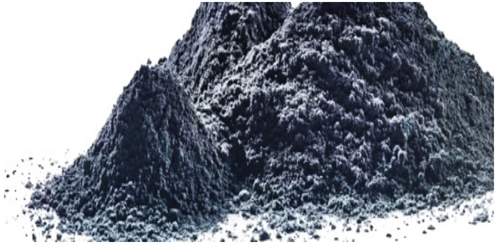
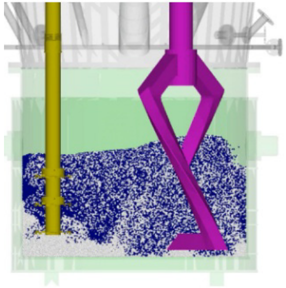
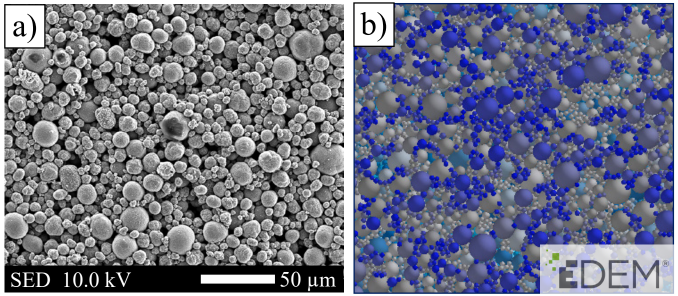
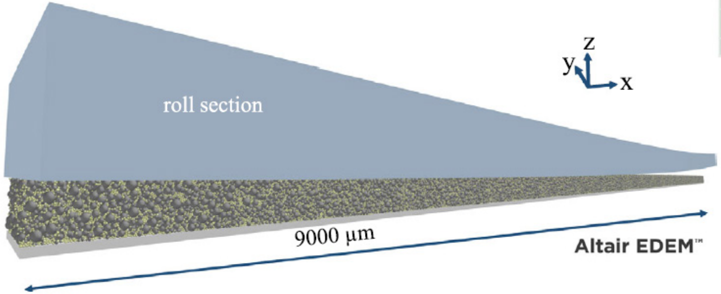
Introducing EDEM simulation technology



- Simulates behaviour of particulate materials at the particle scale
- Powered by the **Discrete Element Method** (DEM)
- **Fundamental investigation** of process mechanics at macro and micro scales
- **Virtual prototyping and optimization** of equipment and process operation
  - **Understand how the electrode microstructure is affected during manufacturing**
  - **Simulate different materials and process conditions**
  - **Control the microstructure to optimize electrode performance**







Schreiner, D., Klinger, A. and Reinhart, G. (2020) 'Modeling of the calendering process for lithium-ion batteries with DEM simulation', *Procedia CIRP*. Elsevier B.V., 93, pp. 149–155

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Expanding the World First Powder Database

15,000 new material models for powders

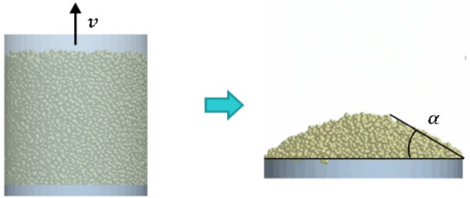
Key Industries

- Batteries
- Pharmaceutical
- Process Manufacturing

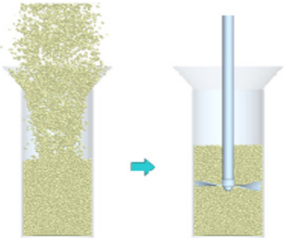
BENEFITS :

- Eliminate manual calibration of the powder
- Understand powder flow and behavior

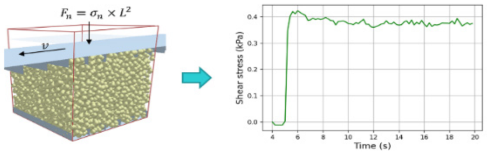
Static Angle of Repose



FT4 Powder Rheometer



Direct Shear tester



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Integration Ready for Multiphysics & AI

PM-FlexTire™

Available via the APA

EDEM-HyperStudy Connector

Altair Software

3rd Party Software

MBD	FEA	CFD	AI
			HyperStudy
			romAI
MotionSolve	OptiStruct	AcuSolve	
	SimSolid	uFX	
		OpenFOAM	
Adams	Ansys Mechanical		
RecurDyn		Ansys CFD	

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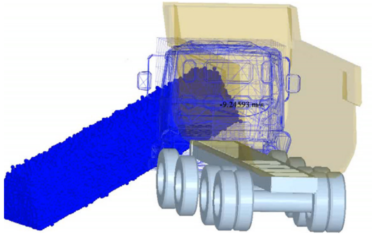

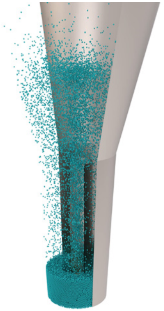

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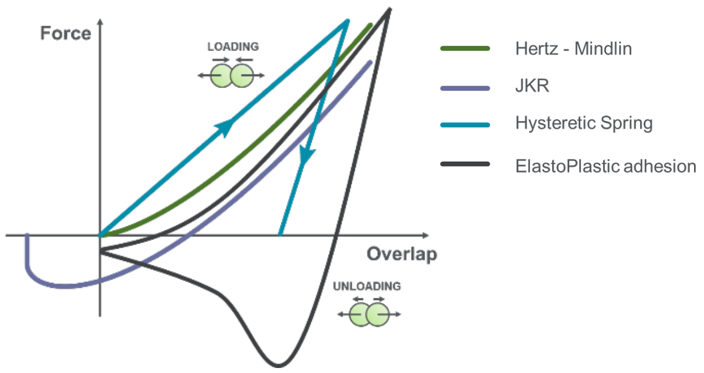
PARTICLE MODELING

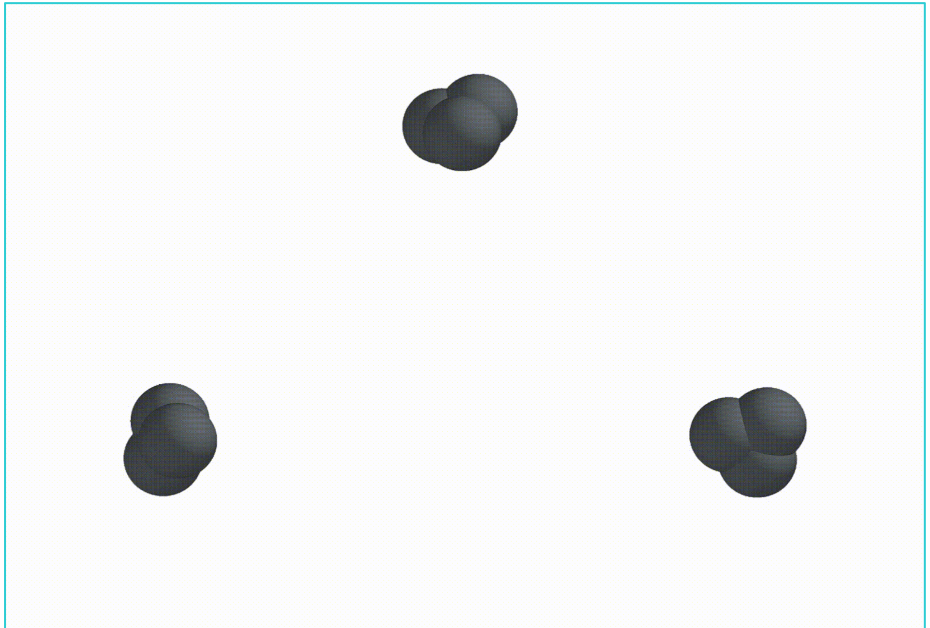
What is DEM?

- Discrete Element Modelling – a way of simulating discrete matter
- The bulk behavior emerges from the collective interaction of each individual object

Soft-sphere Method

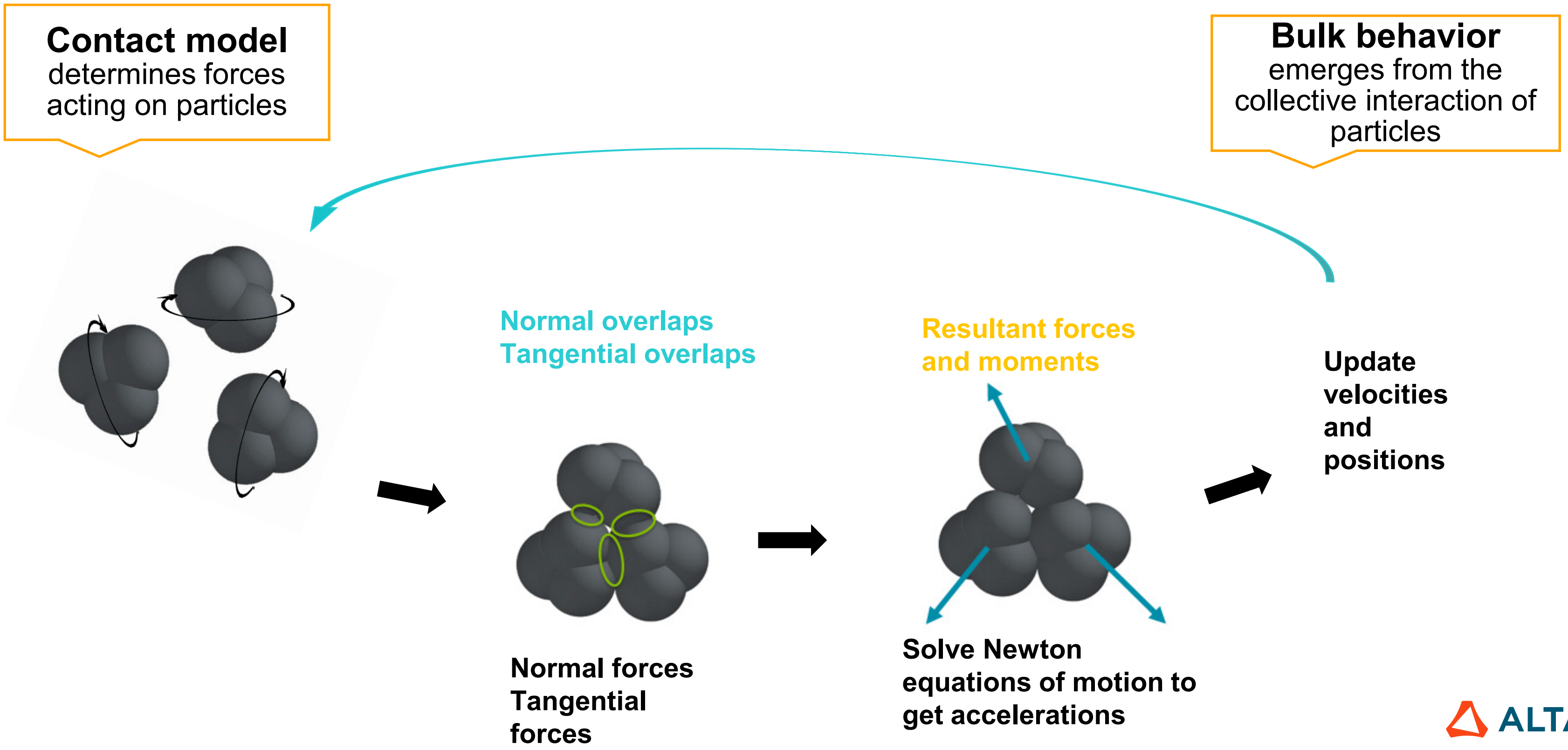
Rigid particles but small overlaps allowed
Evaluates forces accurately



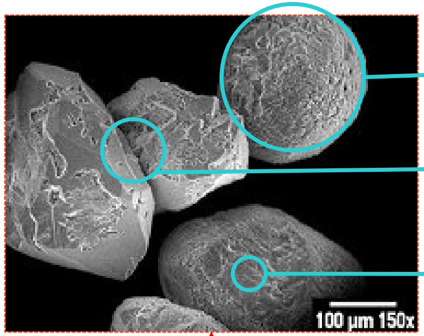


Motion of Particles

The DEM Method



How Particle modeling?



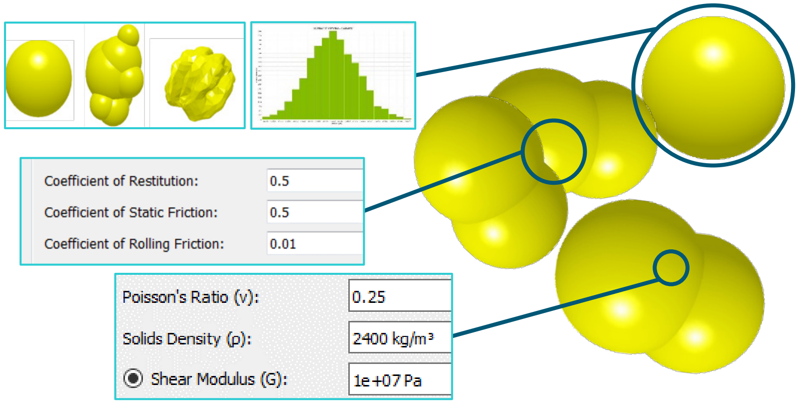
Micro Mechanical properties

Morphology:
- Shape & Size

Interaction forces
- Friction, repulsion, adhesion

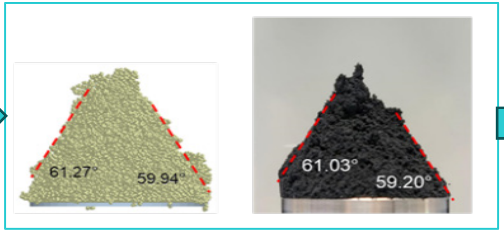
Material properties:
- v, ρ, G

Meso-scopic modeling



Macro behaviors

- Capture the macro-mechanical behaviour by CALIBRATION
- Achieve high computational efficiency



[1] Pantaleev, S., Yordanova, S., Janda, A., Marigo, M., & Ooi, J. Y. (2017). An experimentally validated DEM study of powder mixing in a paddle blade mixer. *Powder Technology*, *311*, 287–302.

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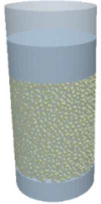
Standard Test for Battery process

Quasi-static flow regime
- Non-critical state consolidation
- Critical state consolidation

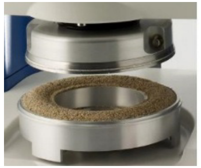
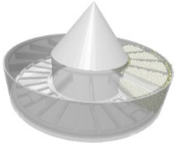
Dynamic flow regime
- Low stress free surface flows
- Highly dynamic systems

lab-scale

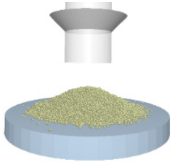
Uniaxial compression

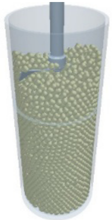
Direct shear

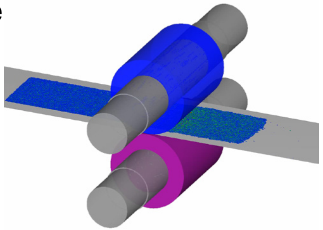
Angle of repose

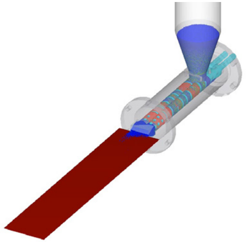
FT4 Flow Energy

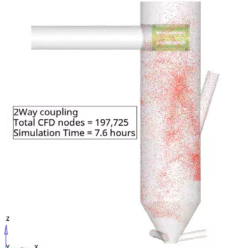
Industrial-scale



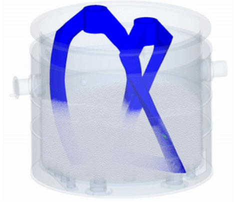
- Calendering



- Hopper
- Screw granulation

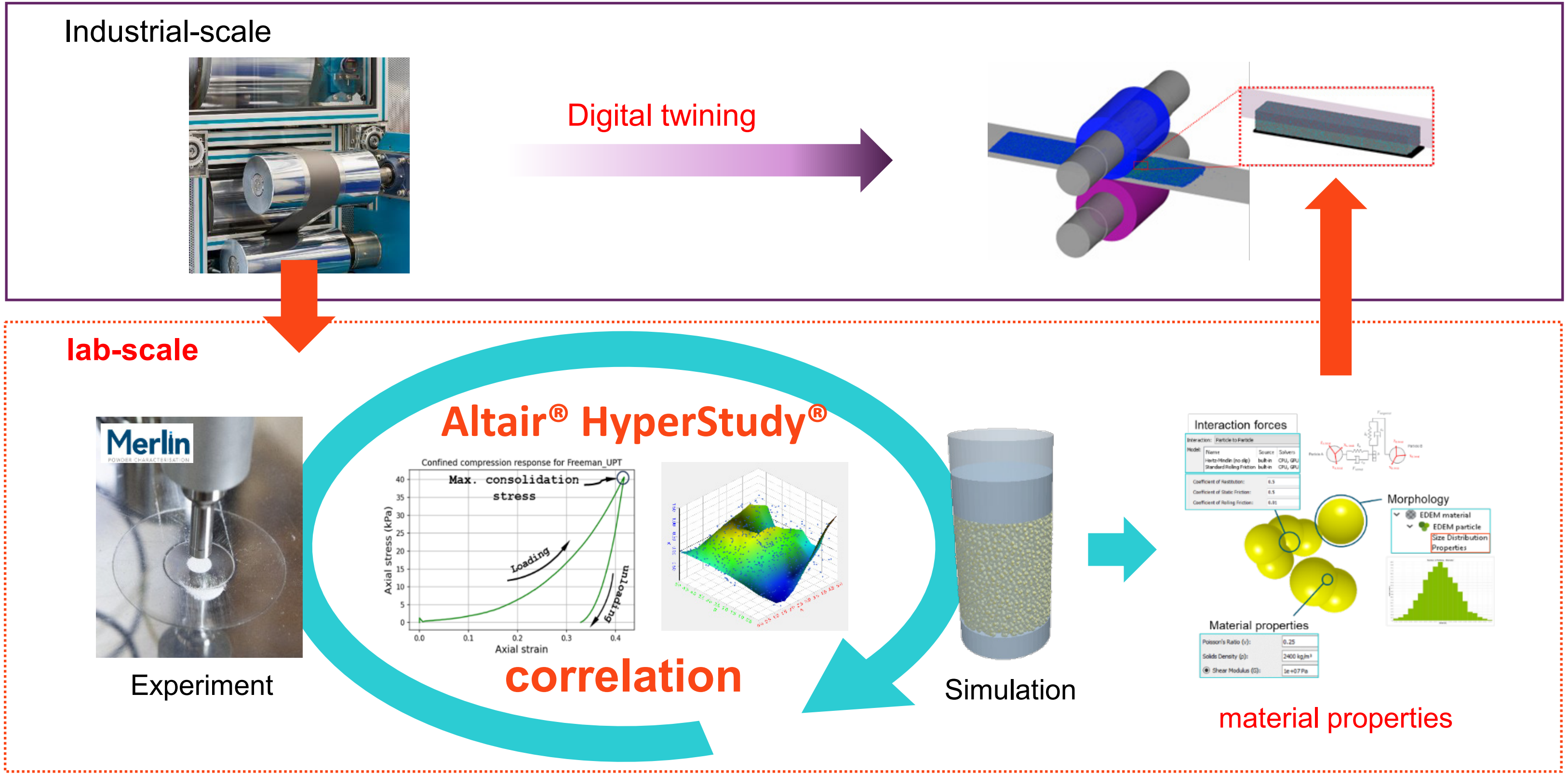


- Jet milling
- Powder drying



- Mixing
- Granulation

Automation for calibration using EDEM+HyperStudy



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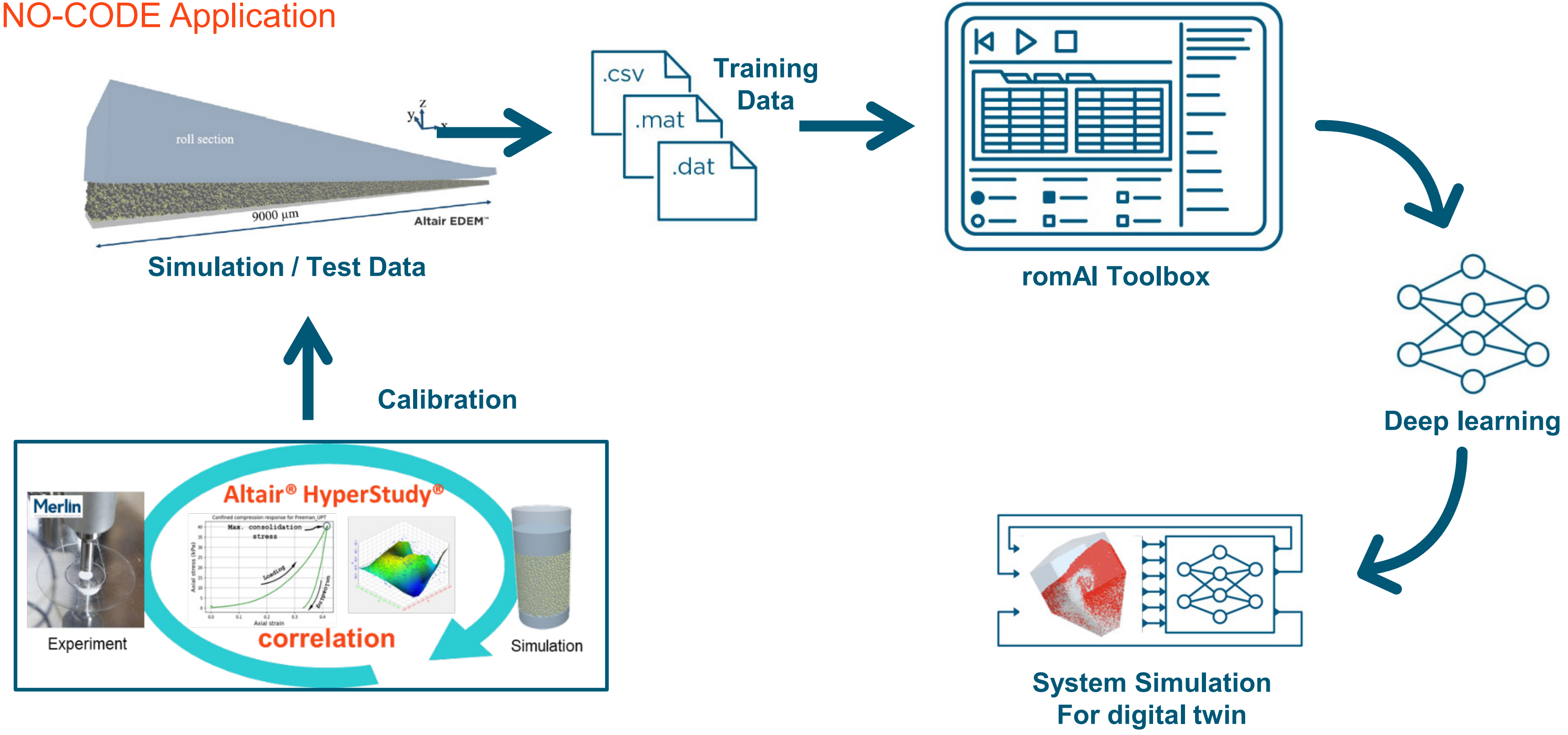
AI model generation with Altair® romAI™

NO-CODE Application



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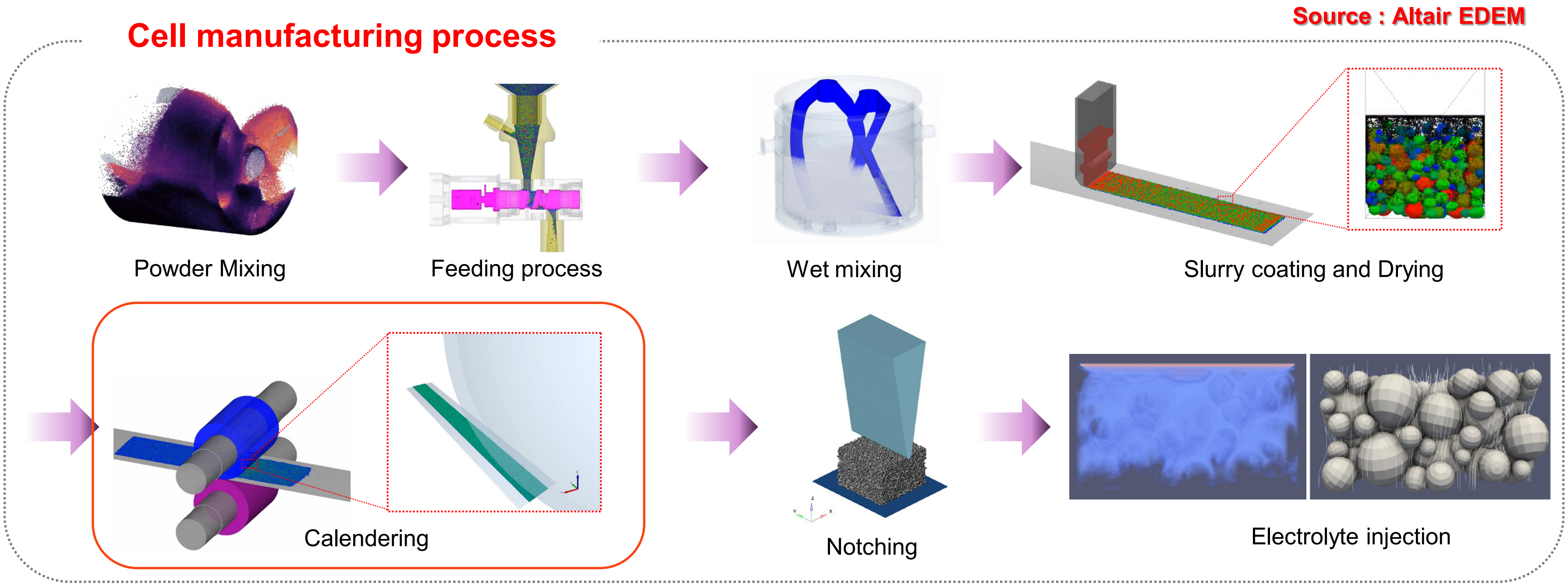
CALENDERING PROCESS USING EDEM + OPTISTRUCT

Particle Level Simulation for Battery Manufacturing Process

- DEM is the most suitable tool for simulating the battery cell manufacturing process.



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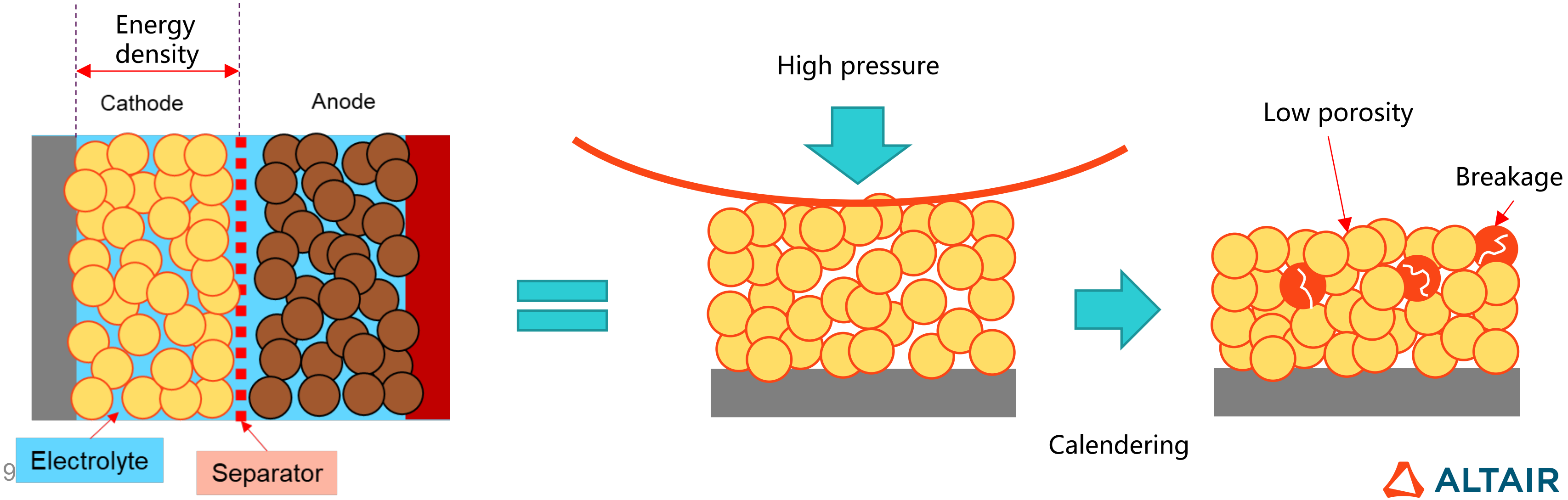
Use Cases of LIB manufacturing process

Process	Calibration method	KPI	Value to customer	Results from simulation	Solutions
Packing	Bulk density Angle of repose	Maximizing the bulk density for high energy density	Minimizing experiments with material variations	Packing density	EDEM
Calendering	Bulk density 1axis compression	Optimizing the process condition for the Optimal microstructure		Porosity tortuosity Connectivity	EDEM Optistruct
New material	Bulk density 1axis compression	Optimizing the blending ratio and PSD for high energy density		Mass ratio PSD Shear modulus	EDEM, AI
Mixing	Rheometer	Optimizing the process condition for mixing uniformity	Higher efficiency, lower losses, better quality	Mixing index	EDEM, AI
Multi roll mill (No solvent)	Bulk density Direct shear test	Optimizing the process condition for the uniform thickness & film strength		Thickness of film Stress of particles	EDEM, AI

Importance of Calendering

- The high energy density of the cell results from the high compressive density of the electrode.
- High pressure Calendering is required for high compression density.
- Particle density increases with high pressure, but efficiency decreases due to particle breakage or reduced voids.



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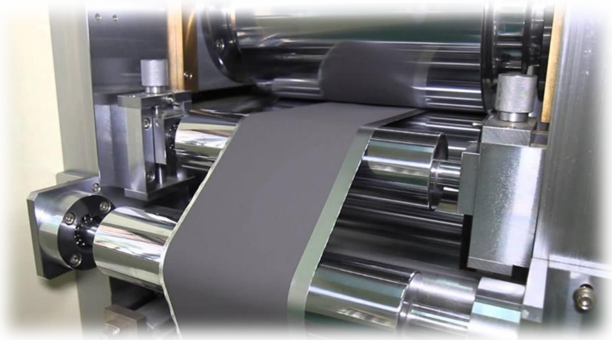
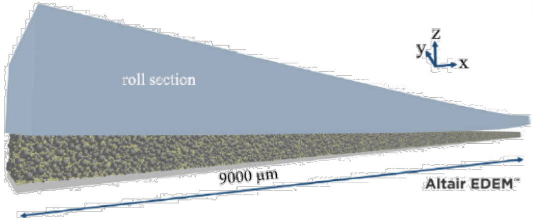
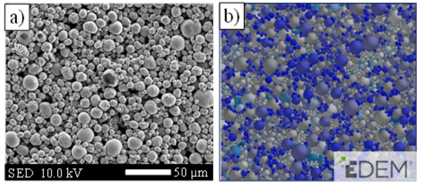
Importance of Calendering

- Particle properties
- Rheology
- Process parameters

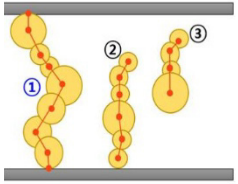




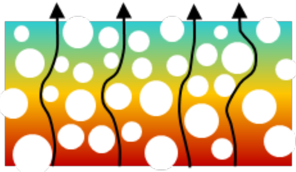


- Energy density
- Resistivity
- Discharge rate
- Service life etc…

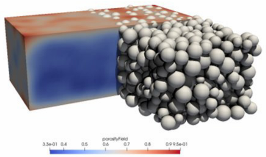
Connectivity



Tortuosity



Porosity



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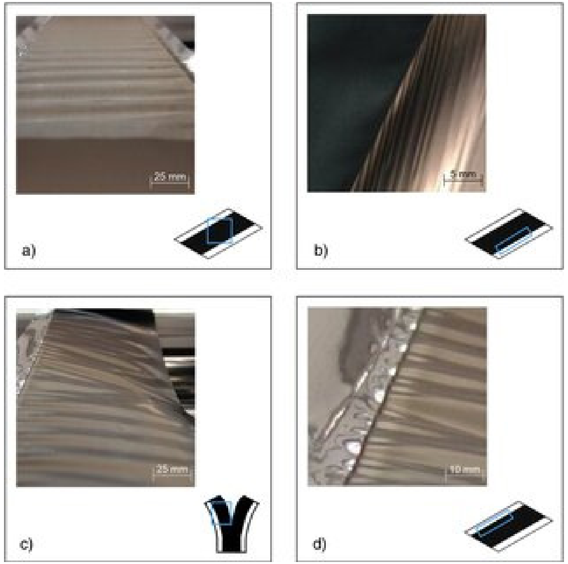
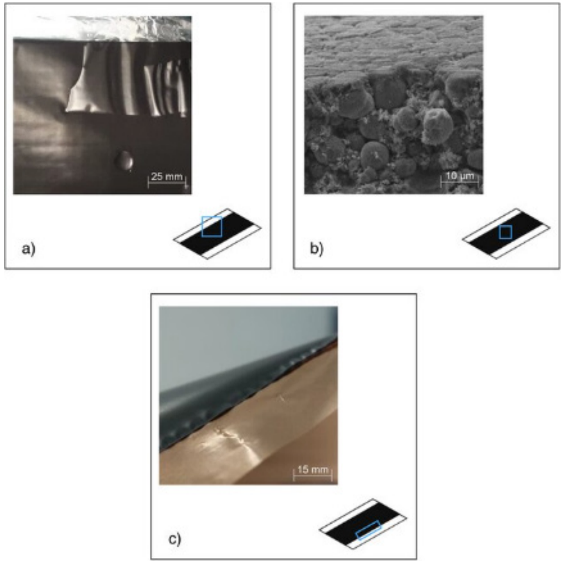
Electrode Defects

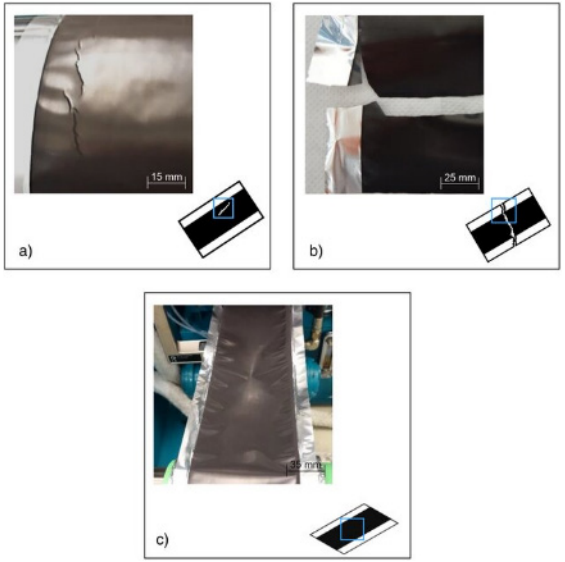
Defect related to geometrical defects	Defect related to mechanical defects



a) electrode corrugation, b) foil embossing,
c) saber effect d) corrugations at the coating edge.



a) local thickness and density fluctuations
b) sealed surface pores c) coating detachment.



a) crack formation in electrode, b) foil tear
c) embrittlement of the electrode.

“Classification of Calendering-Induced Electrode Defects and Their Influence on Subsequent Processes of Lithium-Ion Battery Production”,
Till Günther, David Schreiner, Ajinkya Ganesh Metkar, Gunther Reinhart

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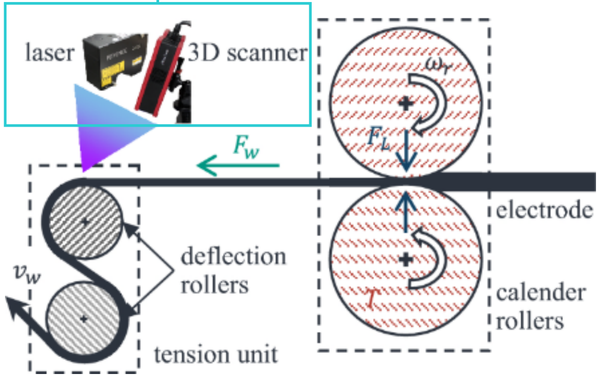
Process variable analysis

- Main parameters

- Bulk density of electrode ρ
- web speed v_W
- angular speed of the rollers ω_r
- temperature T of the rollers
- line load F_L
- web tension F_W



Formation of a longitudinal wrinkle
with the coating edge on the left side

"Analysis of longitudinal wrinkle formation during calendering of NMC811 cathodes under variation of different process parameters" Ann-Kathrin Wurba, Lennart Altmann, Jürgen Fleischer

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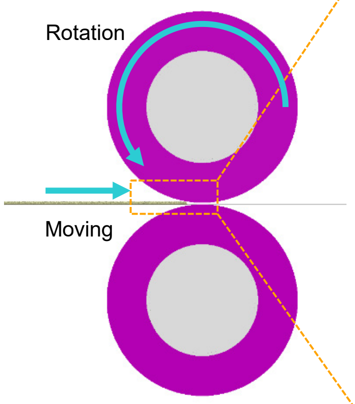
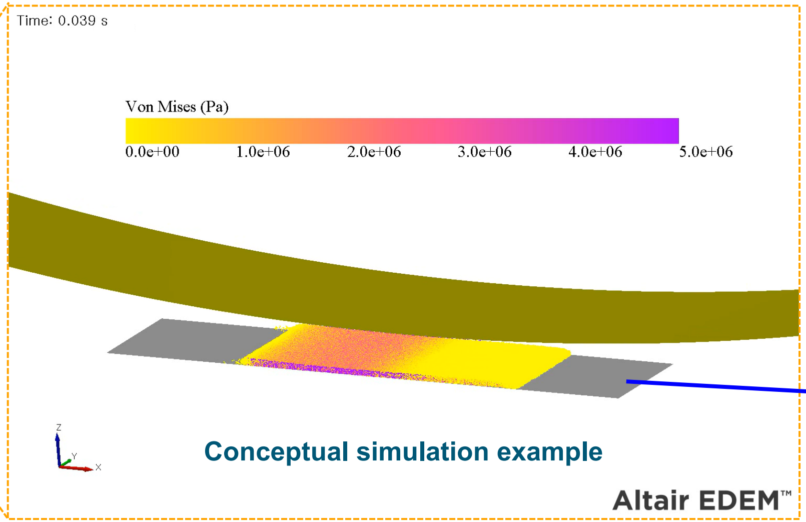
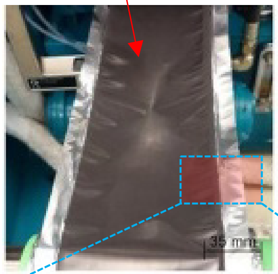
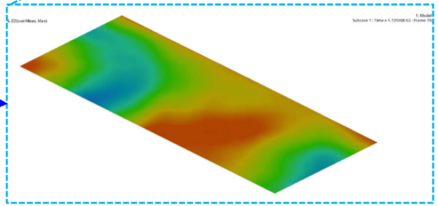
Calendering – concept

- EDEM can provide the evolution of microstructure during press process
- Deformation of foil can be simulated using DEM-FEM 2way coupling
- Easy to optimize the process parameters of press process using Hyperstudy





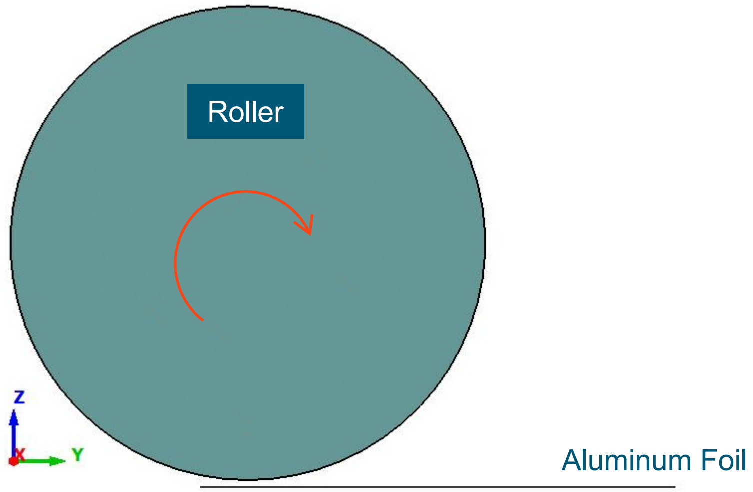




Foil deformation

Calendering – outline

- Calendering using **EDEM-FEA coupling** involves modeling the interaction between particulate mate rials and deformable structures.
- This coupling allows detailed analysis of material behavior under compression such as
    - ✓ Roll force
    - ✓ Stress distributions
    - ✓ Structural deformations



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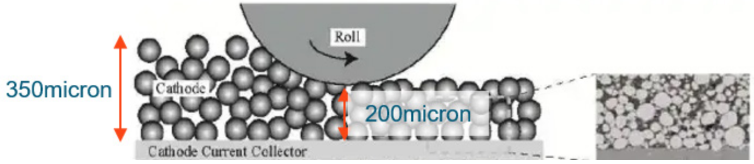
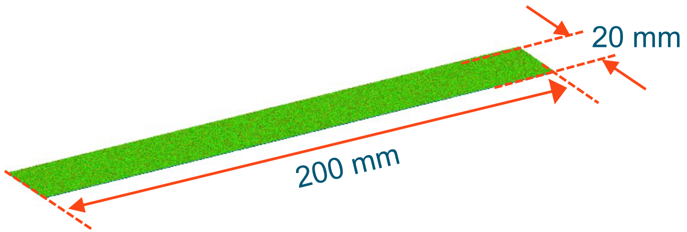
Modeling detail

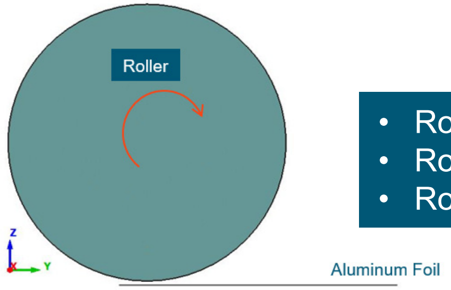
- *Cathode particles are modelled for the dimension such as*
- *Length =200 mm*
- *Width = 20 mm*
- *Depth= 0.35 mm (350 micron)*
- *Roller is moved to compact the cathode material to a depth of 200 micron*
- *Aluminum foil is fixed in vertical (Z-axis) and free in other two axis*
- *Aluminum modelled using Solid (Hexa) elements*



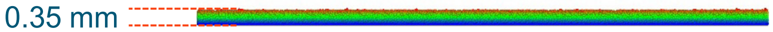
https://iestbattery.com/

Roll press





- Roller rotates at 3 rad/s
- Roller translational velox=city is 0.3 m/s
- Roller Diameter is 200mm



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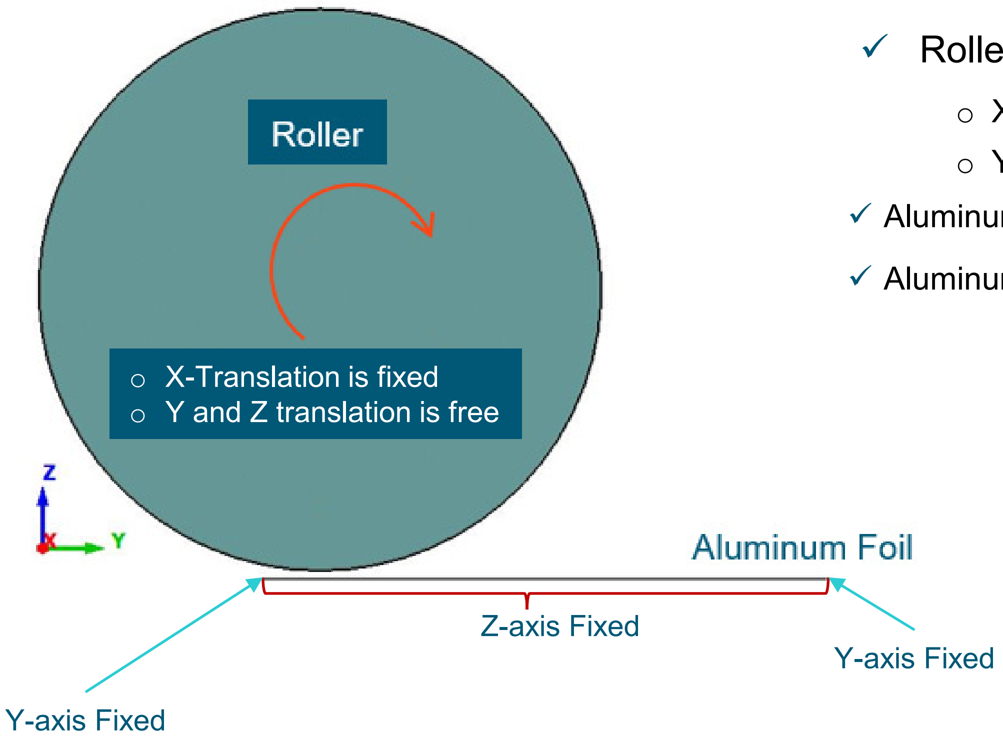
Boundary condition



- ✓ Roller Constrain:
  - X-Translation is fixed
  - Y and Z translation is free
- ✓ Aluminum Foil bottom face is constrained in Z- axis
- ✓ Aluminum Foil Side face is constrained in Y- axis

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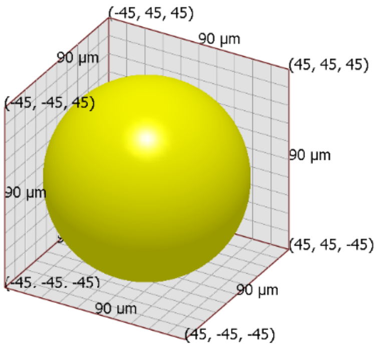
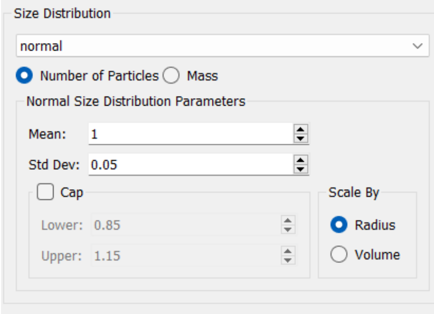
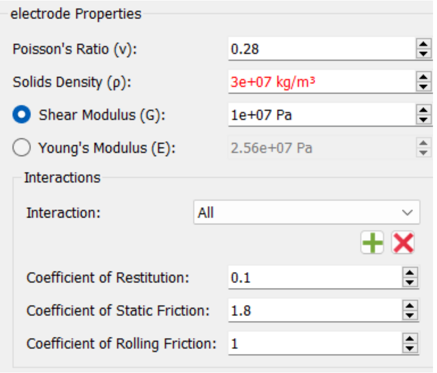
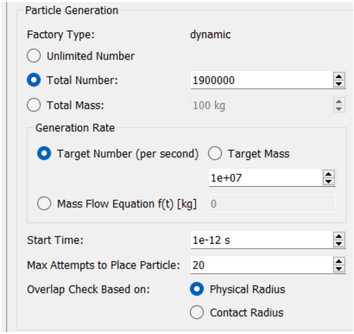
EDEM setting

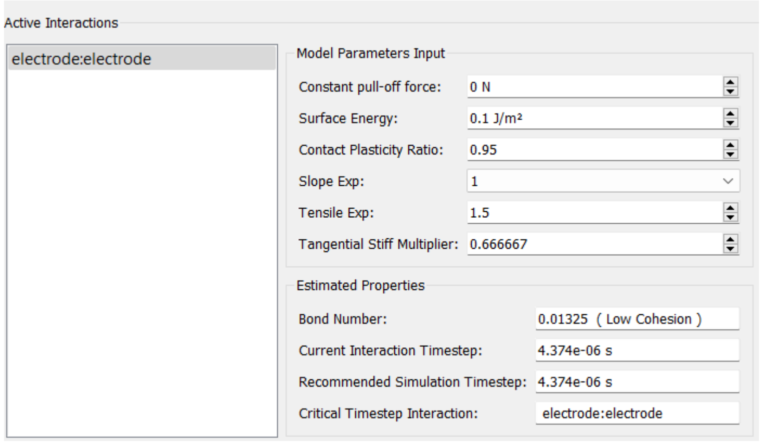








- Physics for particle to particle



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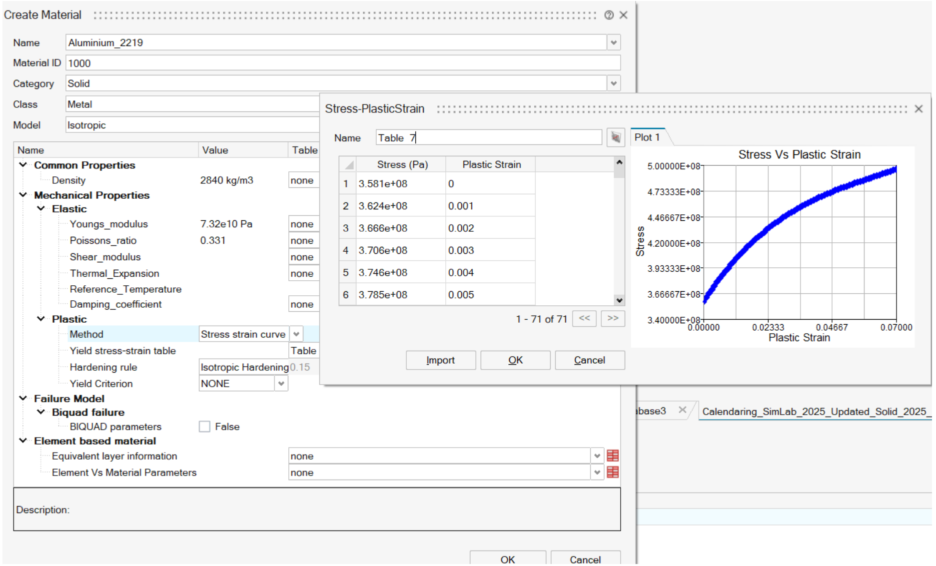
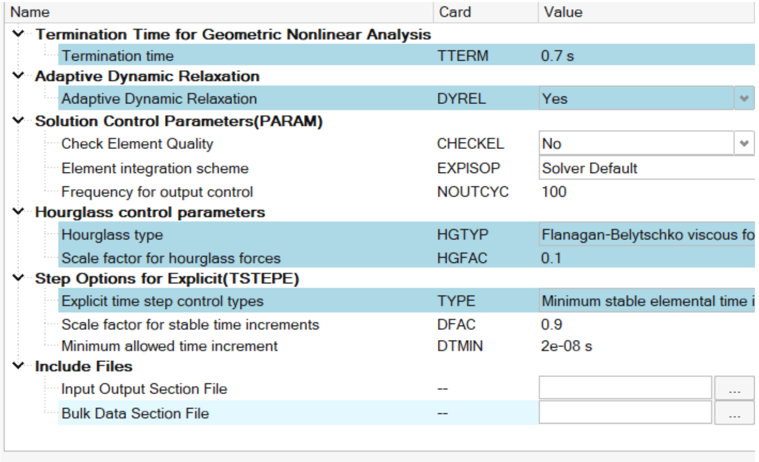
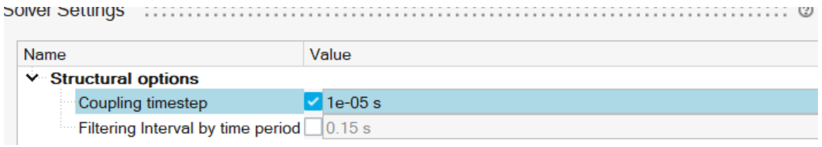
Simlab(Optistruct) setting

- Nonlinear material properties for Al foil







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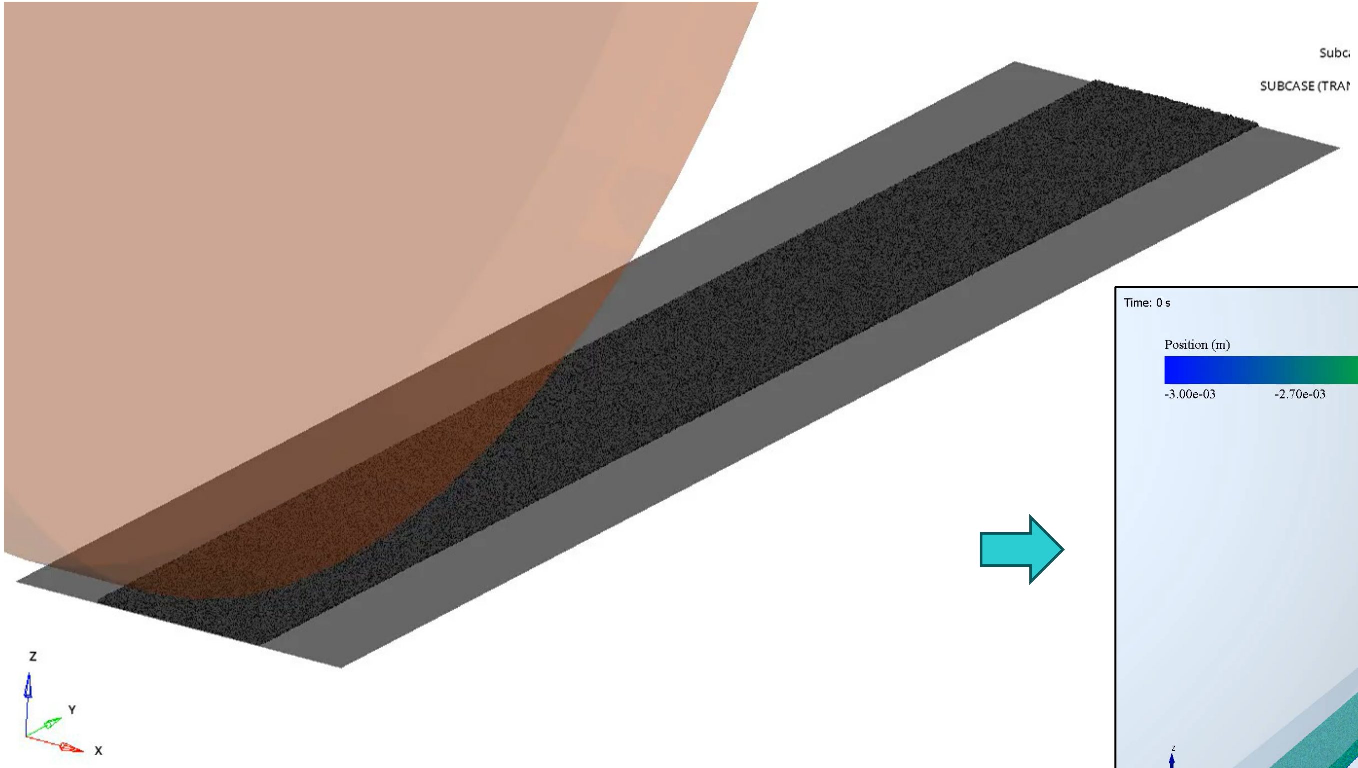
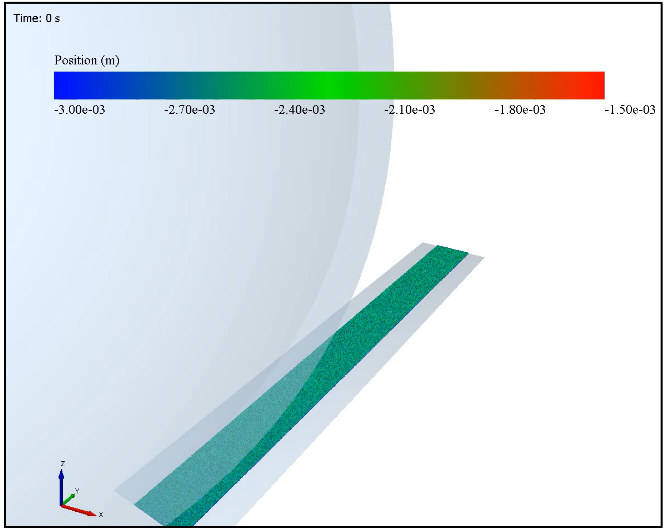
Simulation Overview





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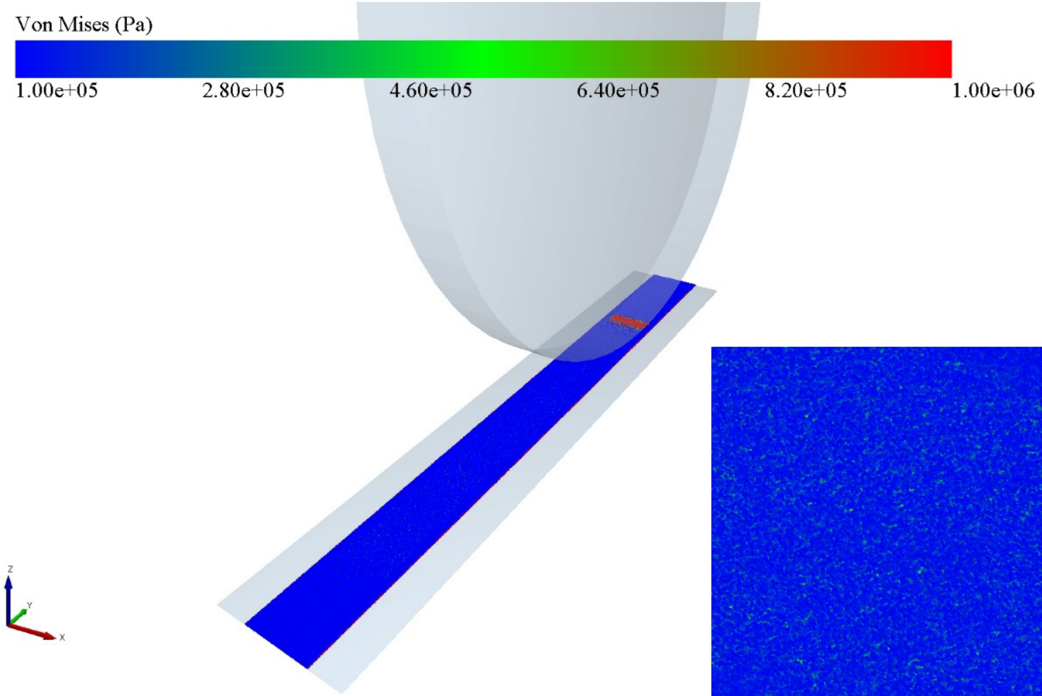
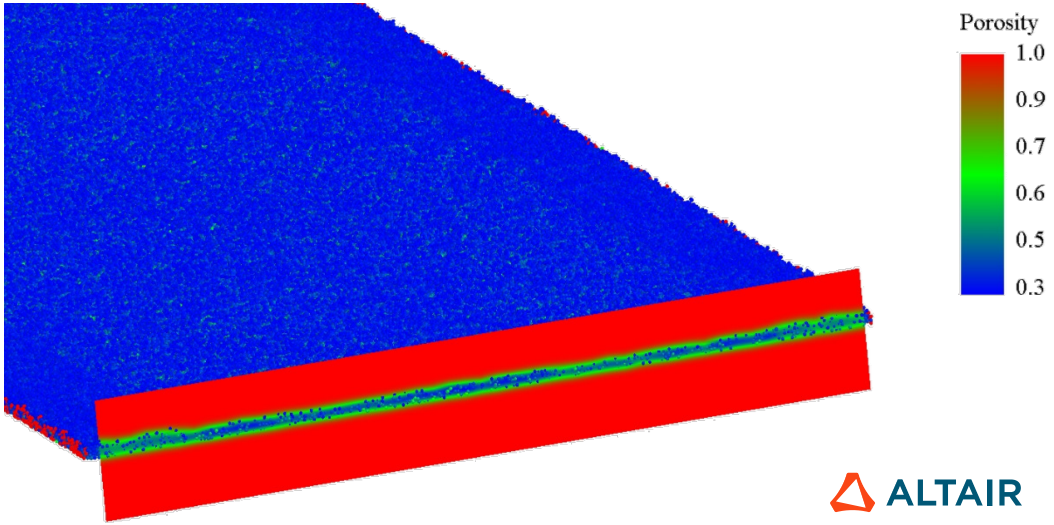
Particle Stress & Porosity





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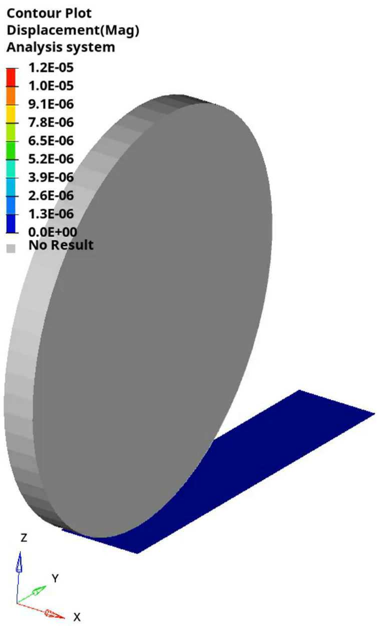
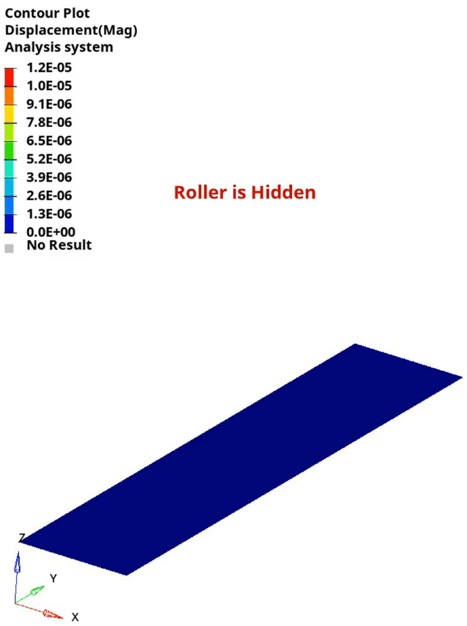
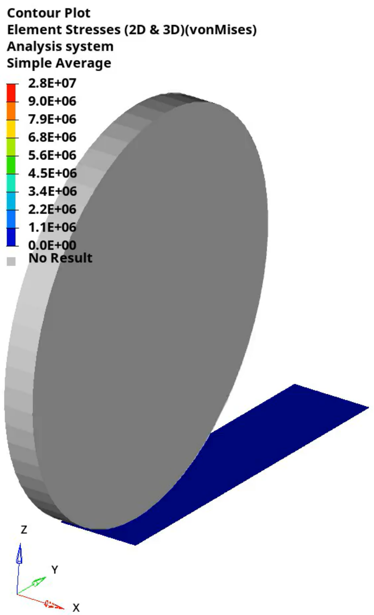
Aluminium Foil

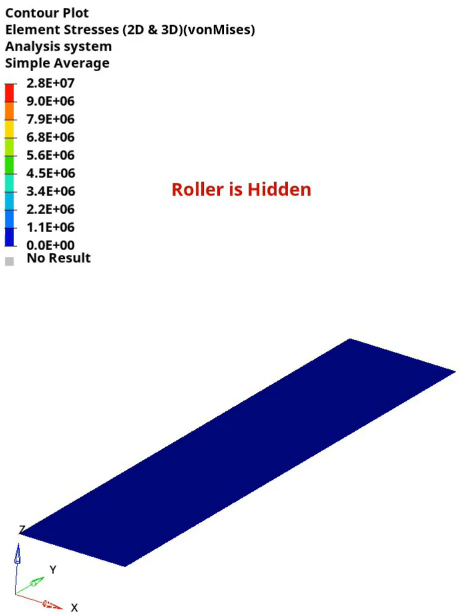
Displacement





VonMises Stress





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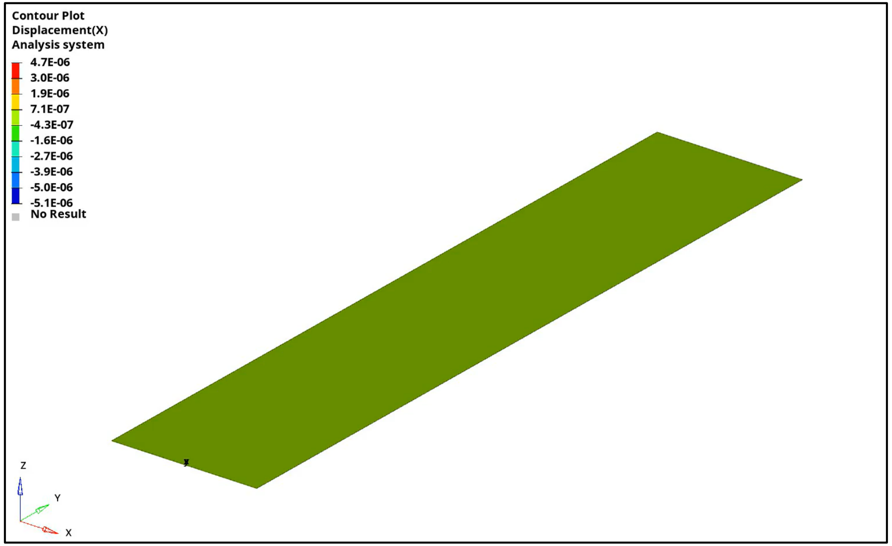
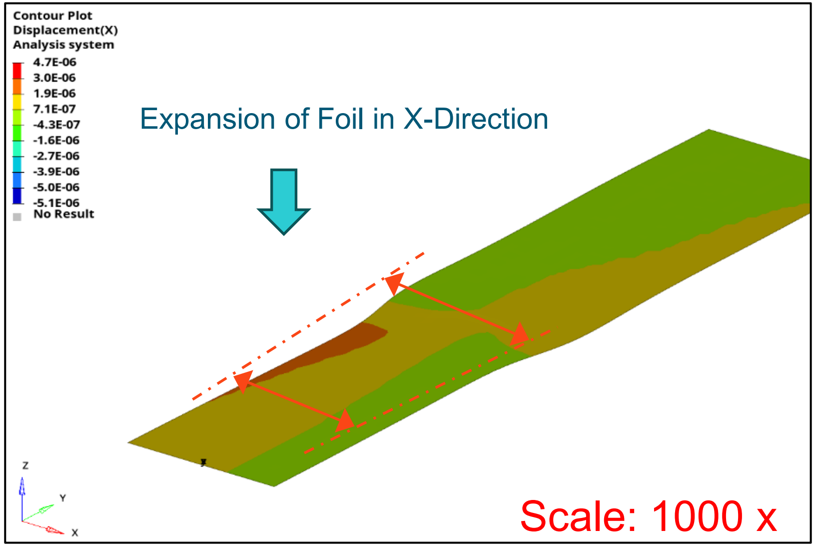
Aluminium Foil Displacement





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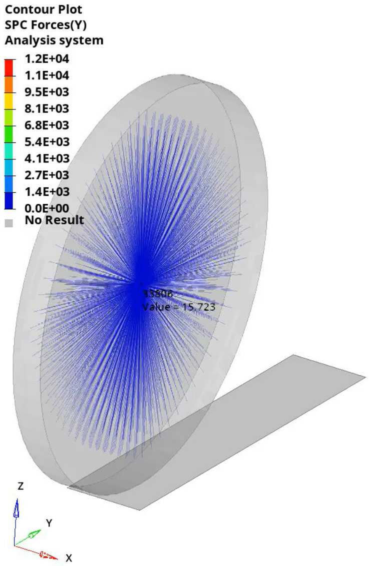
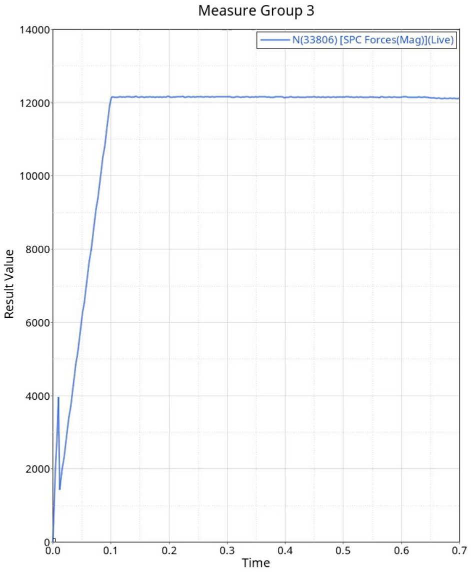
Force

Roller Reaction Force





Aluminium Foil Reaction Force

ROLL PRESSING PROCESS USING EDEM + ROMAI

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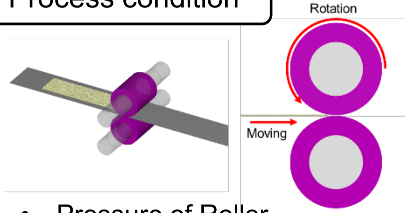
Overall process

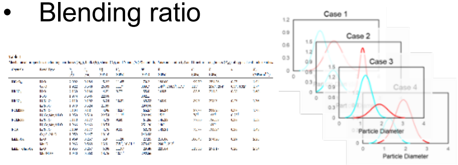
Process condition



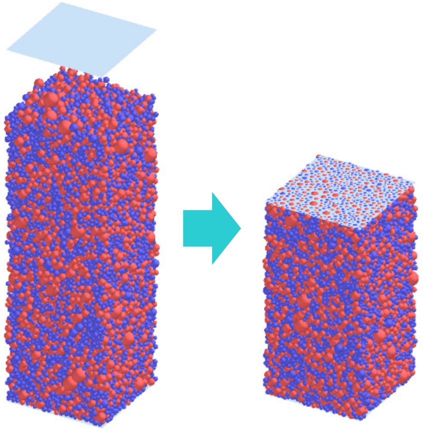
- Pressure of Roller
- Gap size

Material condition

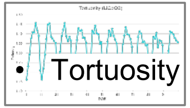
- Particle size distribution
- Shear modulus of particle
- Blending ratio



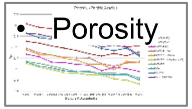
DEM simulation



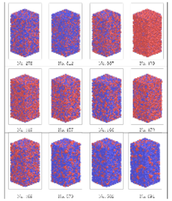
Microstructure DB



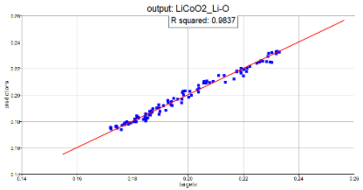
- Tortuosity

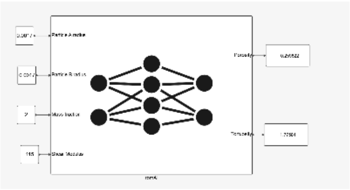


- Porosity



romAI





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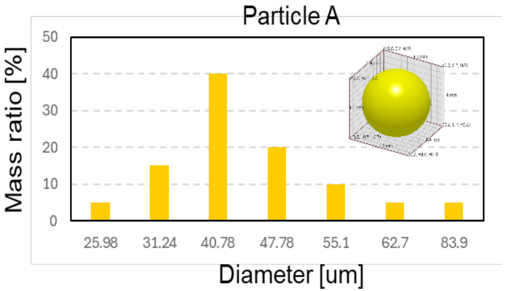
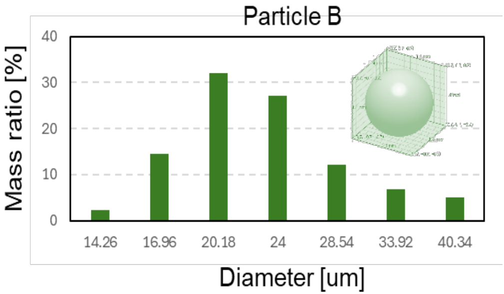
Particle size distribution

- Variable parameters
  - Mass ratio of A and B
  - Scale of D50 of each particle
  - Shear modulus, Poisson's ratio of each particles
- Fixed parameters
  - Total mass of particles
  - PSD of each particle





Crystals	Bond Type	G (GPa)	E (GPa)	ν
$LiCoO_2$	Li-O	99.79	254.36	0.27
	Co-O	115[c]	236[a], 264[c]	0.3[a], 0.32[c]
$LiNiO_2$	Li-O	83.5	214.3	0.28
	Ni-O			
$LiNiO_2$	Li/Ni-O	89.7	228.7	0.27
	Li/Ni-O			
NCM333	Li/Ni-O	87.78	223.95	0.28
	Li/Co/Mn/Ni-O	78[d]	199[d]	0.25[d]
NCM622	Li/Ni-O	77.00	196.53	0.28
	Li/Co/Mn/Ni-O		180[e]	
NCA	Li/Ni-O	75.77	193.24	0.28
	Co/Al/Ni-O			
$LiMn_2O_4$	Li-O	106.43	274.26	0.29
	Mn-O			
$LiMn_{1.5}Ni_{0.5}O_4$	Li-O	113.30	291.17	0.28
	Mn/Ni-O			

Liu Xiao (2024), *Mechanical properties modeling of cathode materials for lithium-ion batteries based on bond valence model*, Materials Today Communications, vol 39

DOE space - full factorial

- 4 factor, 10 level : 10000 cases for simulation
- 4 factor, 3 level : 81 cases for deep learning

# of Level	10	10	10	10	
Properties	Particle A Scale	Particle B Scale	Mass fraction	Shear Modulus	Poisson's ratio
Level	0.7	0.7	1:9	75.8	0.28
	0.811	0.811	2:8	77.0	0.28
	0.922	0.922	3:7	78.0	0.25
	1.033	1.1033	4:6	83.5	0.28
	1.144	1.144	4.5:5.5	87.8	0.28
	1.256	1.256	5:5	89.7	0.27
	1.367	1.367	6:4	99.8	0.27
	1.478	1.478	7:3	106.4	0.29
	1.589	1.589	8:2	113.3	0.28
	1.7	1.7	9:1	115.0	0.32

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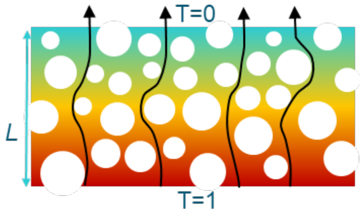
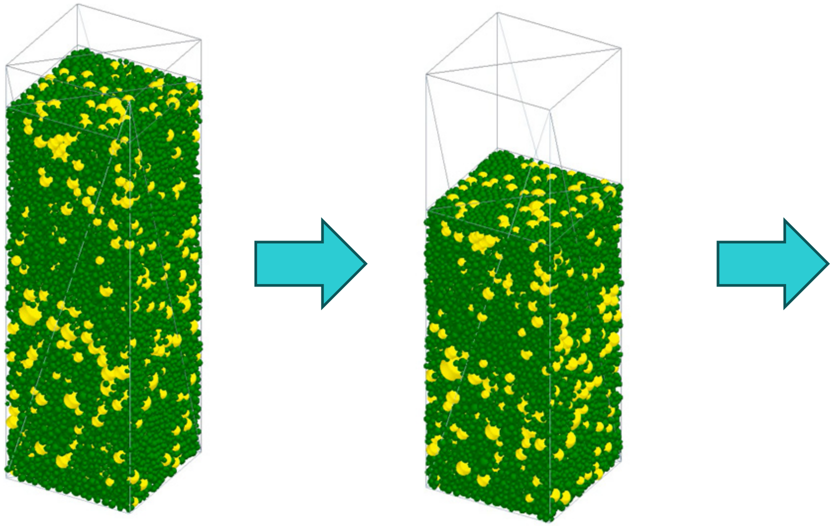
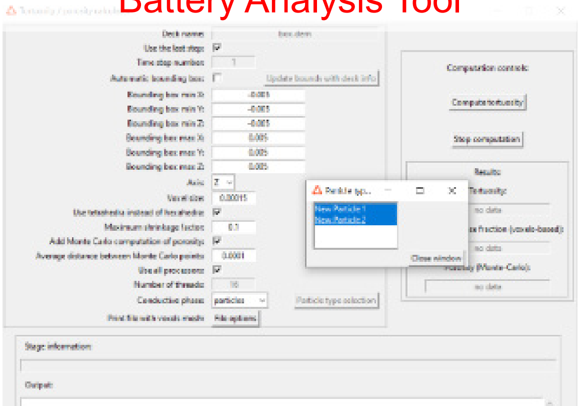
Simulation Modeling

- Periodic boundary is used
- Particle is generated by using volume packing
- Pressing condition is from the actual roll pressing process





Battery Analysis Tool



Diffusive Tortuosity (τ) computed as

$$\tau = \frac{straight\_flux}{tortuous\_flux} = \frac{k}{k'} (\geq 1.0) \quad \text{with } flux = k\frac{A(T_1 - T_0)}{L}$$

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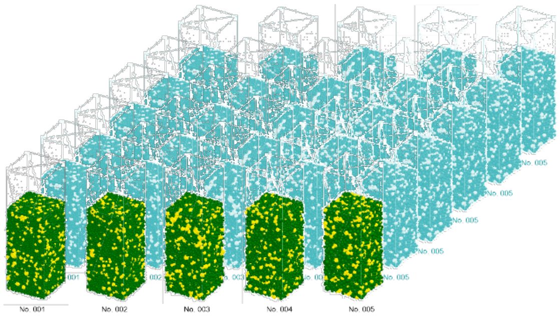
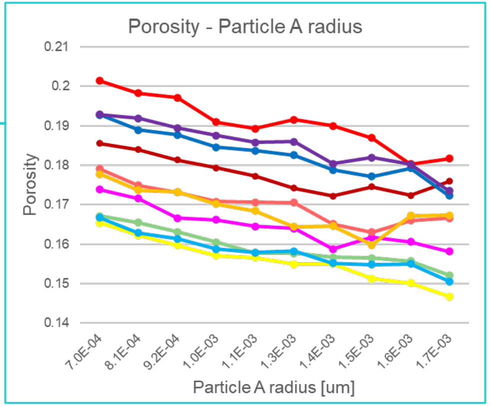
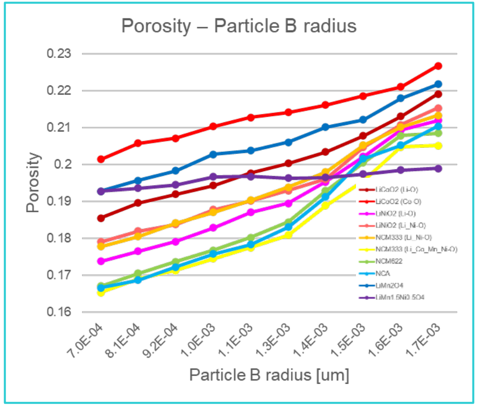
Result

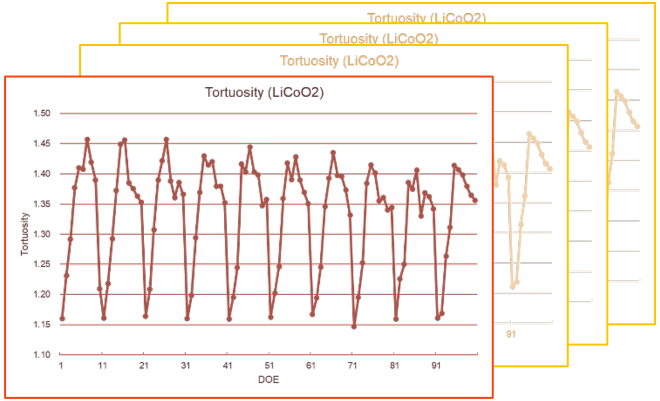
- Porosity and Tortuosity
- Microstructure 81ea



Microstructure

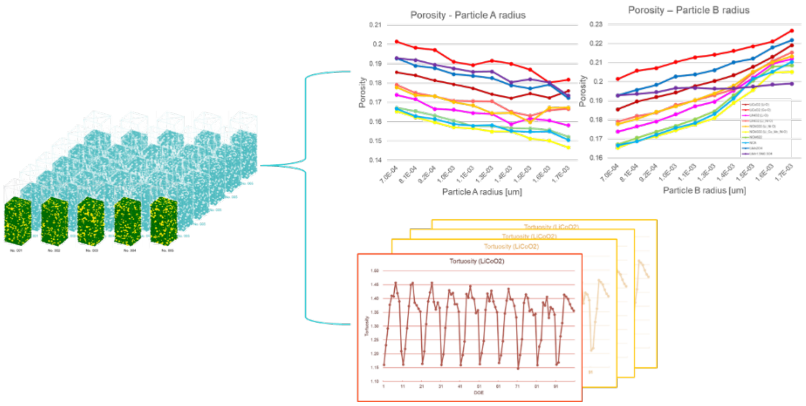


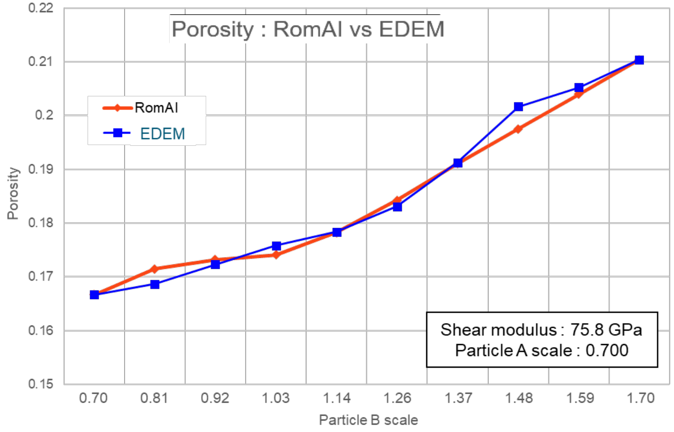


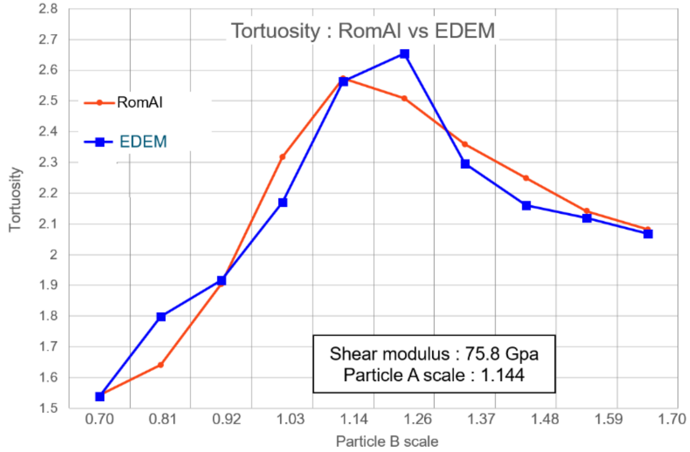


Deep learning - romAI

- R square : 0.93 for Tortuosity, 0.98 for Porosity
- By reducing simulation cases from 10,000 to 81, less than 1% of the initial time cost was required







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SUMMARY

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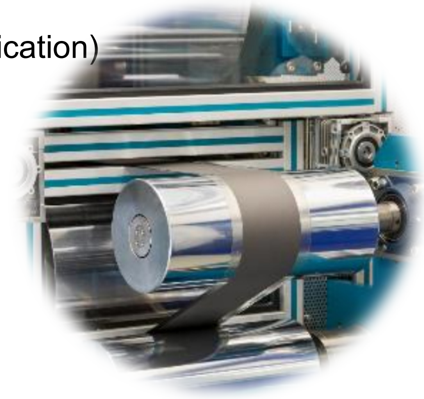
Advanced feature of EDEM for battery

❖ Unique Physics model

1. Edinburgh-Elasto-Plastic-Adhesive Model
2. Liquid Bridge and Transfer Model
3. Slurry model (Hydrodynamic Lubrication)
4. Breakage model

❖ Battery Analysis tools

1. Porosity, permeability, connectivity
2. Easy to connect with Data Analytics
3. Tortuosity Analysis



❖ Pre-Processing

1. Powder Database
2. Material Calibration tool

❖ Multi-physics

1. DEM-CFD : EDEM-AcuSolve
2. DEM-FEM : EDEM-Optistruct

❖ AI convergence

1. romAI
2. HyperStudy ML

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THANK YOU

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#ONLYFORWARD

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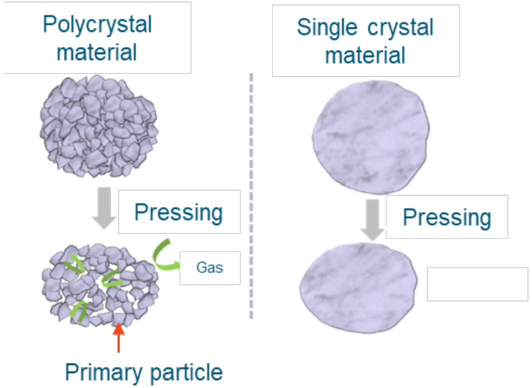
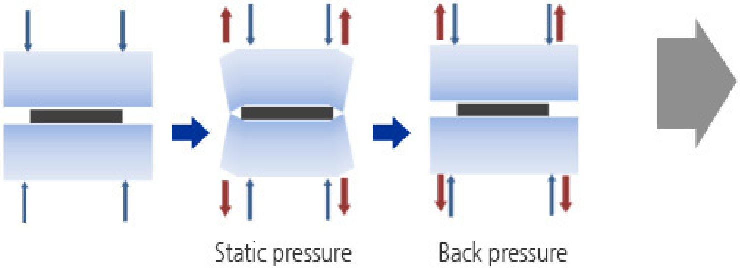
BACK DATA

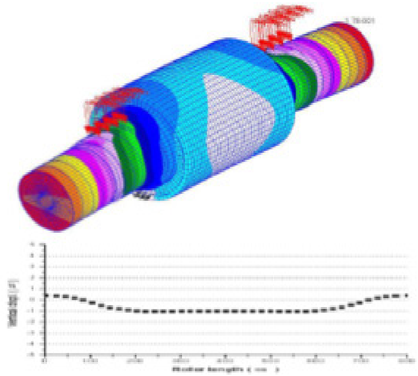
Future

- Modeling closer to the actual process scale.
- Additional research on the actual boundary conditions is needed.
- The anisotropy of aluminum foil needs to be considered.
- The profile of roller can be considered for structural analysis.
- And Heat transfer between electrode and roller can be considered



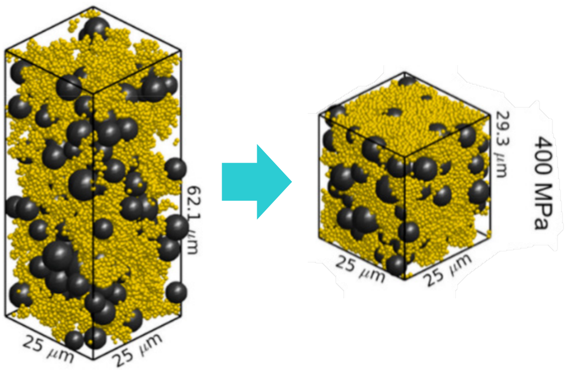


http://www.cisro.co.kr/

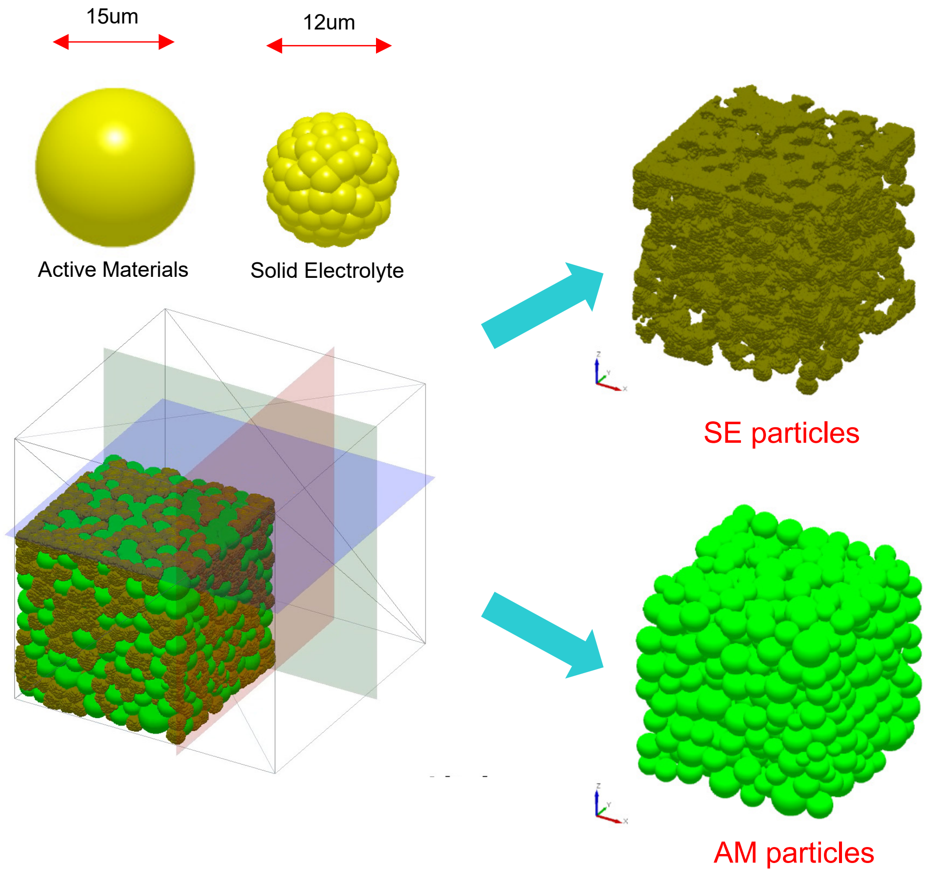


All Solid-State Battery

- Simulation of isotropic pressurization process
- Simulation of deformation of solid electrolyte
- Reference paper



Effect of mold pressure on compaction and ion conductivity of all-solid-state batteries revealed by the discrete element method, October 2021Journal of Power Sources, Magnus So, Gen Inoue, Ryusei Hirate, Keita Nunoshita, Shota Ishikawa, Yoshifumi Tsuge.



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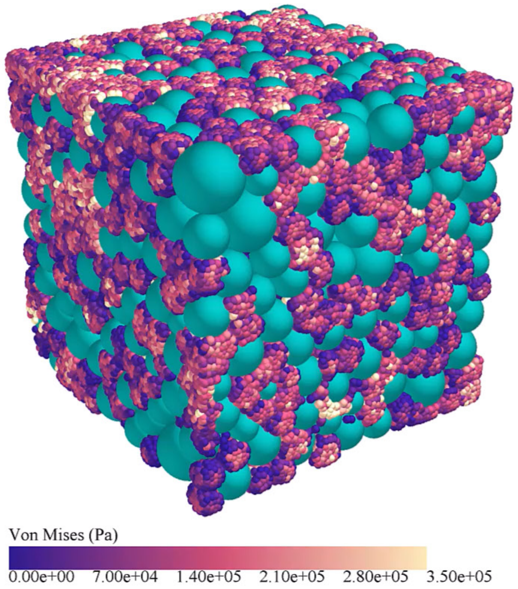
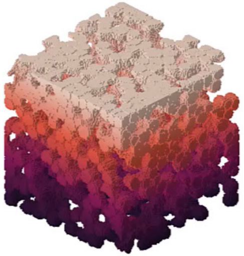
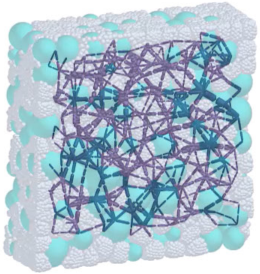
Maximize the battery performance when simulating its microstructure by:



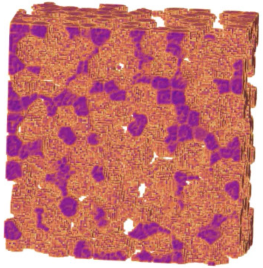
Obtain the components stress during compaction



Analyzing the microstucture tortuosity



Predict the electrode percolation



Identify the porosity distribution

Battery Industry customer

EV OEM

TESLA
BYD
HYUNDAI MOTOR GROUP

Cell manufacturer

CALB
LG Energy Solution
CATL
acc AUTOMOTIVE CELLS Co
SAMSUNG SAMSUNG SDI
SK on

Equipment industry

JEIL M&S
NARA
LG Electronics
Hanwha Corporation/Momentum

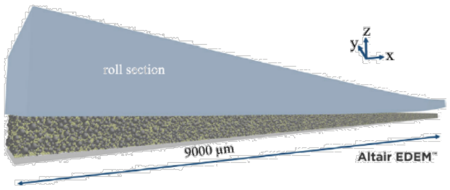
Material industry

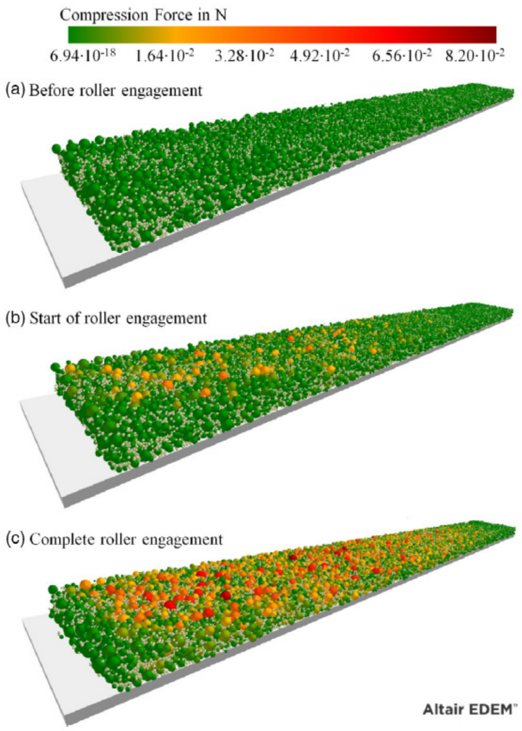
umicore
posco HOLDINGS
LG Chem
EcoPro BM
SUMITOMO METAL MINING

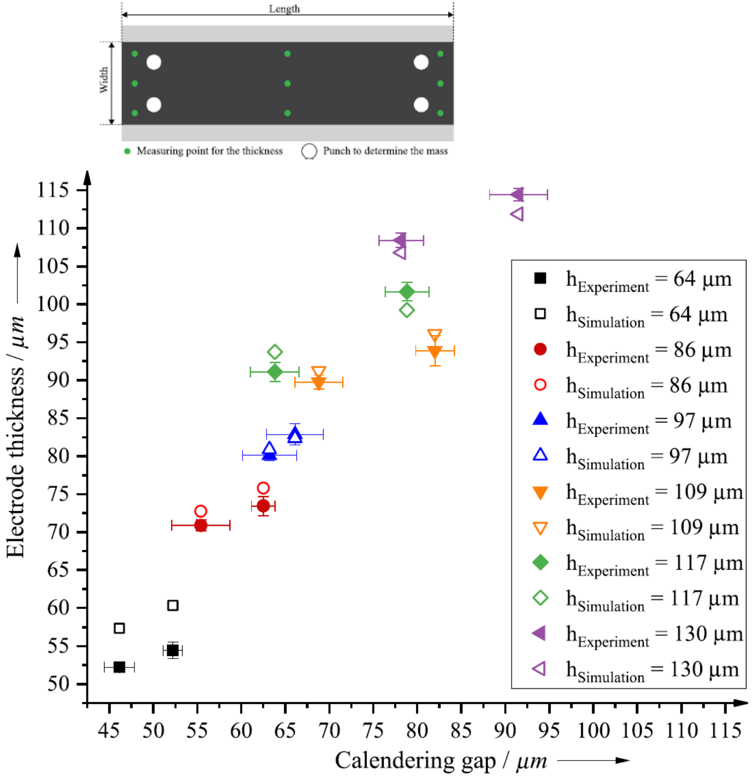
Research

KETI Korea Electronics Technology Institute
RIST 재단법인 포항산업과학연구원
NEXTRODE
tusail
TUM
University of Sheffield

Battery Manufacturing Simulation – calendering







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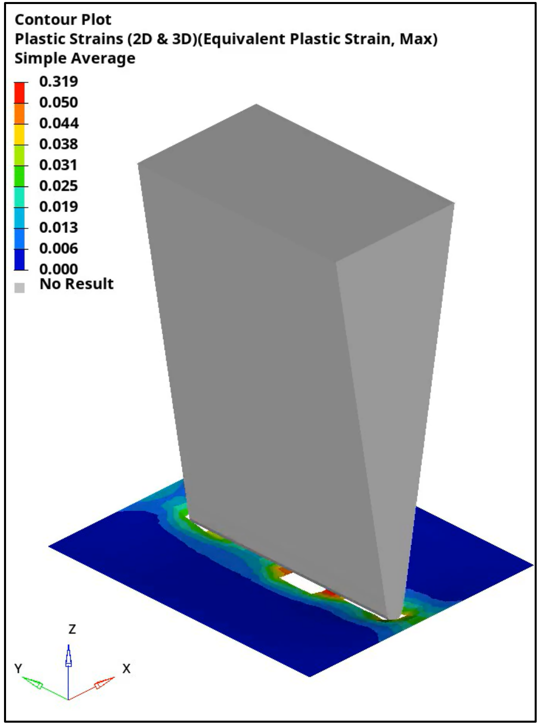
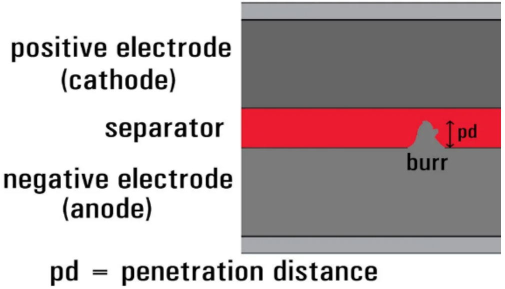
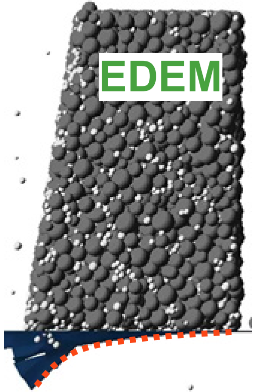
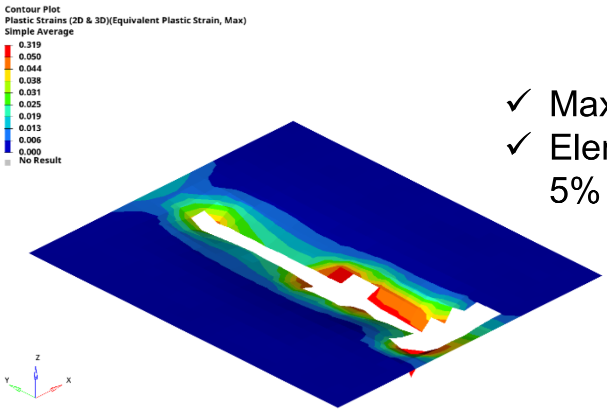
Notching: Plastic Strain







https://www.leica-microsystems.com/science-lab/industrial/burr-detection-during-battery-manufacturing/



- ✓ Maximum Plastic Strain= 31.9%
- ✓ Elements exceeding plastic strain 5% is damaged

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