Multiscale modelling of Li-ion battery and battery-protective materials

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Background story and problem definition

Li-ion battery technology is expected to be the energy storage for choice for EVs in the coming years.

Advantages:

Better energy & power performance

Higher volume & weight efficiency

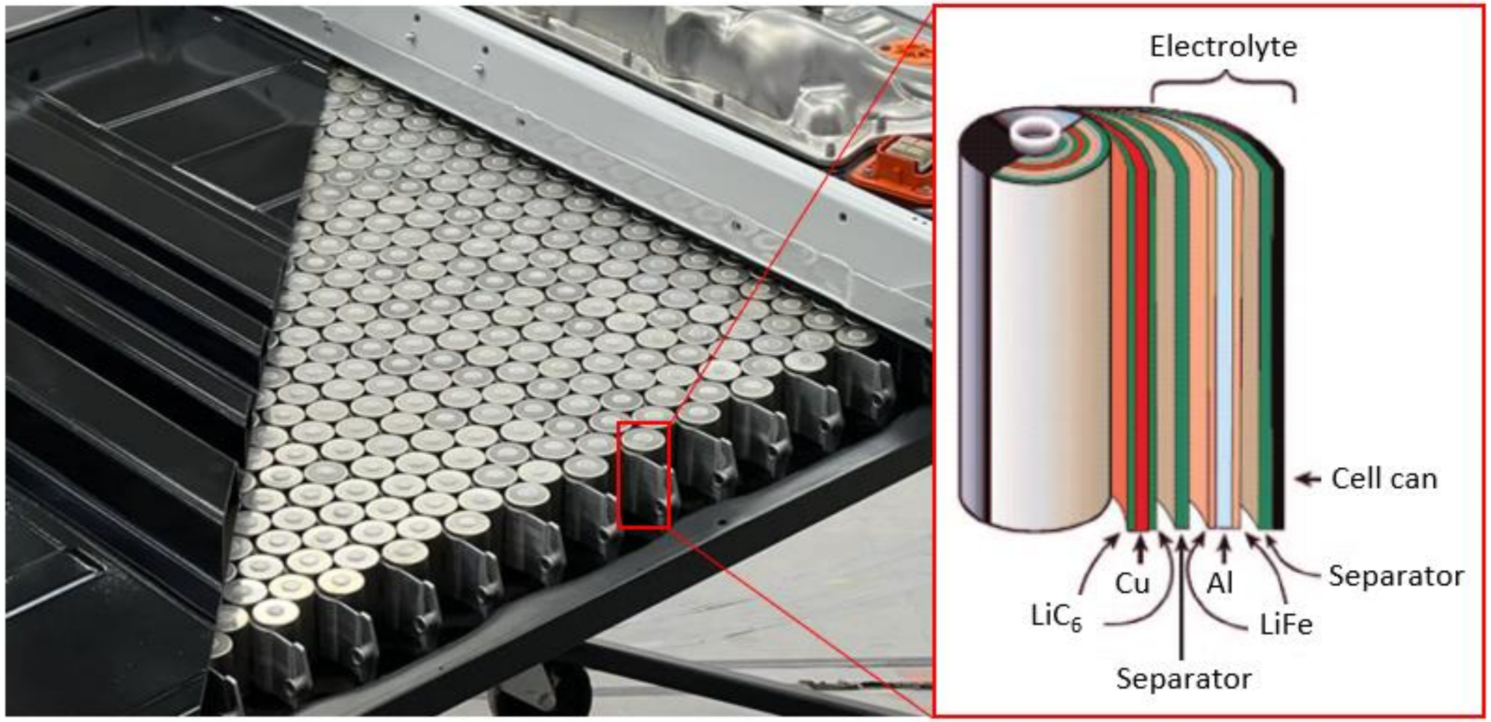
Disadvantages:

Battery life

Safety

Driving range

Charging time



Thermal runaway of Li-ion cells

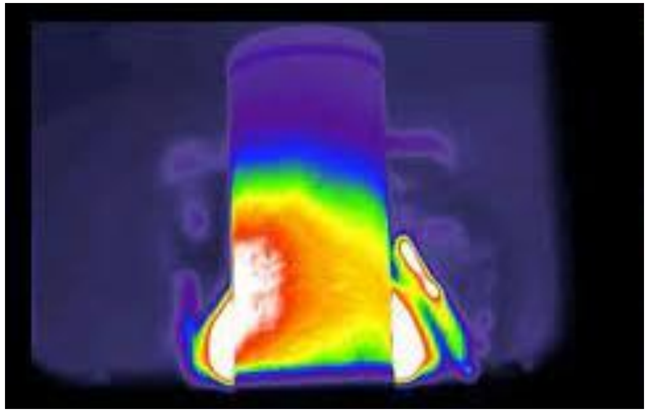
Optimal range
15-35 ºC

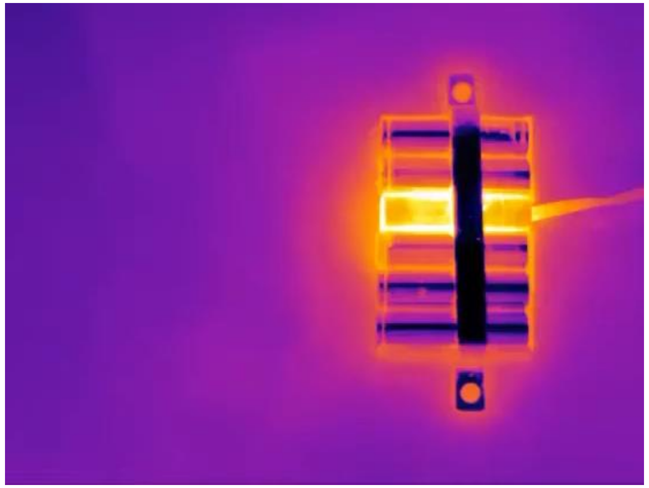
Below range:
Capacity drops
Slower charging
Reduce battery life

Above range:
Battery degradation
Prone to thermal runaway
Lower efficiency

External abusive conditions:
External heating
Over charging
Over discharging

Thermal runaway:
Smoke
Flames
Gas venting
Explosions



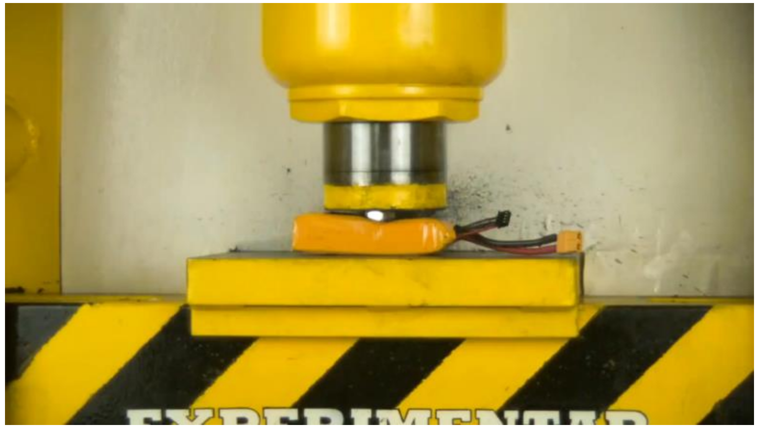


Mechanical abuse of Li-ion cells

Compressive loads

- Voltage drop
- Temperature increase
- Thermal runaway

- Affects battery life
- Can become inoperative
- Fire ignition
- Explosions
- Short-circuit



State of art: Battery modelling

Thermal modelling:

- Temperature discharge
- Thermal runaway
- Heat dissipation

+

Mechanical modelling:

- Compression test
- Mechanical integrity
- Stress measurements

=

Thermo-mechanical coupled model:

Investigation of mechanical properties with controlled temperature changes

Thermo-mechanical model

Steady-state heat conduction

$$\nabla^{\mathrm{T}}\mathbf{q} + Q = 0$$

$$q = \begin{pmatrix} q_x \\ q_y \\ q_z \end{pmatrix} = -\begin{bmatrix} k_{xx}, & k_{xy}, & k_{xz} \\ k_{yx}, & k_{yy}, & k_{yz} \\ k_{zx}, & k_{zy}, & k_{zz} \end{bmatrix} \begin{pmatrix} \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial y} \\ \frac{\partial T}{\partial z} \end{pmatrix} = -k\nabla T$$

$$\nabla^T = [\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}]$$

$$-\nabla^T(k\nabla T) + Q = 0$$

Heat dissipated by convection and radiation is ignored here!

Transient heat conduction

$$c\frac{\partial T}{\partial t} - \nabla^T(k\nabla T) + Q = 0$$

Thermoelastic effect:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}^M = C_{ijkl}(\epsilon_{kl} - \epsilon_{kl}^T)$$

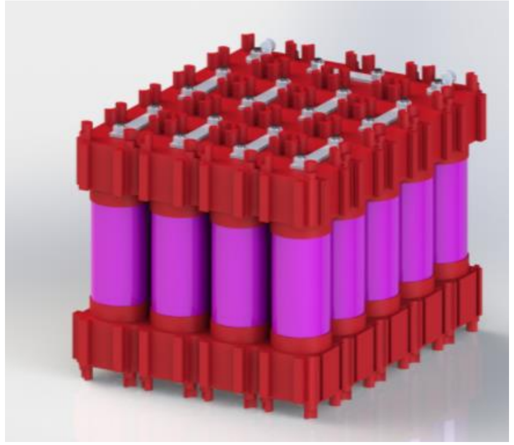
$$\epsilon_{kl}^T = \alpha\Delta T\delta_{kl}$$

$$\delta_{kl} = \begin{cases} 1 & if \quad k = l \\ 0 & if \quad k \neq l \end{cases}$$

$$\sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \alpha\Delta T\delta_{kl})$$

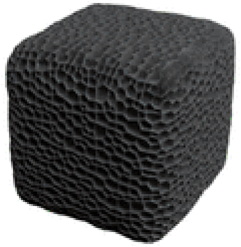
Project aim and overall framework

Battery pack enclosure: load bearing + heat dissipation

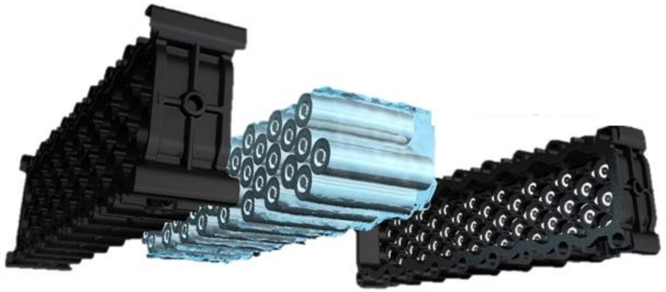


Composite material will ‘wrap’ cells to protect them from mechanical and thermal abuses, and facilitate the load transfer in case of collisions

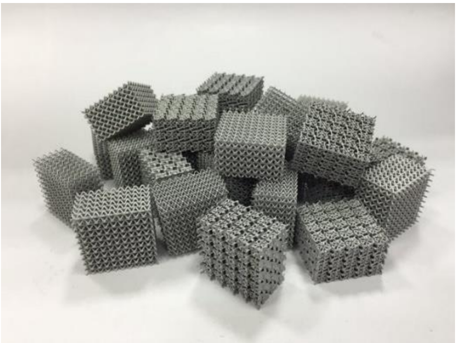
Composite structure can have different designs (porous, coolant filled, lattice structure)



Porous foam



Coolant filled



Lattice structures

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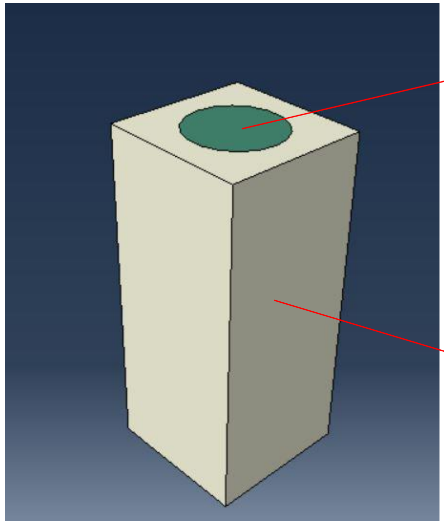
[1]-Wang et al. Nano Lett. 2022, 22, 10, 3931–3938

[2]- 3M, XING mobility, 2020

[3]-https://medium.com/@revrandom/3d-printing-is-grid-locked-in-lattice-structures-fd9e053ee959

Overall framework

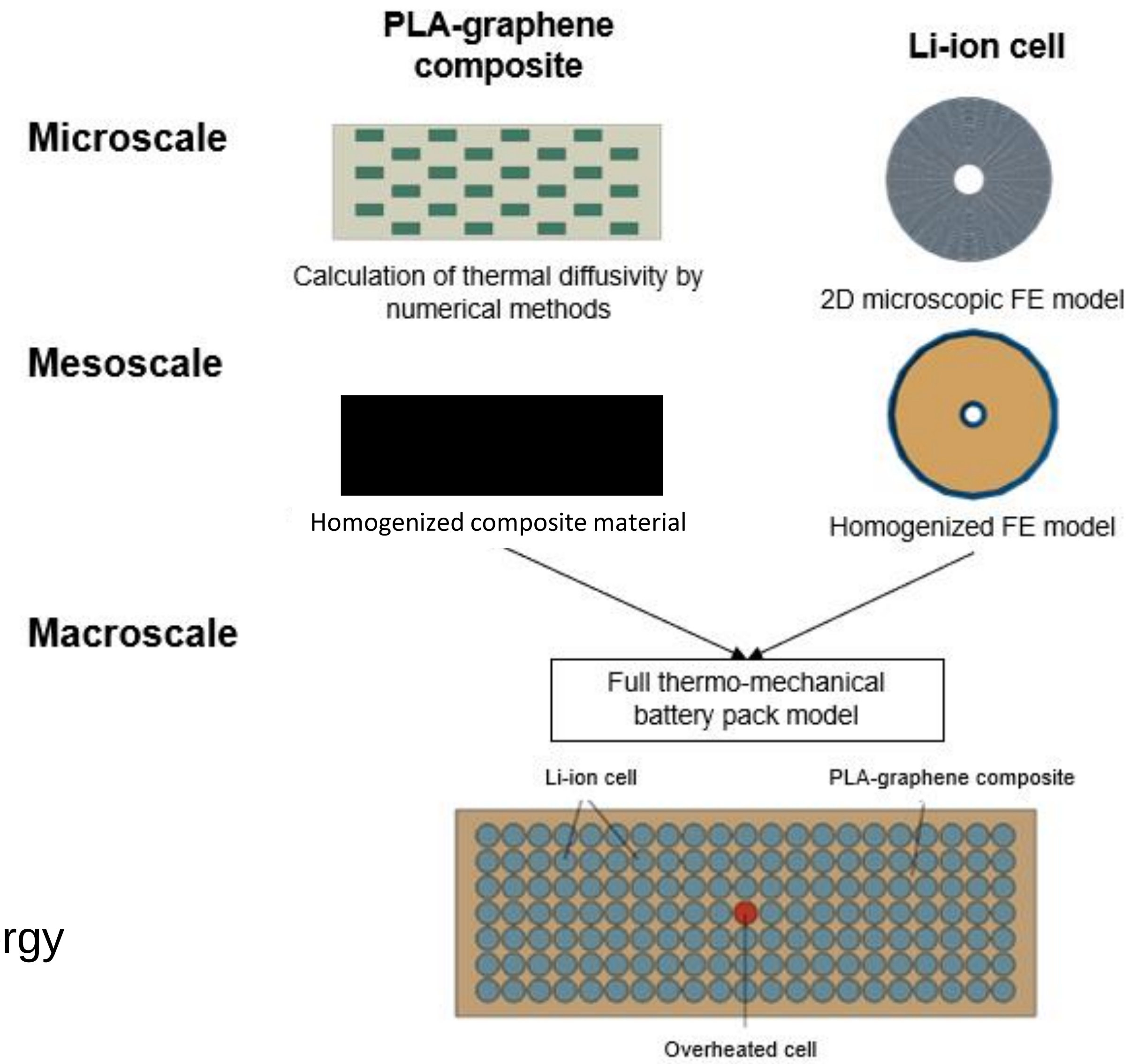
- Multiscale characterisation and modelling
- Thermal-mechanical multiphysics modelling



Battery cell

Multifunctional porous casing (Thermal management & Energy absorbing)

Experimental unit composed of Li-ion cell + protective encasing



Microscale modelling

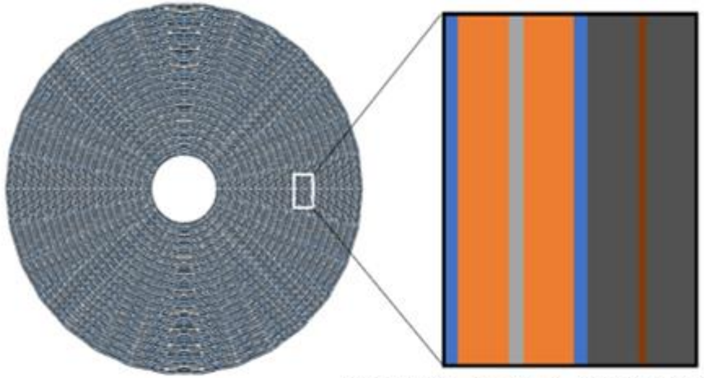
Microscale modelling

Issues with last model:

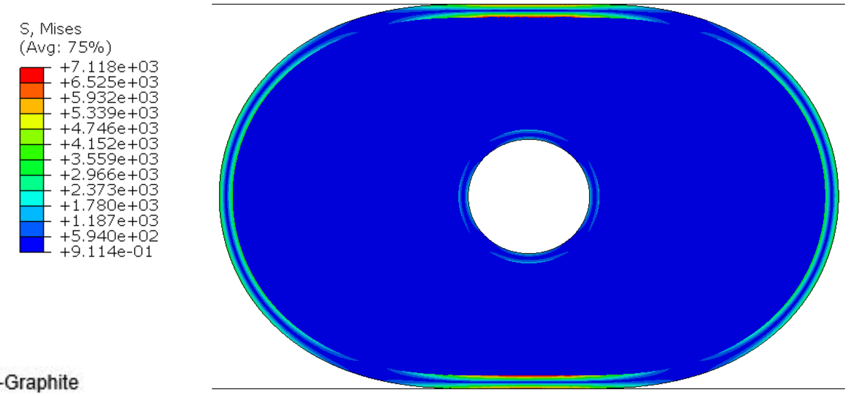
- Perfect-bond between layers
- Bad meshing in thinnest layers

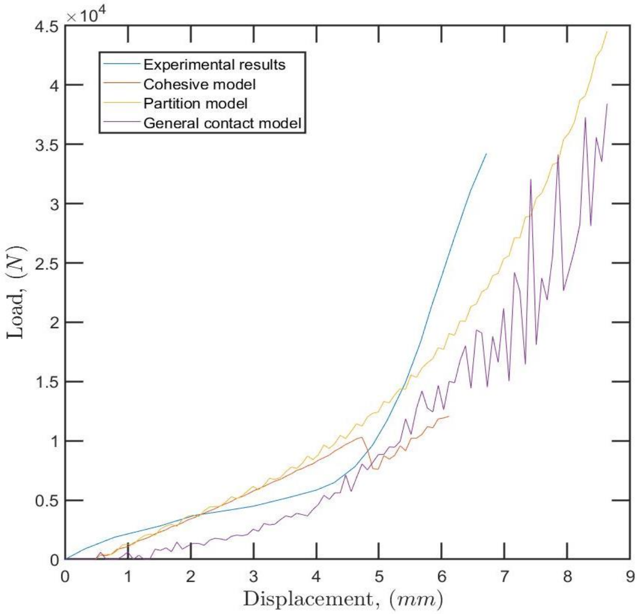
Improvements in latest model:

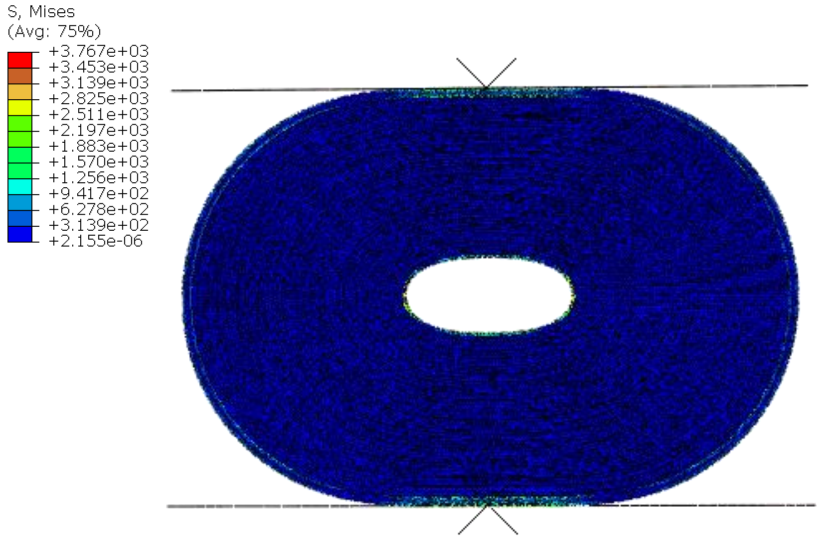
- Layers are bonded using 3 different approaches
- Fine meshing in thin elements
- Closest results obtained by partition and cohesive models



Sep-$LiFePO_4$-Al-$LiFePO_4$-Sep-Graphite-Cu-Graphite





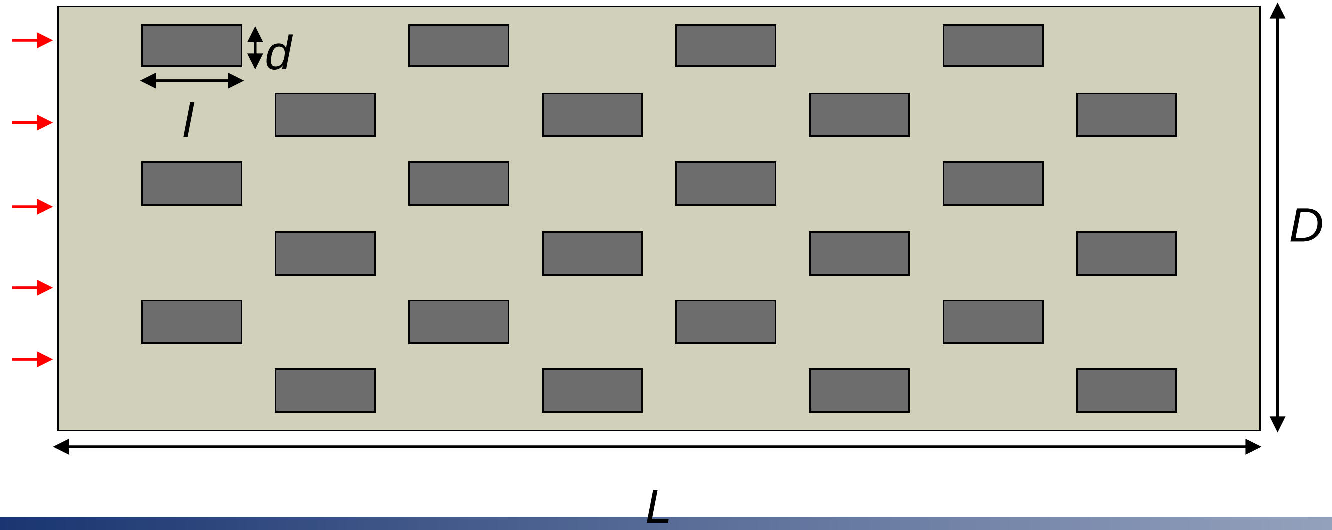


Thermal properties via numerical methods

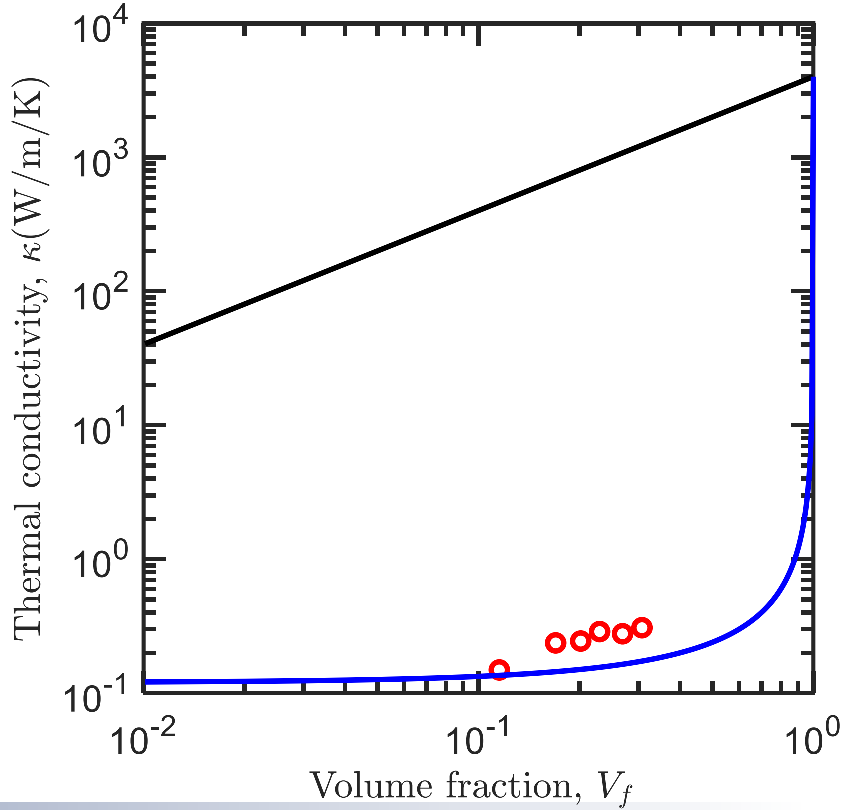
- Temperature profile obtained from numerical simulation
- Temperature profile obtained from PDE heat equation, with same BCs (100°C)
- Both data compared by PDE code, fitting the thermal diffusivity value

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

- Investigation at different range of volume fraction v_f



	Size (μm)
L	450
D	160
l	30 - 40
d	10 - 20



Mesoscale modelling

Constitutive model

- **Homogenization** of the jellyroll by **rule of mixtures.**

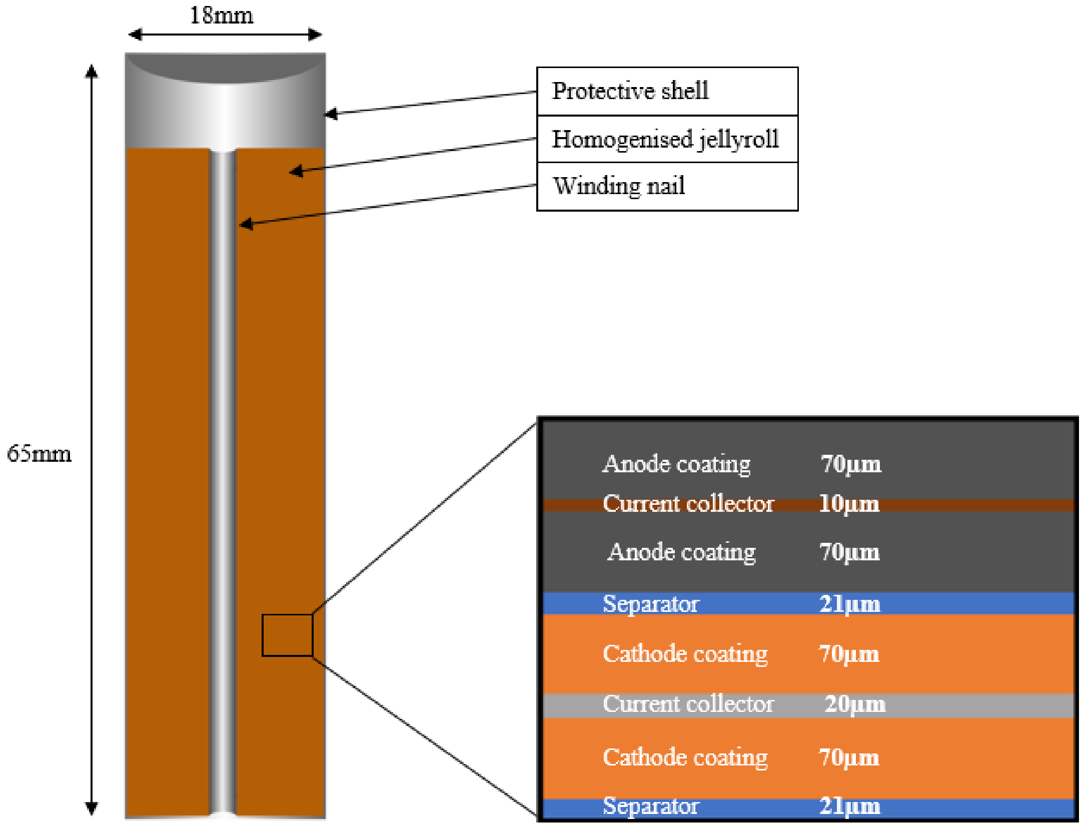
$$E_c = fE_f + (1 - f)E_m$$

- **Johnson-Cook plasticity** is used for model the yielding behaviour of the **jellyroll** (composite material).

$$\sigma^0 = [A + B(\epsilon^{-pl})^n](1 - \hat{\theta}^m)$$

- **Von-Mises plasticity** model was utilised to predict the plastic behaviour of the **metallic shell and winding nail.**

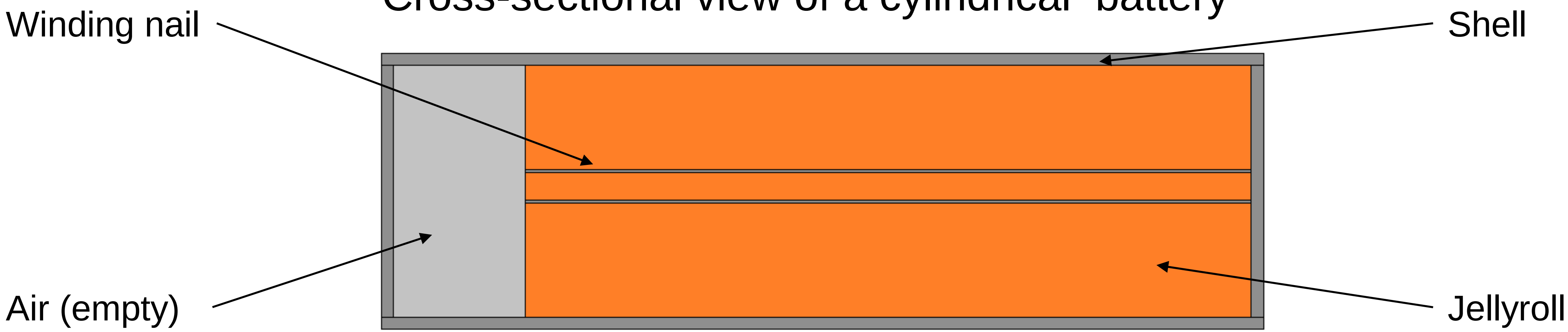
$$\sigma_v = \sqrt{\tfrac{1}{2}[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2]}$$



Material properties

Component	Material	Plasticity model
Winding nail	Stainless steel	Isotropic, Johnson-Cook
Shell	Stainless steel	Isotropic, Johnson-Cook
Jellyroll	NCO electrode	Isotropic, Johnson-Cook

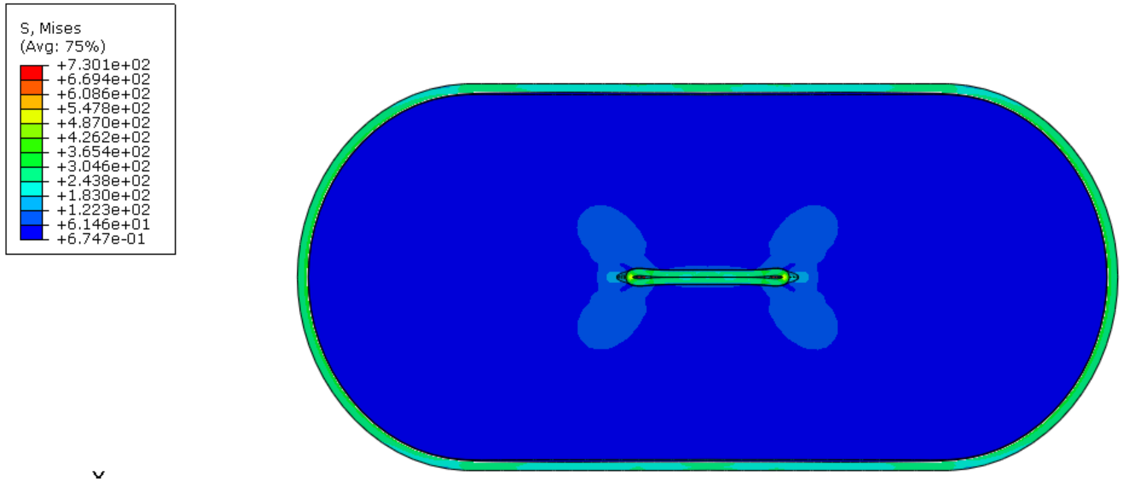
Cross-sectional view of a cylindrical battery

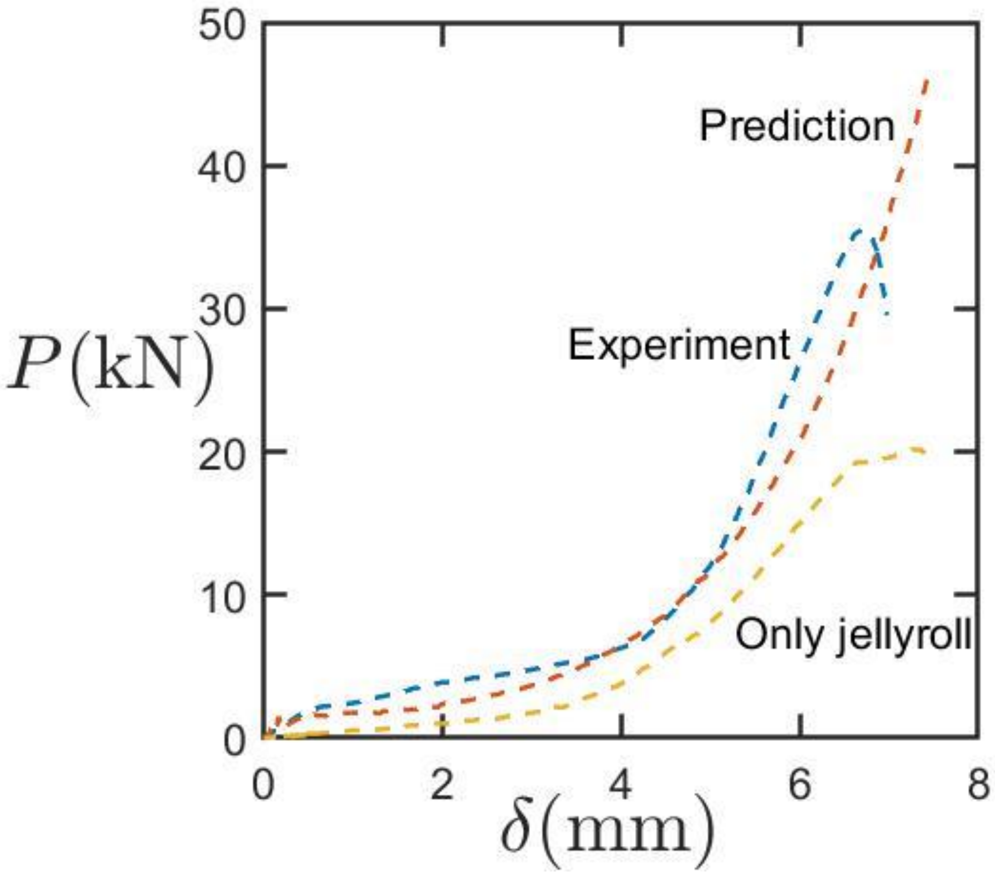


Mesoscale mechanical model

Homogenized model:

- Rule of Mixtures for mechanical properties
- Material properties obtained from literature review [4]
- Compressive test cell data obtained from [5]
- Very good agreement



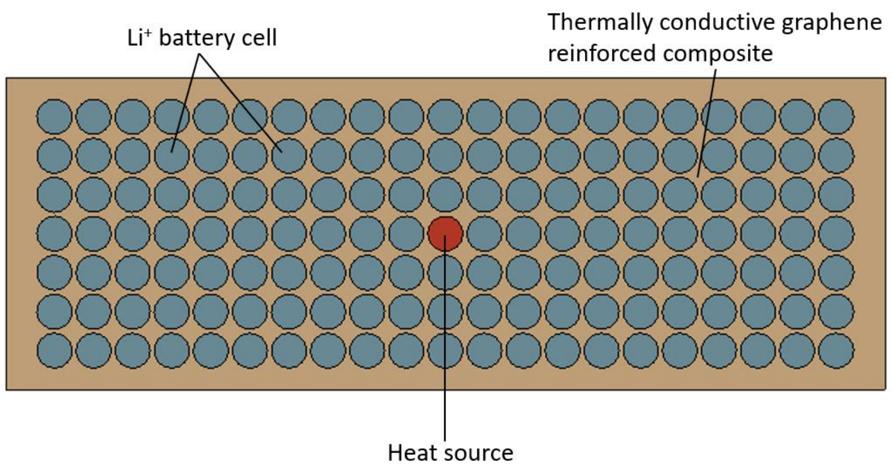


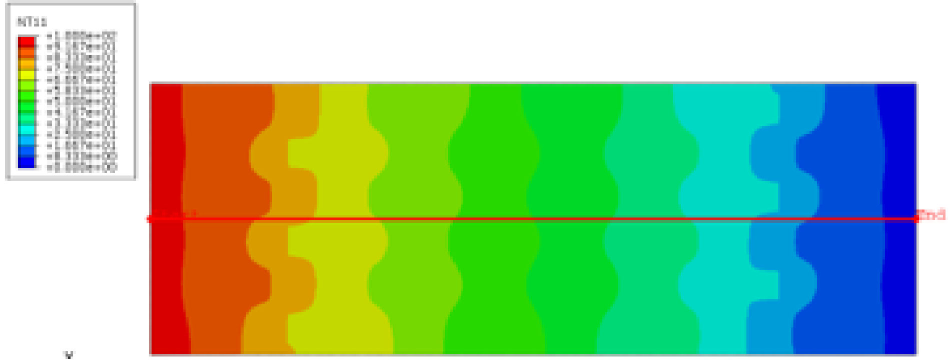
[4]-Jun et al, Dynamic mechanical int. 2015, 53, 97-110
[5]- Binghe et al, Mechanical integrity 2018,91, 315-326

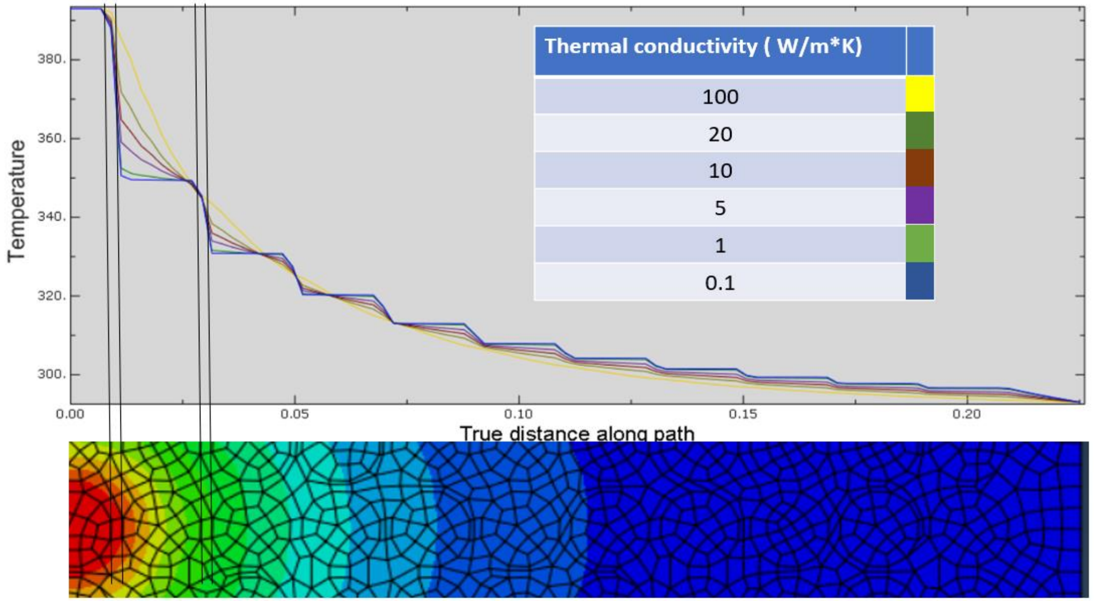
Macroscale modelling

Macroscale thermal analysis on battery pack

- Simulation of an overheated cell inside a battery pack.
- Investigation of heat propagation and thermal conductivity importance of matrix.







Thank you for listening

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