Prediction of Electrode Calendering Defects Through Finite Element Modelling

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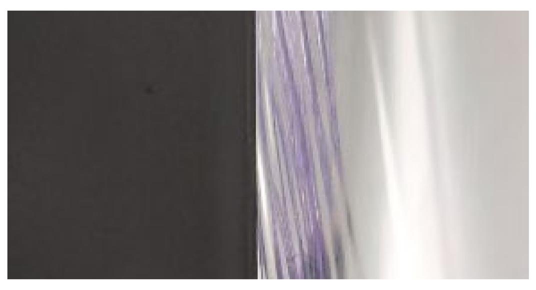
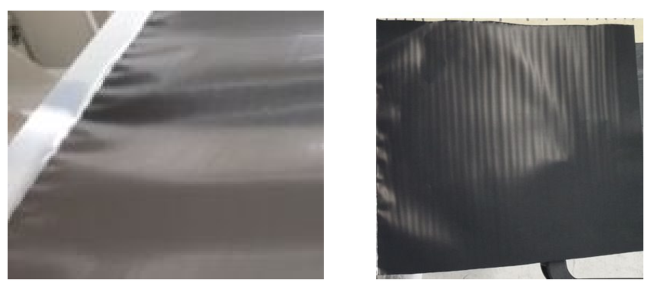
Abstract

- Calendering is the last electrode processing step where the battery performance and mechanical stability can be controlled
- This process can produce defects in the current collector, such as embossing and corrugation, that are detrimental to the cell assembly process and net manufacturing yield.



Embossing

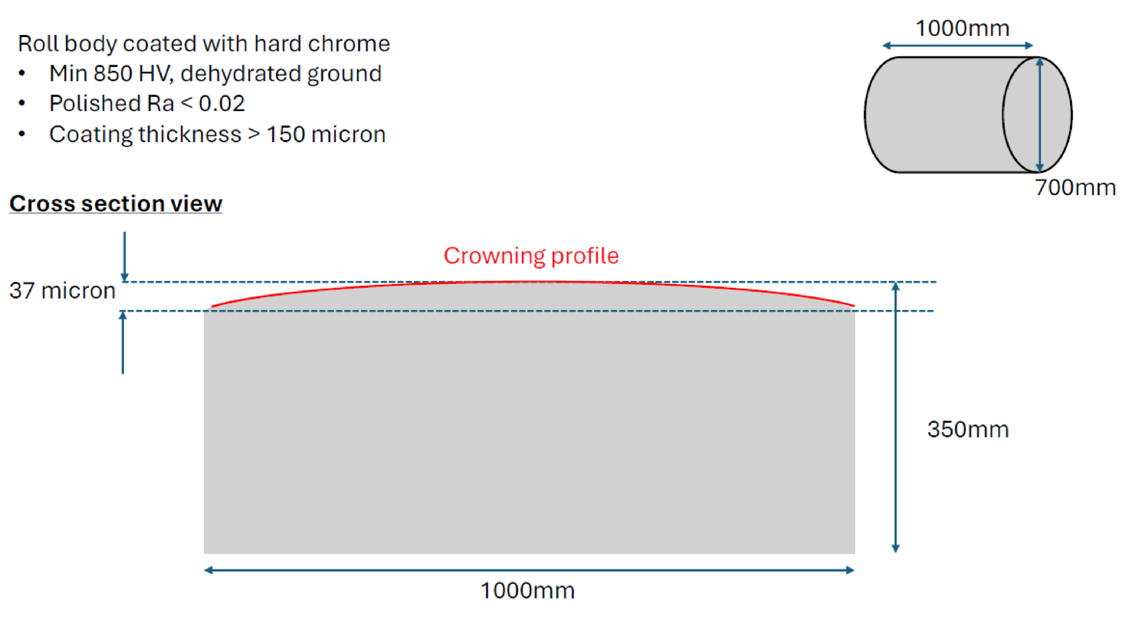


Edge (left) & longitudinal (right) corrugation

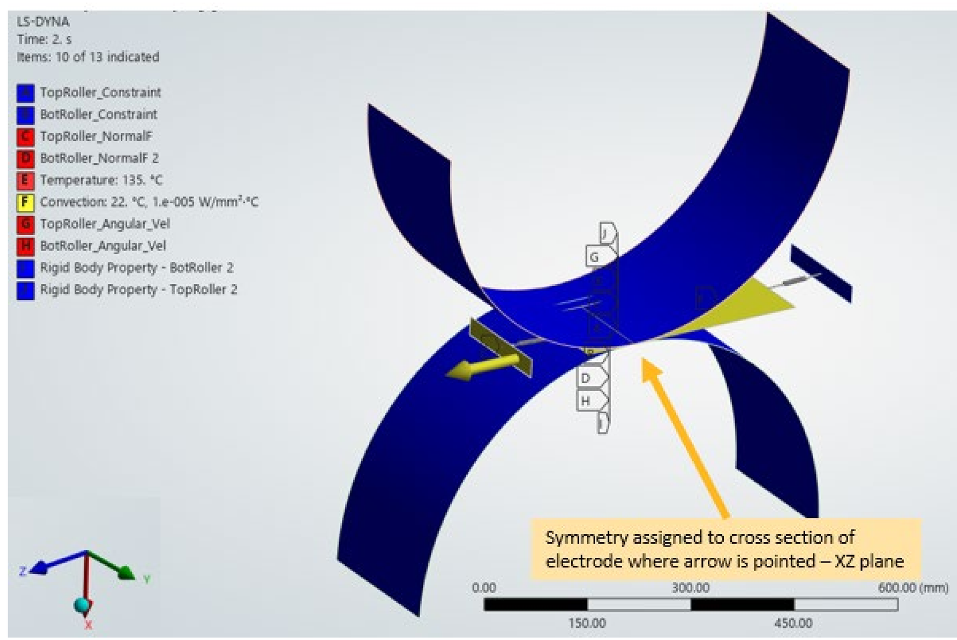
- While these are usually managed through live process adjustments and discarding defective material, it would be valuable to forecast and mitigate these in advance of production runs.
- Working towards this goal, UKBIC, in collaboration with Ansys, have developed a thermomechanical model of the calendering process
- The model has been used to verify and enhance existing knowledge about how certain calendering defects are initiated
- With further development, this will allow for physics-driven definition of process control strategies to mitigate these defects.

Method

- Small section of calendering roller and electrode foil taken as simulation domain
- Symmetry taken along centreline of roller, crowning profile of UKBIC roller imported into model
- Both electrode and foil considered isotropic & homogeneous, rollers assumed to be rigid
- Simulation performed as fully coupled thermo-mechanical analysis, including conduction/convection
- Ansys Mechanical used for mesh generation and majority of finite element model setup
- Ansys LS-DYNA, which is best suited to perform time-explicit structural simulations, used to complete model setup, solves the numerical model and post-process results
- Model takes 1-2 days to simulate 1 second of physical time on Ansys's 128-core machine



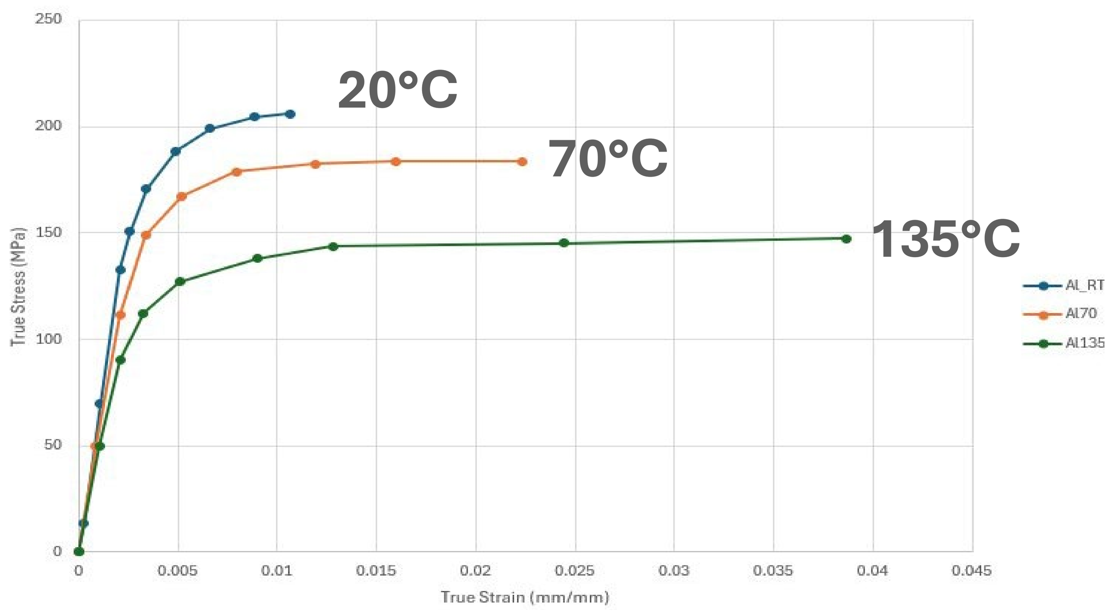
Schematic of UKBIC crowned calendering roller



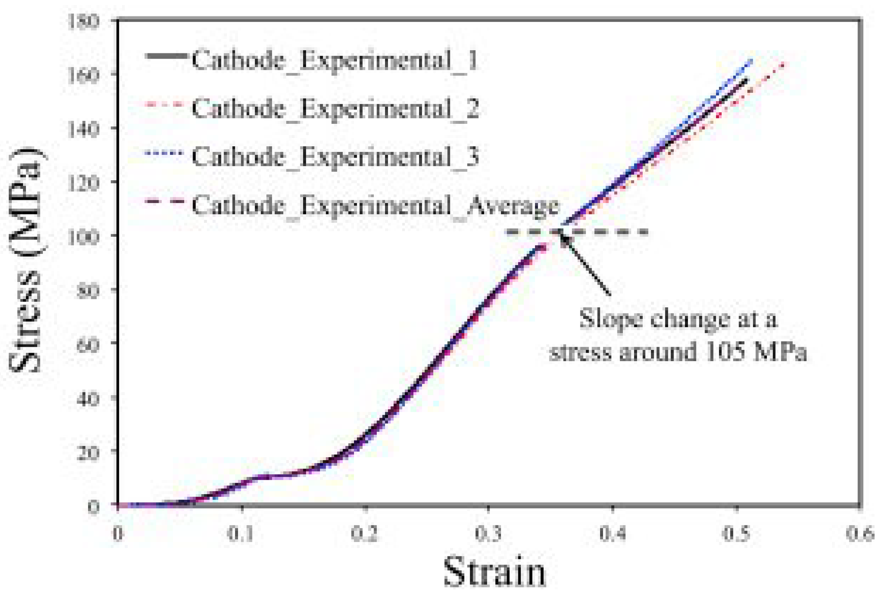
Outline of structural model boundary conditions

Material Property Inputs

- Case of interest is UKBIC in-house coated cathode material on aluminium foil
- Capturing electrode & foil non-linear and temperature-dependent properties is critical to predicting the correct structural behaviour
- Tensile tests of UKBIC aluminium foil at different temperatures (shown below) were conducted by an external test house

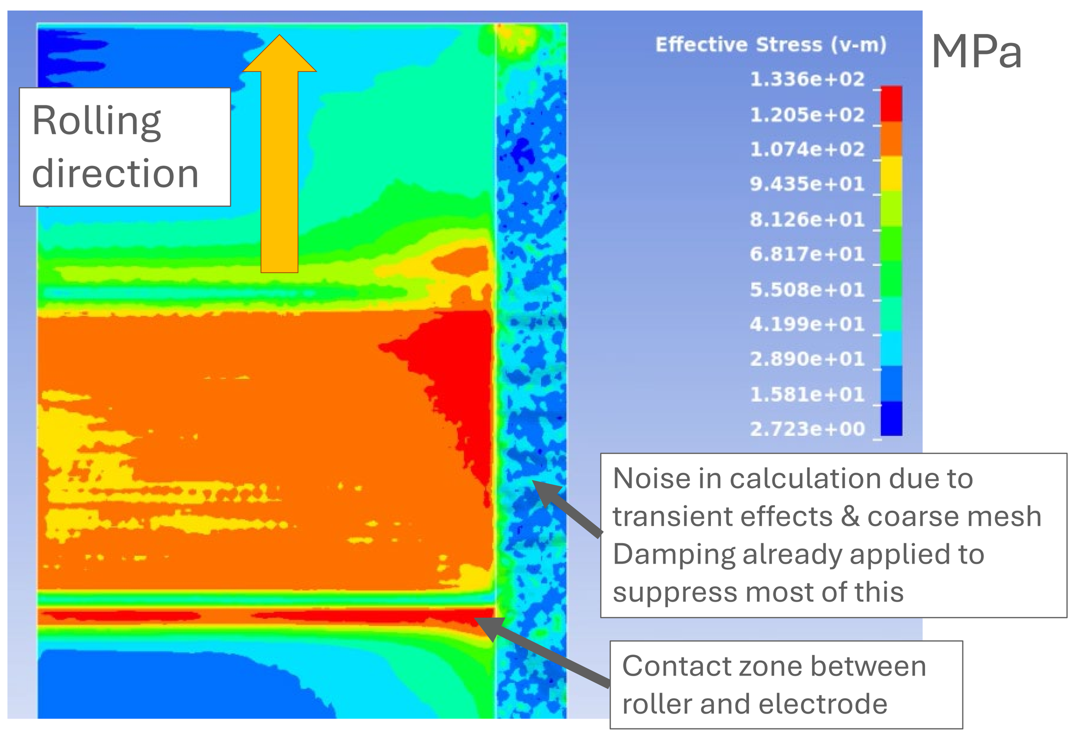


- Initial nano-indentation tests with UKBIC cathode not successful due to repeatability issues
- Stress-strain response of calendared, room temperature cathode taken from literature by Zhang et al. (2017) [1]



Stress & Embossing Prediction

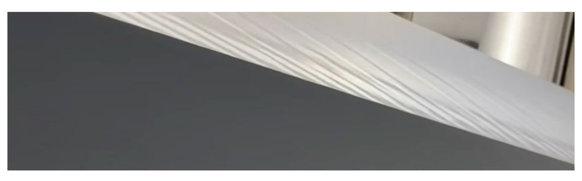
- The model is able to predict the local stress & strain field within the electrode as a natural consequence of solving the finite element model
- Comparing the predicted local stress with material failure strengths allows the model to predict whether web breaks may occur with a given combination of line load, web tension and line speed



Von Mises Stress plot of current collector foil

- Model also qualitatively predicts embossing, although not a full collapse due to coarse foil mesh and zero Poisson ratio assumed for the cathode coating

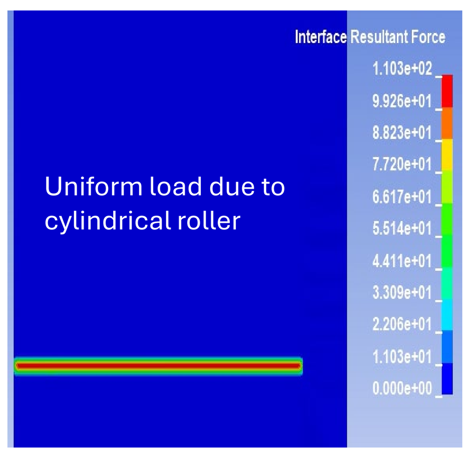
Sample model prediction of foil embossing



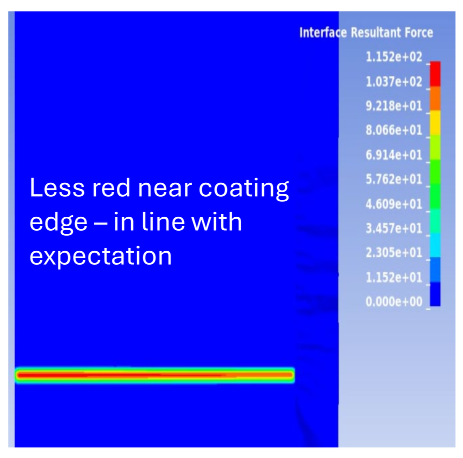
Test observation – more clear & frequent plastic collapse

Impact of Roller Crowning

- UKBIC's calendar rollers on the Industrial Scale-up Line (ISL) are not perfectly cylindrical – they have a 'crowning profile'
- The roller has a slightly larger radius near the centre compared to the edges of the roller
- While the deviation is only ~35 microns, this can have a large impact on calendering defects, especially if the full width of the roller is used
- Performing an experimental DOE of roller geometry is not practically possible with this scale of equipment
- The developed model provides a far more rapid way to assess not only the impact but the physics behind how crowning affects the formation of calendering defects
- A crowned roller reduces the clamping force on edges of coated region (as shown by interface force plots below)

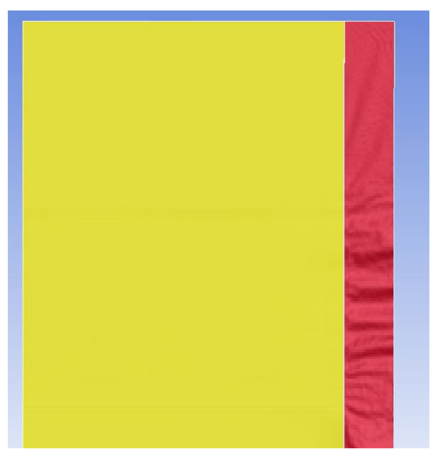


Interface force on flat roller

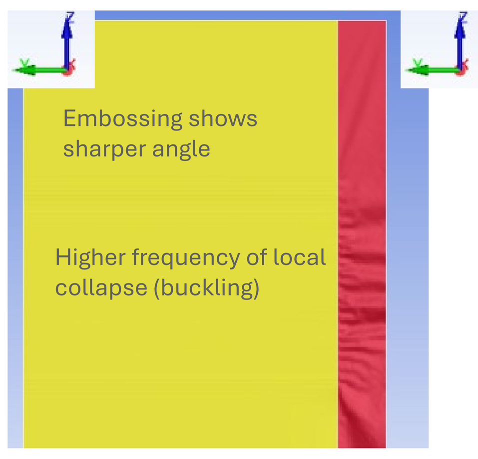


Interface force on crowned roller

- This makes the mass free zone less stiff and thus more prone to buckle for the same applied compression force



Embossing with flat roller



Embossing with crowned roller

Conclusion & Next Steps

- The produced model can make qualitative predictions of calendaring defects
- The structural material property definition of the coated cathode needs refinement to quantitatively predict these defects and validate the model against experiments
- There is some evidence that the mesh is insufficiently refined despite it being computationally taxing to run already with its current coarse mesh
- UKBIC is currently working with Micromaterials Ltd. to acquire better quality nano-indentation measurements of our uncalendared cathode
- Further collaboration with Ansys and the Nextrode Consortium are being planned to further optimize the model and produce results with reduced turn-around time
- The modelling approach will later be extended to cater to UKBIC's in-house anode along with customer electrodes

References

1. Zhang, Chao & Xu, Jun & Cao, Lei & Wu, Zenan & Santhanagopalan, Shriram. (2017). Constitutive behavior and progressive mechanical failure of electrodes in lithium-ion batteries. Journal of Power Sources. 357. 126-137. 10.1016/j.jpowsour.2017.04.103.

Presenter bio

Amin is a Process Simulation Engineer at the UK Battery Industrialisation Centre interested in developing physics-based simulation models of battery manufacturing processes, which can help de-risk the scale up of current and emerging battery chemistries to gigafactory-scale.

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