Multiphysics Modelling of Structural Battery Composites, Half-cell Representation of a Coated Carbon Fibre Positive Electrode

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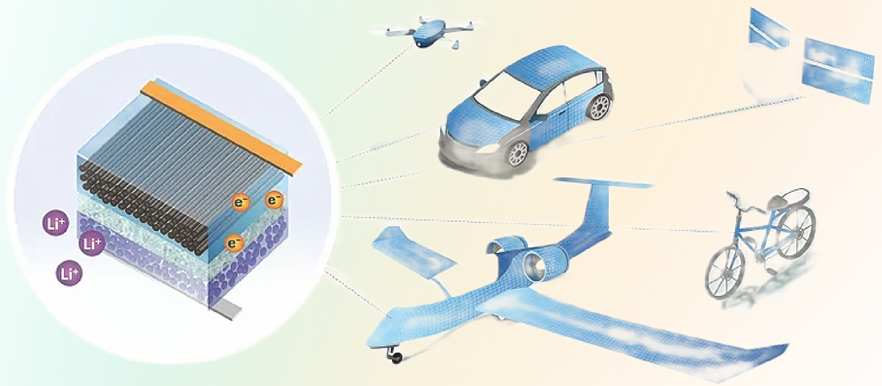
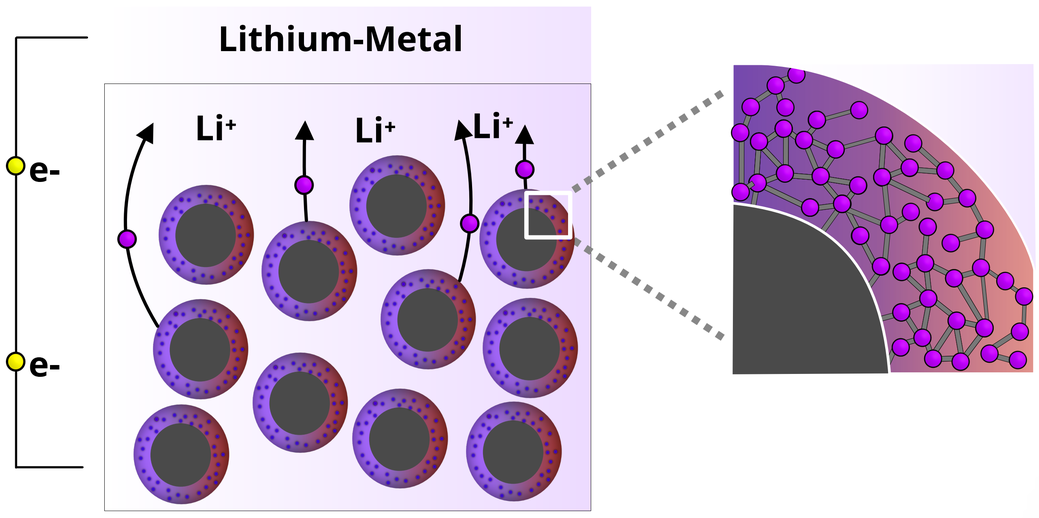
What is a structural battery?

- Multifunctional material that can store electrical energy and transfer mechanical load simultaneously.
- Carbon fibre-based negative electrode acting as lithium host.
- Two phase electrolyte, the solid phase transfer loads between carbon fibres and the liquid phase facilitates Li-ion exchange between electrodes.
- $LiFePO_4$ (LFP), coated carbon fibres as positive electrode using electrophoretic deposition.
- Li-insertion induced expansion of the coating material.





Half cell model of the fibre-based positive electrode

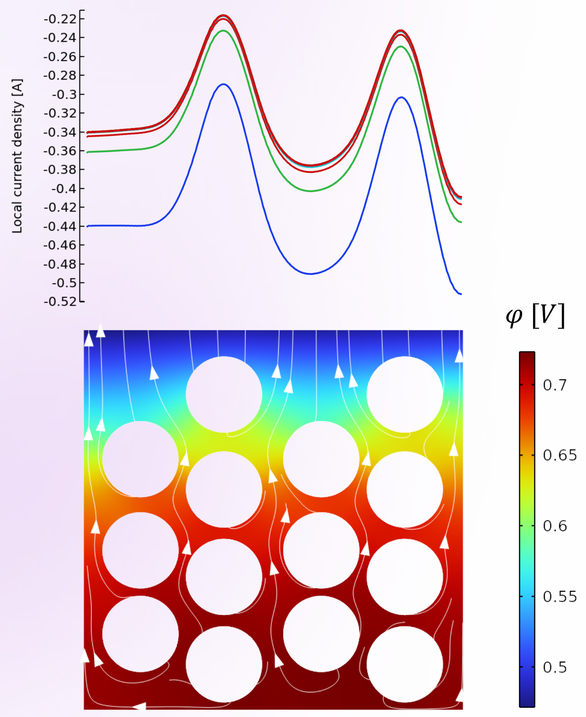
- Half cell representation, allowing assessment and characterization of the individual electrode against a known reference potential.
- Considering homogeneous properties of the underlying LFP coating structure.

$$\left.\begin{aligned} -\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} &= \mathbf{0} \\ F[c_{Li} - c_X] + \boldsymbol{d}\cdot\boldsymbol{\nabla} &= 0 \\ \partial_t(c_i) + \boldsymbol{J}_i\cdot\boldsymbol{\nabla} &= 0 \end{aligned}\right\}$$ Solved using finite element method.

- Butler-Volmer kinetics.
- Weak form implementation in COMSOL Multiphysics 6.1.

Model results

- Predicts ionic migration between electrodes, boundary currents, as well as diffusion of Li in the coating material.
- Allows for prediction of internal stress state, caused by the lithium insertion induced swelling of the coating material.
- Two-way coupling between chemical potential and mechanical stresses, i.e. application of mechanical stresses causes voltage change, and vice versa.
- Material parameters such as diffusion coefficients and exchange current density can be calibrated from physical tests, improving the accuracy of the model.



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