Modelling Lithium Flow from Power-Law Creep in 2D

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Lithium metal is a promising anode material for batteries because of the capacity, which is much larger than that of graphite anodes. However, there are still many challenges related to the stability of the lithium metal during deposition and dissolution. A common fault mechanisms is the formation of irregular structures such as dendrites, whiskers, or porous 'mossy' lithium. Experiments indicate that lithium metal batteries with a liquid electrolyte perform better when being cycled under pressure[1,2].

Lithium is a soft metal, that is easily deformed. Under sustained pressure, lithium is able to creep. The main creep mechanism under battery conditions is power-law creep caused by the movement of dislocations. This can be described mathematically as a strain rate $\dot{\epsilon} \sim (\Delta p)^{6.6}$ which is driven by the difference in pressures on different surfaces. The exponent 6.6 has been determined experimentally[3,4].

We assume the liquid electrolyte will fill the voids and remain at atmospheric pressure, as is common in many cell designs, and the separator will transfer pressure from the cathode onto the anode. Applying stack pressure on such a battery will then lead to flattening of the rough anode due to an inhomogeneous pressure distribution.

In this contribution, we present a two-dimensional model in the Lagrange frame that describes the flow of lithium during irregular dissolution. The spatial structure of the anode with a forming void is resolved through finite elements in a spherically symmetric system, with a phase field that describes the fraction of solid lithium in every element. This way we can model dissolution and track the deformation of the lithium anode.

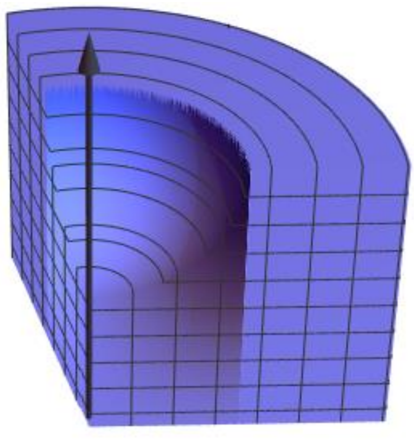

Figure 1: cross-section of an example system with axisymmetric finite elements and a void on the anode surface, showing the symmetry axis

Keywords*:* battery, lithium metal, power-law creep, solid mechanics.

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