A coupled-field model of lithium-ion battery charging and its isogeometric analysis

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ABSTRACT

Lithium-ion batteries are known to be the highest energy density rechargeable storage medium and thus they are of interest for several applications, e.g., electric vehicles, mobile devices and cordless machines. A lithium-ion battery's construction consists of two electrodes, a separator in between and an electrolytic solution which allows for transport of charge in form of lithium ions. In the electrodes an intercalation reactions occurs.

In [1] we formulated a model for the growth of electrode-electrolyte interfaces in lithium batteries in the presence of an elastic prestress. The model accounts for the kinetics of lithium transport through a solid electrolyte and, within the interface, for the kinetics of lithium ion adsorption by the anode, for electrostatics, and the elastic field. We specifically account for the effect of the elastic field through an asymptotic analysis of a nearly flat interface between two semi-infinite elastic bodies and use the model as a basis for assessing the effect of prestress on the stability of planar growth and the potential of prestress as a means of suppressing the formation of deleterious dendrites. Here, in this study we investigate a possible process which leads to a deviation of a planar electrode's interface and thus results in dendritic growth. To account for the above mentioned volumetric swelling and phase segregation, a various number of fields has to be coupled and leads to a complex mathematical description based on fourth order partial differential equations (Cahn-Hilliard type). Numerical treatment by using the isogeometric concept has been used already for similar type of problems and has proven to be reliable and efficient.

We present a linear stability analysis that results in explicit analytical expressions for the dependence of growth rates, and of the critical unstable wavelength for the interfacial roughening, on the state of prestress and on fundamental parameters such as surface diffusivities, surface energy, deposition kinetics, and elastic moduli. This model is studied in the light of experimental observations concerned with the effect of applied pressure on a lithium/dioxolane-dimethoxy ethane electrolyte systems. With reasonable choices of parameters and some calibration, the model accounts for the observation that a modest applied pressure indeed results in a substantial reduction in the roughening of the lithium surface during cycling. Example calculation will be shown for an arbitrary shaped surface and a three-dimensional cathode as studied in [2]. Finally, the phase segregation and the mechanical stress state in different particles are presented.

REFERENCES

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