Stresses Due to Intercalation of Non-Spherical Lithium Storage Particles

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Abstract

Due to computational considerations most models of lithium storage particles in batteries incorporate spherical particles. However most storage particles used in battery electrodes tend to be irregular in shape with sharp edges and extended aspect ratios. The change of the relative surface area to the volume of the particle can lead to a change in the stress response of the particle for the same material parameters. In order to study the effect of these edges on the stress response, we perform a parameter study on intercalation of lithium into cubic and ellipsoidal particles with different aspect ratios. We use a coupled stress-diffusion model developed previously [1,2] where we identified three non-dimensional parameters that govern the stress response of these particles, the non-dimensionalized current, the non-dimensionalized partial molar volume and the maximum lithiation strain. Our work shows that the effect of the stress on the concentration within spherical particle can be quite significant and we aim to identify the effect of these parameters on particles with non-spherical geometry.

The parameter study was performed using COMSOL Multiphysics®. A 3-d model was set up of a single quadrant of the particle, be it cubic or ellipsoidal. Symmetry boundary conditions were then applied to the inner faces in order to recreate the entire particle. A PDE interface was used to input the coupled stress diffusion equations. The gradient of the hydrostatic stress is a required component of our equation which was calculated using the structural mechanics module. The boundary condition applied to the surface of the particle was one of flux, which was done through a PDE physics interface.

Our results show that a change in material properties can lead to differences in both the value of maximum stress as well as its location in the particle, due to the interplay of diffusion and stress responses. In Figure 1, we see a plot of the maximal stresses in an ellipsoidal particle as a function of aspect ratio for the case of extraction of lithium from a particle. The results show that the maximum stress occurs at $\sqrt{0.5}$ followed by $\sqrt{2}$. Our results indicate that the aspect ratio plays a key role in determining the effect of stress assisted diffusion by changing concentration gradients.

In Figure 2 contours of the principal stress are plotted for the case of extraction of lithium from a cubic particle, which show that the edges and the corners of cubic particles show different stress responses. The differences in the ratio of the surface area to the volume locally causes a

change in the effective rate of extraction per unit volume at different points, which leads to different stress responses within the same particle.

Our model highlights the fact that if storage particle geometry could be controlled by using the appropriate manufacturing techniques, then the stress response of the lithium intercalation particles can be improved.

Reference

1. R Purkayastha, R.M McMeeking ‘A Linearized Model of Lithium Ion Batteries and Maps for their Performance and Failure’, Journal of Applied Mechanics, 79 (2012) 031021.1 – 031021.16
2. R. Purkayastha, R.M. McMeeking, ‘A Parameter Study of Intercalation of Lithium into Storage Particles in a Lithium-Ion Battery’ Computational Materials Science, 80 (2013) 2-14

Figures used in the abstract

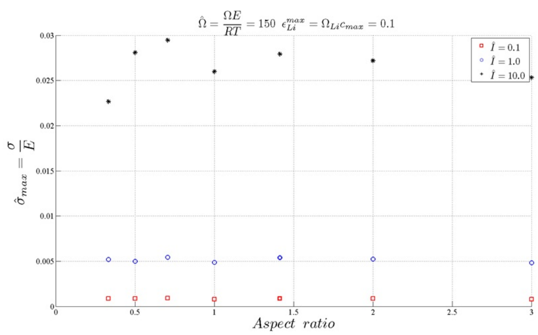

Figure 1: Plot of maximum stresses in an ellipsoidal particle as a function of aspect ratio

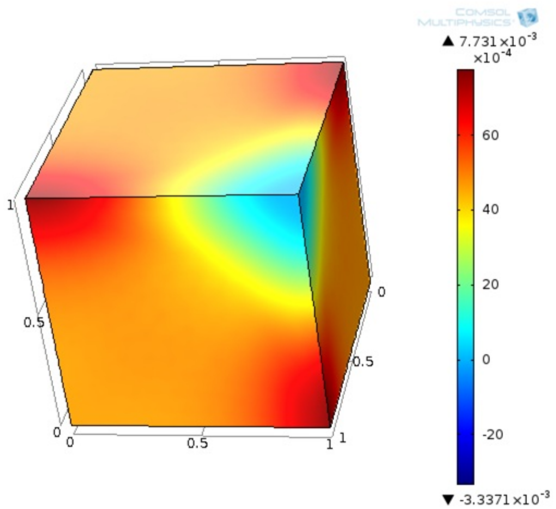

Figure 2: Contour plot of maximum principal stress in a cubic particle from which lithium is being extracted