IGA for anodes of lithium-ion batteries

M. Werner*, **S. Homberger and K. Weinberg**

* Universität Siegen
Department Maschinenbau
Institut für Mechanik und Regelungstechnik - Mechatronik
Lehrstuhl für Festkörpermechanik
Paul-Bonatz-Str. 9-11, 57076 Siegen
e-mail: marek.werner@uni-siegen.de

ABSTRACT

To satisfy the world's hunger for energy sources combined with the usage of cordless machines, the improvement of rechargeable storage media based on a lithium-ion technology is of great interest. In lithium batteries, a great variety of chemical compositions like $LiCoO_2$, $LiFePO_4$, $LiMn_2O_4$, $Li_4Ti_5O_{12}$, $LiNiMnCoO_2$ or $LiNiCoAlO_2$ are used as cathode material and pure substances like graphite or silicon are employed as anode material. Especially the second highest abundance within the earths crust (after oxygen) makes silicon from the industrial point of view very attractive.

The ion intercalation into the host material comes along with a high volumetric change and thus leads to pulverization and capacity fade of the anode. Here, in this study we investigate an ion intercalation into different shaped electrode particles which induces a volumetric swelling and phase segregation. Therefore mechanical, thermal, chemical, electrical and diffusion field equations are coupled [1]. This leads to a complex description based on fourth order partial differential equations. The numerical solution of the arising problem is solved by using a NURBS based finite element method.

Exemplary, the isoparametric study involves several single particle shapes like a topology optimized pillar [2], a helix or a round particle due to the superb spline properties. Within IGA a curved geometry can be modeled precisely by using a moderate number of elements. To avoid transition from amorphous to crystalline silicon ordering, mainly structures of the order of a few microns edge length are considered. Also the adaption of the field dependent physical parameters like the elastic moduli for nano-scaled materials is vital. Most of the physical values are reported for a temperature of 298 K (STP), so we will restrict our consideration to an isothermal framework.

REFERENCES

[1] Werner, M. and Weinberg, K. *Coupled Thermal and Electrochemical Diffusion in Solid State Battery Systems*. Advanced Structured Materials, vol 108. Springer, Cham

[2] Werner, M. and Weinberg, K. *Towards structural optimization of lithium battery anodes* Proc. Appl. Math. Mech. **18**:1–2.