Institut für Numerische Simulation
Rheinische Friedrich-Wilhelms-Universität Bonn

hausdorff center for mathematics

Einladung zu einem Vortrag im Seminar
Materialwissenschaften und Mathematik

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spricht zum Thema

Multiscale Material Modelling for Li-Ion Batteries

Zeit: **Donnerstag, den 14. April 2011, 16.00 Uhr**
Ort: **Endenicher Allee 60, Seminarraum 2.040**

gez. **Prof. Dr. Michael Griebel**, **Prof. Dr. Stefan Müller**

Abstract: During a typical charge/discharge cycle of a Li-ion battery the active intercalation materials experience a volume change of up to 10%. This causes fracturing and loss of contact of the active particles and finally the degradation of the whole cathode/anode. A careful understanding of these mechanical-electrochemical degradation mechanisms is mandatory to fulfil the high quality and lifetime requirements in automotive applications.

Here we present a new multiscale modelling approach for degradation of Li-ion batteries. The centre of our approach is a one-particle micromechanical diffusion model. The driving force for diffusion is deduced from basic thermodynamics and statistical physics and allows the modelling of phase-change materials. The arbitrarily shaped and positioned particles are then coupled to the pseudo two- dimensional electrochemical "dualfoil" battery-cell model. Various coupling schemes between our micromechanical particle model and the electrochemical battery-cell model, which couples the microstructure to the charge/discharge cycles of "real-world" battery applications, will be discussed.

The parameters of our one-particle micromechanical diffusion model can be directly obtained from ab-initio DFT calculations if they are experimentally not accessible or in cases where new computer-designed materials are to be evaluated.

Strengths and limitations of our multiscale modelling approach will be discussed thoroughly, in particular with focus on the needed experimental input. Finally, we discuss extensions of our model like many-particle microstructural models (including e.g. binder, conductive additives, etc.) and the explicit modelling of crack-growth.