Institut für Baumechanik
und Numerische Mechanik

Gottfried Wilhelm Leibniz Universität Hannover
IBNM, Appelstr. 9a, 30167 Hannover

Leibniz Universität Hannover

Prof. Dr.-Ing. U. Nackenhorst

www.ibnm.uni-hannover.de

edited by:
Dr. Jorge Urrea

Tel.: +49 (0)511.762-**4897**
Room: 3408 - **121**
E-Mail: **jorge.urrea**
@ibnm.uni-hannover.de

Master thesis - *Masterarbeit*

for

Student Name

Student No.: XXXXXXXX

Project received: XX.XX.XXXX	Workload: 720 h (24 CP)
Submission of project until: XX.XX.XXXX	Duration: 6 months
First examiner: Prof. Dr.-Ing. U. Nackenhorst	Supervisor: Dr. Jorge Urrea
Second examiner: Prof. Dr.-Ing. Vorname Nachname	

Impact of mechanical stresses on Li-ion battery performance
Auswirkungen mechanischer Spannungen auf die Leistung von Li-Ionen-Batterien

Li-ion battery cells have been widely used to supply electric portable devices such as mobile phones, laptop computers and cameras. The expected use of Li-ion batteries (LIBs) for high-power and high-capacity demanding systems, as electric vehicles, and for storage systems for renewable energy sources makes contained capacity fading and power loss nowadays priorities for the world-wide research community. Whereas experimental studies are the backbones of batteries investigation, modeling can provide fundamental contributions, particularly in tailoring material performances and degradation.

Within the scope of this master thesis, a simple coupled electro-chemo-mechanical model for solid polymer electrolytes should be selected from the literature and implemented using, e.g., MatLab, Python, or Abaqus. The model should be applied to study the effect of the coupling on the performance of the battery electrolyte. The prediction of the solid polymer electrolyte conductivity is expected to change considerably when mechanical contribution is included in the analyses, suggesting that stresses and deformations should be properly accounted for in batteries design.

Required knowledge (to be covered in self-study where applicable): Fundamentals of Mechanics of Solids and the Finite Element Method, obtained, for example, from the *Mechanics of Solids* master course offered by the IBNM institute. Basic programming knowledge is mandatory.

This project will be supervised/written in English language.

Literature:

[1] GRAZIOLI, D., MAGRI, M., & SALVADORI, A. (2016). Computational modeling of Li-ion batteries. Computational Mechanics, 58(6), 889-909.

[1] BUCCI, G., CHIANG, Y. M., & CARTER, W. C. (2016). Formulation of the coupled electrochemical–mechanical boundary-value problem, with applications to transport of multiple charged species. Acta Materialia, 104, 33-51.

[2] GRAZIOLI, D., VERNERS, O., ZADIN, V., BRANDELL, D., & SIMONE, A. (2019). Electrochemical-mechanical modeling of solid polymer electrolytes: Impact of mechanical stresses on Li-ion battery performance. Electrochimica Acta, 296, 1122-1141.

[1] ANAND, L., & GOVINDJEE, S. (2020). A small deformation chemoelasticity theory for energy storage materials. In *Continuum Mechanics of Solids* (pp. 320-326). Oxford University Press.

The entire workload contains the following steps:

1. Preparing a milestone plan for a regular discussion of progress with the supervisor. The milestone plan needs to be handed in one week after receiving the task description. In case of circumstances, the milestone plan needs to be updated as agreed upon the supervisor. All versions of the milestone plan are to be submitted within the appendix of the thesis.
2. Literature review on recent advances in the computational modeling of Li-ion batteries.
3. Summarizing the theoretical background.
4. Development of FEM code implementing the coupled electro-chemo–mechanical boundary-value problem.
5. Evaluation of the numerical solution consistency showed by some simulation examples, e.g., showing the species concentration and induced stresses/strains in 1D and 2D as well as a convergence study.
6. Documenting all steps and results regarding established scientific standards.
7. Self-evaluation of the own work using the attached evaluation matrix.
8. Creating a poster for the invitation to the presentation.
9. Presenting (15 to 20 minutes) the project within a colloquium.

In addition to an abstract in English and in German, five content describing key words have to be stated. The written report is to be submitted in one printed version. Additionally, all data are to be attached digitally.

Evaluation matrix:

Content[1]: 50%

Literature research • Coupled diffusion-deformation theories for Li-ion baterries. • Numerical methods to solve coupled diffusion-deformation models.			10
Theoretical basics • Theory of the coupled electro-chemo–mechanical boundary-value problem, with applications to transport of multiple charged species, and the corresponding constitutive theory. • Fundamentals of the Finite Element Method.			15
Solution of the given problem, meeting the objectives • Simulation results showing the consistency of the numerical approximation. • Convergence study. • Implemented code using an open source software.			25

[1]Weighting within "contents" is done by the supervisor corresponding to the type of task.

Appearance of the written report: 15%

Style of writing, written expression, grammar, spelling			3
Visualization, figures			3
References			2
Structure			3
Comprehensibility			4

Working methods: 15%

Time management			4
Independent working			4
Meeting deadlines, reliability			3
Implementing feedback			4

Presentation, colloquium: 20%

Content			8
Structure, slides			4
Delivery			4
Answering questions			4

Evaluation:

Points	0-49	50-54	55-59	60-64	65-69	70-74	75-79	80-84	85-89	90-94	95-100
Grade	5.0	4.0	3.7	3.3	3.0	2.7	2.3	2.0	1.7	1.3	1.0