Mathematical modelling for All-solid-state battery

Tuan Vo[a,b †], Claas Hüter[b], Stefanie Braun[a]

[a]Department of Mathematics, Applied and Computational Mathematics (ACoM), RWTH Aachen University, Schinkelstraße 02, 52062 Aachen, Germany
[b]Institute of Energy and Climate Research (IEK-2), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52428 Jülich, Germany

Mathematical modelling for the next-generation All-solid-state batteries: Nucleation (SE|SSE)$^{(*)}$-Interface

Rechargeable Lithium-ion battery (LIB) is at the heart of every electric vehicle (EV), portable electronic device, and energy storage system [5]. Nowadays, LIBs enable human life more efficient and help to solve global environment issues thanks to EVs' zero emission. However, conventional LIB (c-LIB) is sensible to temperature and pressure, hence, flammable and explosive, which is undesirable. This bottleneck is mainly due to liquid-based electrolyte found in c-LIBs.

All-solid-state battery (ASSB) is one of promising candidates to overcome bottlenecks of c-LIBs. Thanks to solid-state electrolyte (SSE), ASSB is highly stable towards temperature and pressure. Nevertheless, Li-metal dendrite triggered at (SE|SSE)-Interface is the main drawback of ASSB since these dendritic threads extrapolate into SSE grain boundary network, causing crevice, degradation of ionic conductivity, and the probability of short-circuit, which is unfavorable [10].

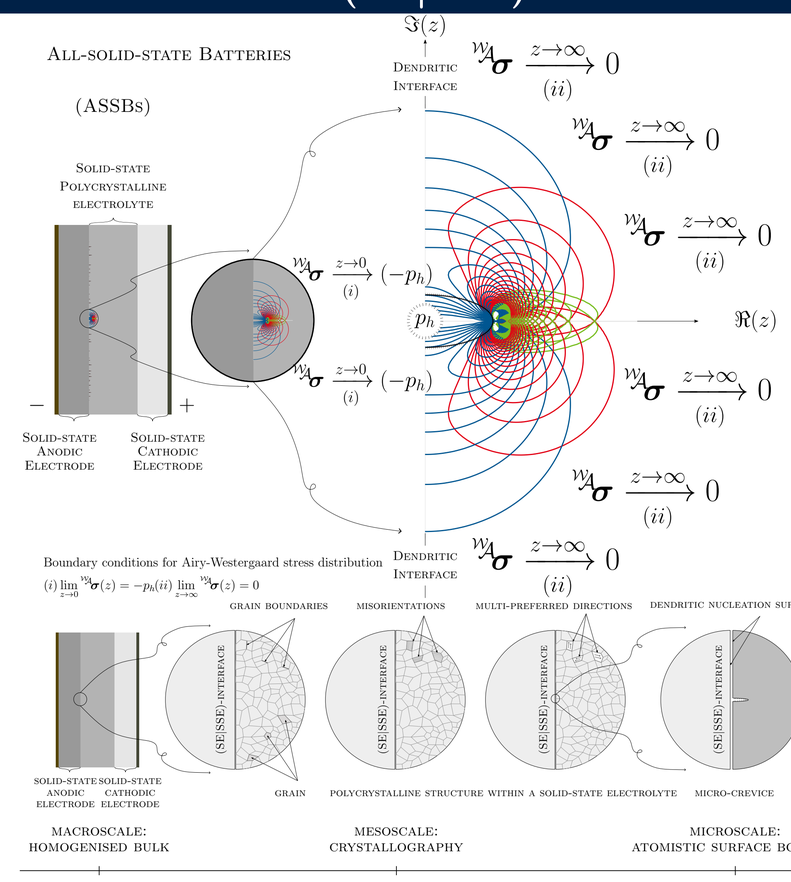
Next-generation All-solid-state battery (ng-ASSB) with a consideration of nucleation criterion defined by

$$\partial_t \dot{\boldsymbol{u}} + \nabla \cdot \left(\overset{4}{\mathbb{C}}^{f_{\text{alocation}}(\lambda,\mu,\boldsymbol{d}^R_{G_i,i=1,\dots,N},\boldsymbol{d}^E;\boldsymbol{x})} : \nabla \boldsymbol{u}^{(s)} \right) + \rho \boldsymbol{b} = -\rho \nabla V_e, \tag{1}$$

$$\text{s.t.} \quad a^{\text{generalised}}_{\text{Griffith}} := a^* = \arg\min_{a \in \mathbb{R}} \iiint_\Omega f(a, \boldsymbol{u}, \theta; \lambda, \mu, \boldsymbol{d}^{(\star)} \otimes \boldsymbol{d}^{(\star)})\, d\Omega - \iint_\Gamma f(a; \gamma)\, d\Gamma \Big|_{\bar{\boldsymbol{u}}} \tag{2}$$

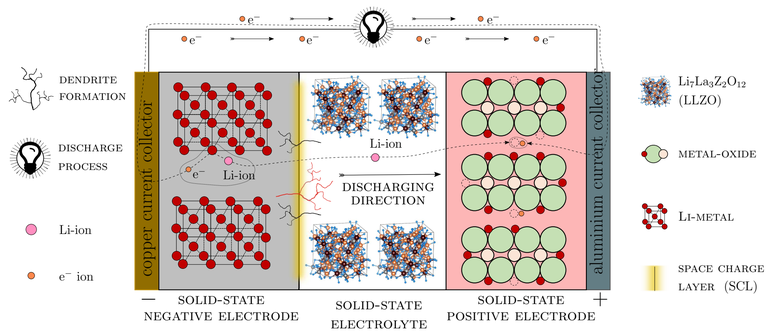
where $V_e : \mathbb{R}^3 \to \mathbb{R}$ is the electric potential applied globally on ASSB. Due to nature setting of ASSB taking the form (SE|SSE|SE) the electric potential becomes uniform. Additionally, $\boldsymbol{u}$ is the displacement field, θ temperature field, a crevice length, λ, μ Lamé constants, $\boldsymbol{d}^{(\star)} \otimes \boldsymbol{d}^{(\star)}$ embedded misorientation structural tensor, and γ cracking-surface energy density, can help to improve ASSB performance [1][2].

Aim: The study is with the purpose of gaining a better insight into dendrite nucleation and formation in ASSB.



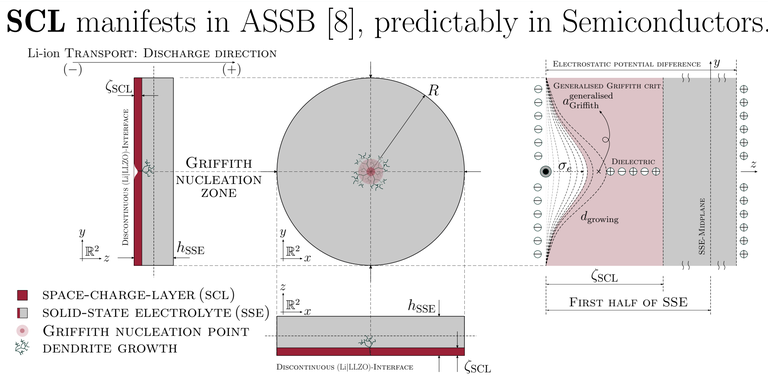
Next-generation All-solid-state battery

Griffith nucleation criterion governs (SE|SSE)-Interface [4].



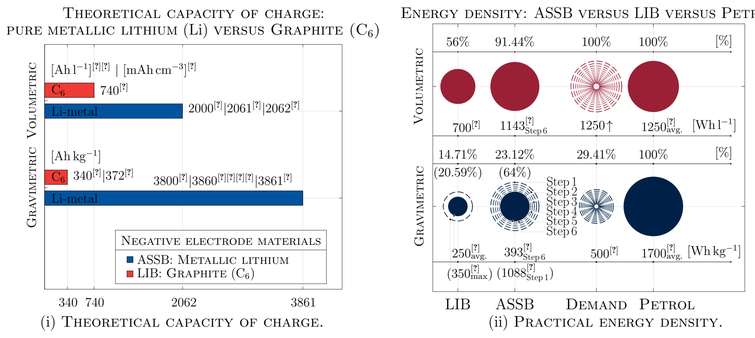
Observation: Space-charge Layer

SCL manifests in ASSB [8], predictably in Semiconductors.



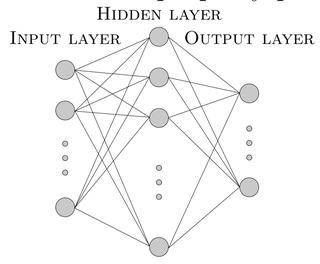
Motivation: Energy density landscape

ASSB enables **energy demand** due to (i), and followed by (ii).



Artificial Neural Networks

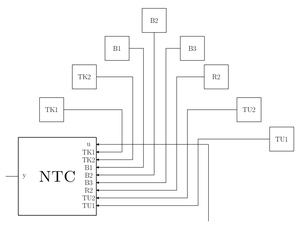
Application: Steel's property prediction.

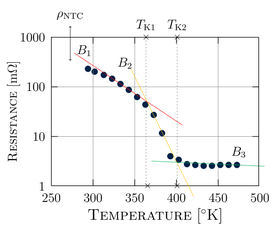


The ANNs scheme enhances bainitic trafo. temperature prediction, validated by [9].

Semiconductor

Application: Start/Stop-System in Starter.
Use-case: BMW B47 (-25°C, 0°C, 120°C).
Optimisation: Pareto @BoschForschung. (Multi-objective optimisation framework)





Negative-temp. Coefficient (NTC) Nd/Gd semiconductor is modelled and validated [7].

Lithium-ion battery

Modelling: Swelling phenomena @FEM [5].
Use-case: Bosch-48-V-Battery.

Nucleation interface: Taking place at the critically dendritic (SE|SSE)-Interface

Coupled fields are Displacement field $\boldsymbol{u}$ and temperature field θ;

$$\boldsymbol{u} : \begin{cases} \Omega \times \mathbb{R}_+ \to \mathbb{R}^3, \\ (\boldsymbol{x}, t) \mapsto \boldsymbol{u}(\boldsymbol{x}, t), \end{cases} \qquad \theta : \begin{cases} \Omega \times \mathbb{R}_+ \to \mathbb{R}, \\ (\boldsymbol{x}, t) \mapsto \theta(\boldsymbol{x}, t), \end{cases}$$

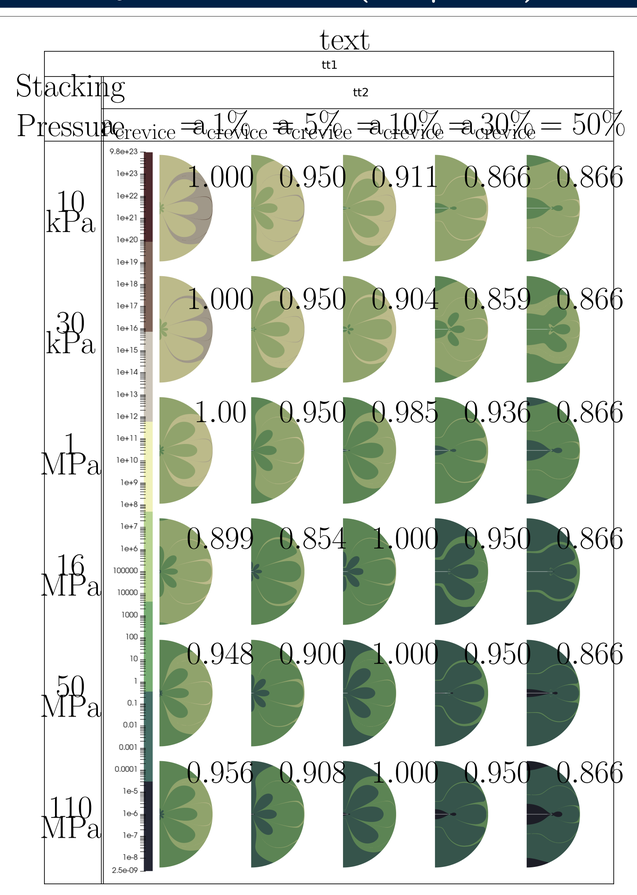
Governing conservation equations used to describe balance of mass, conservation of linear momentum, conservation of angular momentum, and conservation of energy with $\rho(\boldsymbol{x}, t)$ is mass density per unit volume (puv); $\boldsymbol{b}(\boldsymbol{x}, t)$ body force puv; $\boldsymbol{v}(\boldsymbol{x}, t)$ velocity; $e(\boldsymbol{x}, t)$ internal energy puv; $\boldsymbol{q}(\boldsymbol{x}, t)$ heat flux; $r(\boldsymbol{x}, t)$ heat source puv; $\boldsymbol{\sigma}$ Cauchy stress and $\boldsymbol{\varepsilon}$ infinitesimal strain.

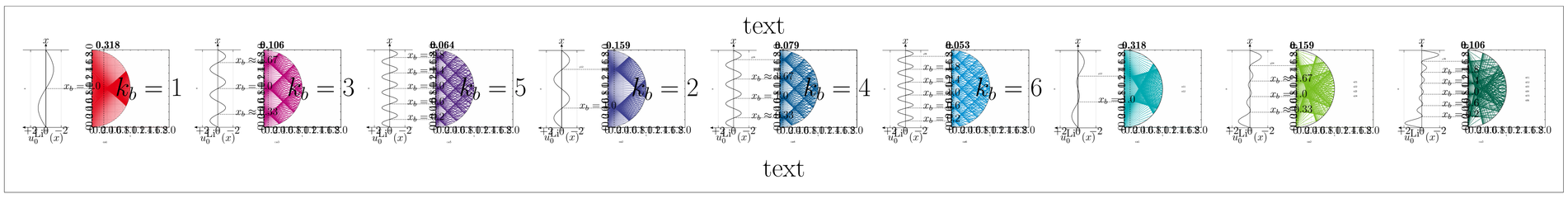
Strain energy is based on the deformation of SSE due to dendrite formation at (SE|SSE)-interface

$$\iiint_\Omega f(a, \boldsymbol{u}; \lambda, \mu, \boldsymbol{d} \otimes \boldsymbol{d})\, d\Omega$$

Surface energy is analysised based on the open crevice cracking at (SE|SSE)-interface affected by prescribed pressure

$$\iint_\Gamma f(a; \gamma)\, d\Gamma$$





Contact

Tuan Vo
vo@acom.rwth-aachen.de

Scan me

..writes his dissertation in Applied and Computational Mathematics at RWTH Aachen University.

References

[1] **T. Vo**, C. Hüter, S. Braun, M. Torrilhon, *Math. modelling for ASSB: (SE|SSE)-Interface*. Poster, Oxford Batt. Modelling Symp., University of Oxford, OBMS23, P. 66, **2023**.
[2] **T. Vo**, C. Hüter, S. Braun, M. Torrilhon, *Next-gen. All-solid-state Battery (#ASSB)*. Poster, SIAM Computational Science and Eng. Conference, CSE23, Amsterdam, **2023**.
[3] **T. Vo**, *Math. modelling for ASSB*. Presentation, Numerical Modelling in Applied Physics with OpenFOAM Summer School, NUMAP-FOAM, University of Cambridge, **2022**.
[4] **T. Vo**, C. Hüter, S. Braun, R. Spatschek, *Mathematical modelling for All-solid-state battery: Griffith criterion*. Doctoral presentation, IEK-2, Forschungszentrum Jülich, **2020**.
[5] **T. Vo**, *Modeling the swelling phenomena of li-ion batt. cells based on a numerical chemo-mech. coupled approach*. Master thesis, Robert Bosch Battery Systems GmbH, **2018**.
[6] **T. Vo**, A. Gallet-Segarra, C. Bertsch, *Integration of Modelica powertrain models into Hardware in the loop env.*. PreMaster, Robert Bosch GmbH, FEBER, EAM-P2695, **2015**.
[7] **T. Vo**, *Simulation environment for NTC-based voltage drop reduction in Start/Stop appl. and its optimization*. Semiconductor. Bachelor thesis, Robert Bosch GmbH, **2014**.
[8] **S. Braun**, C. Yada, A. Latz, *Thermodynamically consistent model for Space-Charge-Layer formation in a solid electrolyte*. J. Physical Chemistry C, 119, 22281-22288, **2015**.
[9] **C. Hüter**, X. Yin, T. Vo, S. Braun, *A pragmatic dataset augmentation approach for transformation temp. prediction in steels*. Comp. Mat. Science, Vol. 176, 109488, **2020**.
[10] **C. Hüter**, S. Fu, M. Finsterbusch, E. Figgemeier, L. Wells, and R. Spatschek, *Electrode-electrolyte interface stability in SSE system*. AIMS Materials Science, 4(4):867-877, **2017**.

Acknowledgments

T. Vo expresses sincere gratitude to the JARA-CSD research project, led by Dr. S. Braun and Dr. C. Hüter, for their crucial support. Special thanks to Prof. Dr. R. Spatschek for hosting at IEK-2, FZ Jülich. Moreover, T. Vo's role as a teaching assistant in the courses of Mathematische Grundlagen I, II, III, IV, and NumPDE at Computational Engineering Science (CES), RWTH Aachen University (2019-2023), was accomplished and enriched thanks to the guidance and mentorship of Prof. Dr. M. Torrilhon, Prof. Dr. M. Schlottke-Lakemper, Dr. R. Speck, Prof. Dr. B. Berkels, Dr. S. Braun, Prof. Dr. J. Kowalski, Dr. A. Jha, Prof. Dr. B. Stamm, Dr. A. Litvinenko, and Dr. M. Kirchhart.

BOSCH

Bosch Spring School on AI in Industry | March 6-7, 2024

Applied and Computational Mathematics | RWTH AACHEN UNIVERSITY | JÜLICH Forschungszentrum