Mathematical modelling for All-solid-state battery

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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.

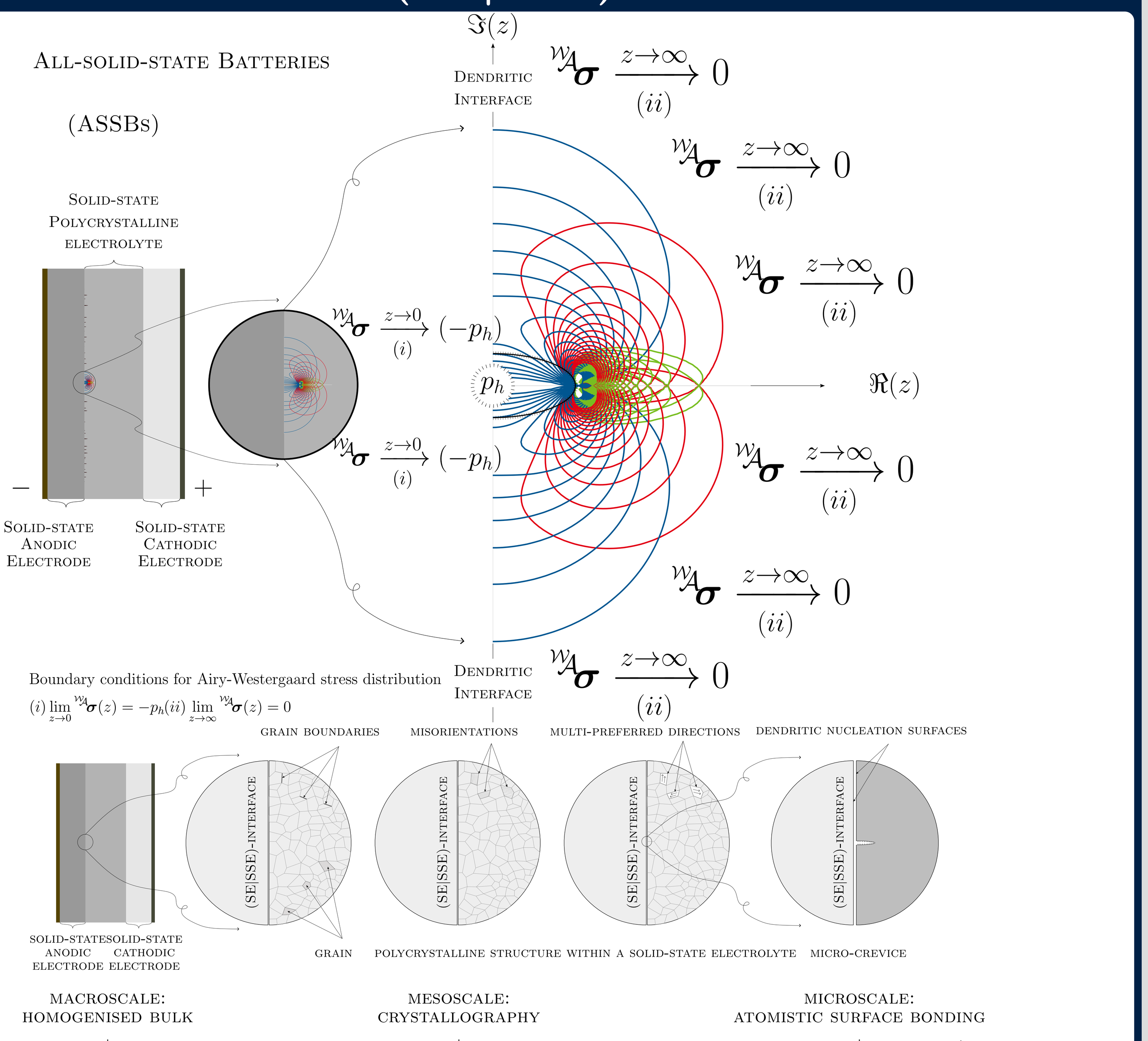
Next-generation All-solid-state battery (ng-ASSB) with a consideration of nucleation criterion defined by

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

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

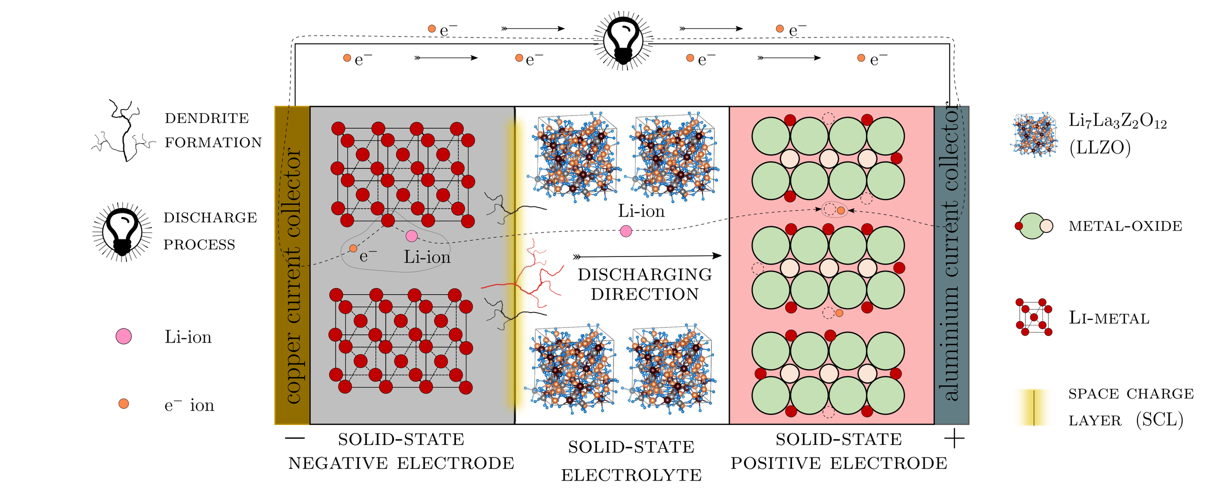
where $V_e:\mathbb{R}^3\to\mathbb{R}$ is the electric potential applied globally on ASSB. Due to nature setting of ASSB taking the form (SE|SSE|SE) the electric potential becomes uniform. Additionally, $\boldsymbol{u}$ is the displacement field, θ temperature field, a crevice length, λ,μ Lamé constants, $\boldsymbol{d}^{(\star)}\otimes\boldsymbol{d}^{(\star)}$ 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.



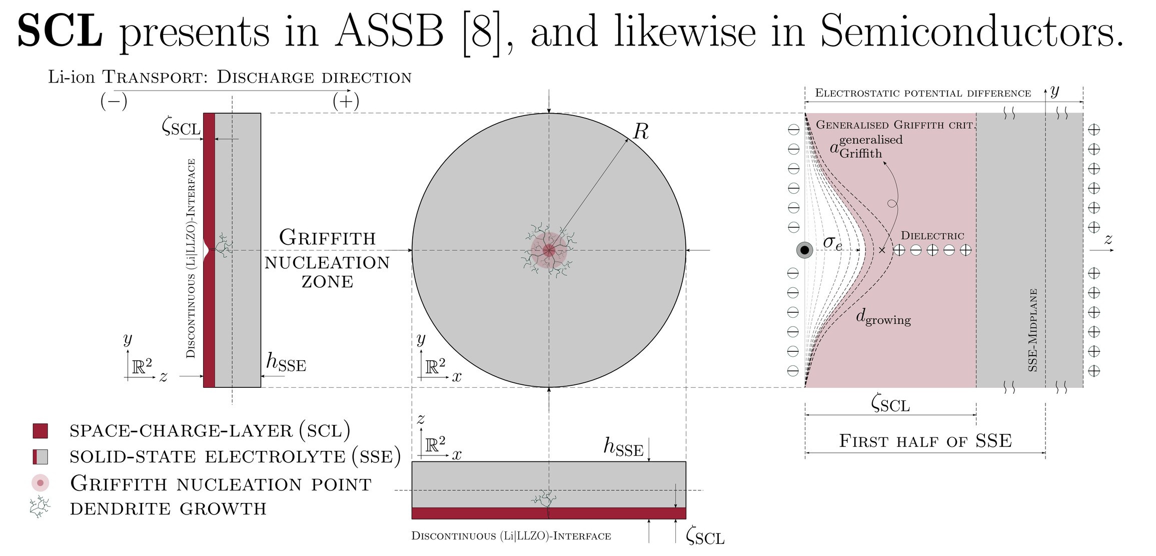
Next-generation All-solid-state battery

Griffith nucleation governs the (SE|SSE)-Interface [10].



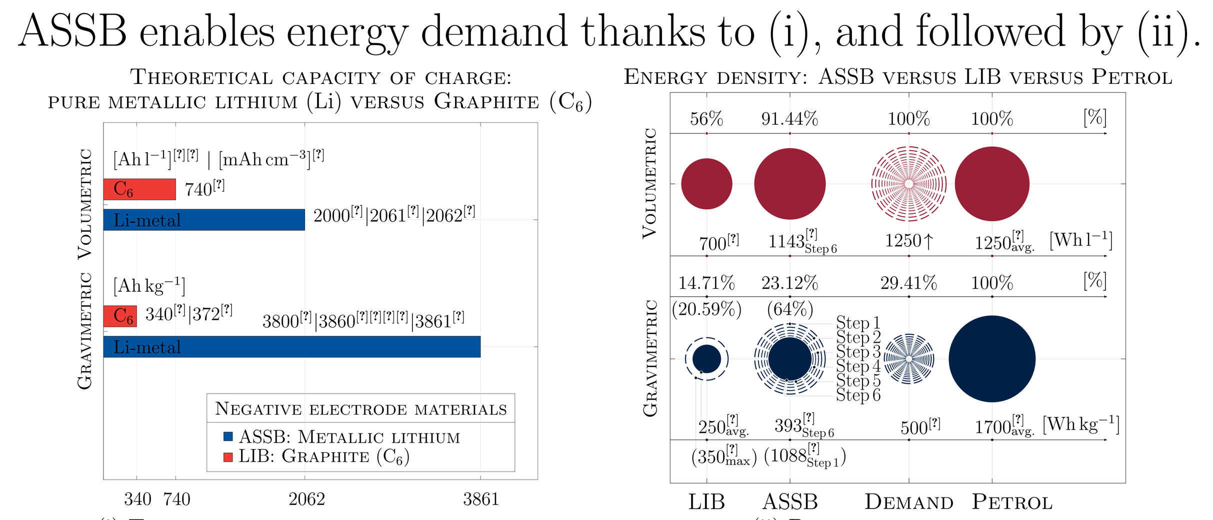
Space-charge Layer

SCL presents in ASSB [8], and likewise in Semiconductors.



Energy density landscape

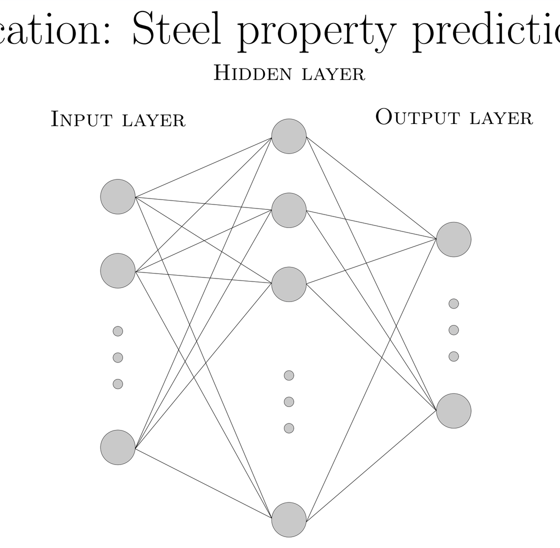
ASSB enables energy demand thanks to (i), and followed by (ii).



(i) Theoretical capacity of charge. (ii) Practical energy density.

Artificial Neural Networks

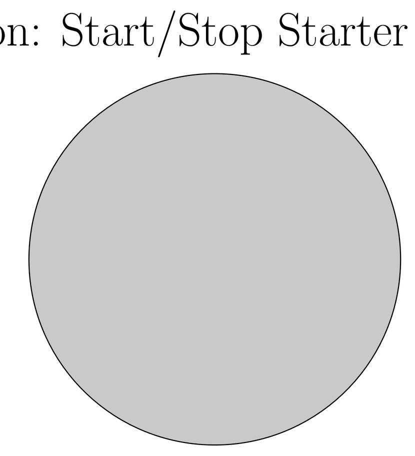
Application: Steel property prediction.



An augmentation scheme for the prediction of the bainitic transformation temperature is validated by means of ANNs [9].

Semiconductor

Application: Start/Stop Starter Motor.



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

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

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

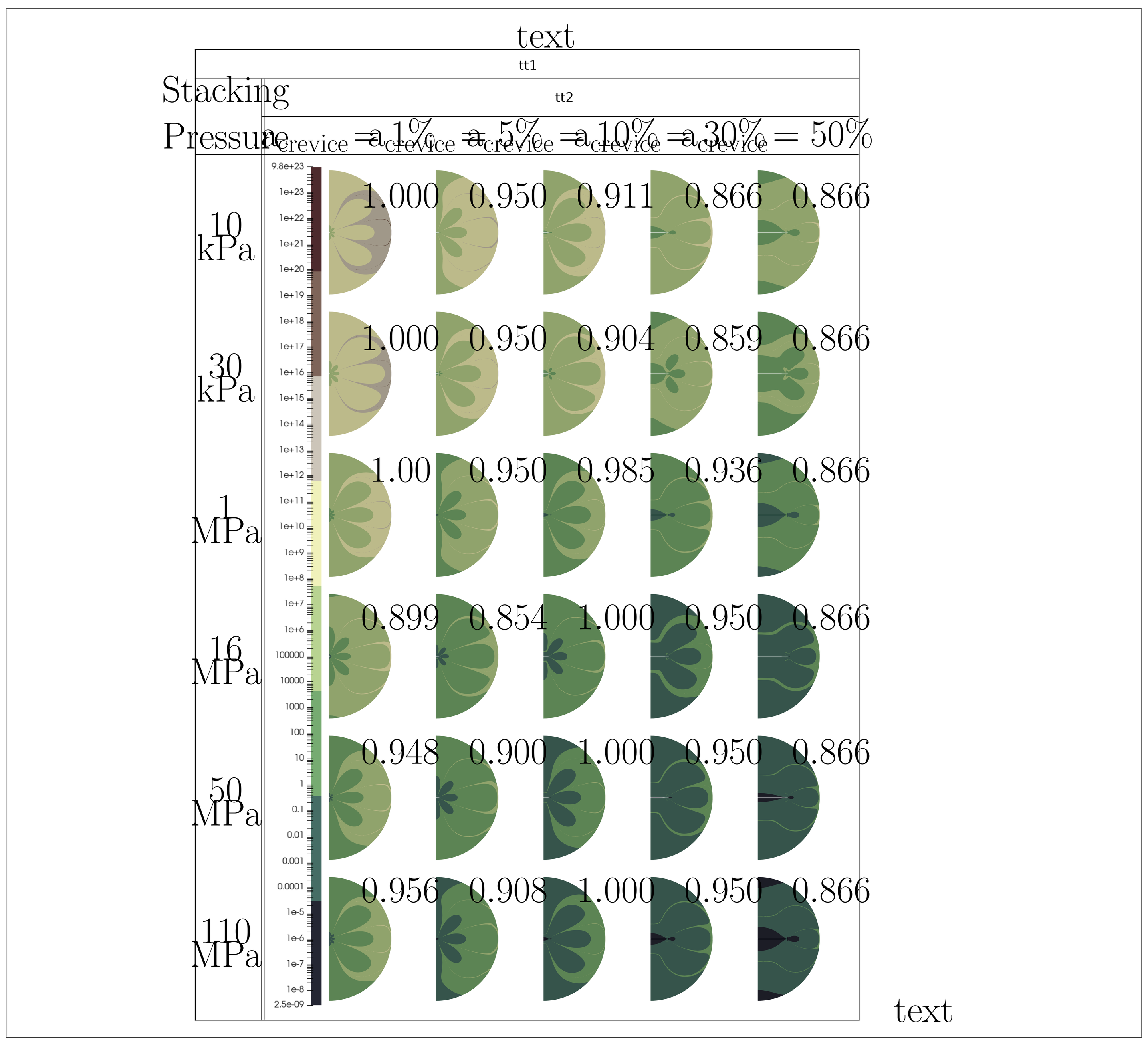
Governing conservation equations used to describe balance of mass, conservation of linear momentum, conservation of angular momentum, and conservation of energy with $\rho(\boldsymbol{x},t)$ is mass density per unit volume (puv); $\boldsymbol{b}(\boldsymbol{x},t)$ body force puv; $\boldsymbol{v}(\boldsymbol{x},t)$ 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.

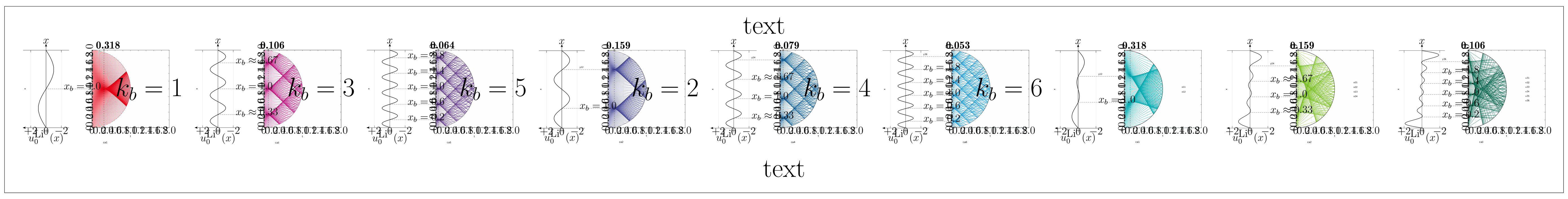
Strain energy is based on the deformation of SSE due to dendrite formation at (SE|SSE)-interface

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

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

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





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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**.

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