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 [10].

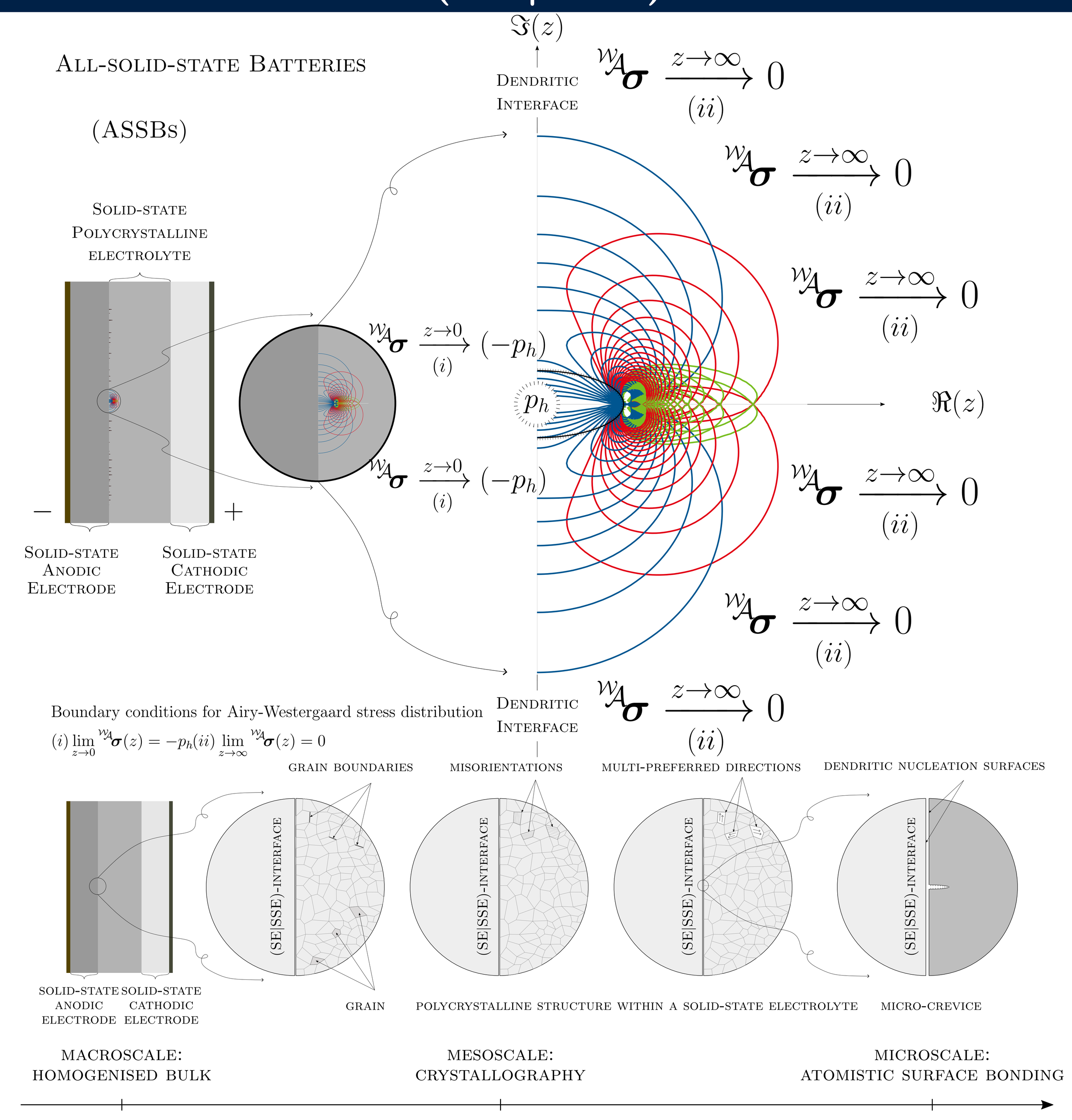
Next-generation All-solid-state battery (ng-ASSB) with a consideration of nucleation criterion defined by

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

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

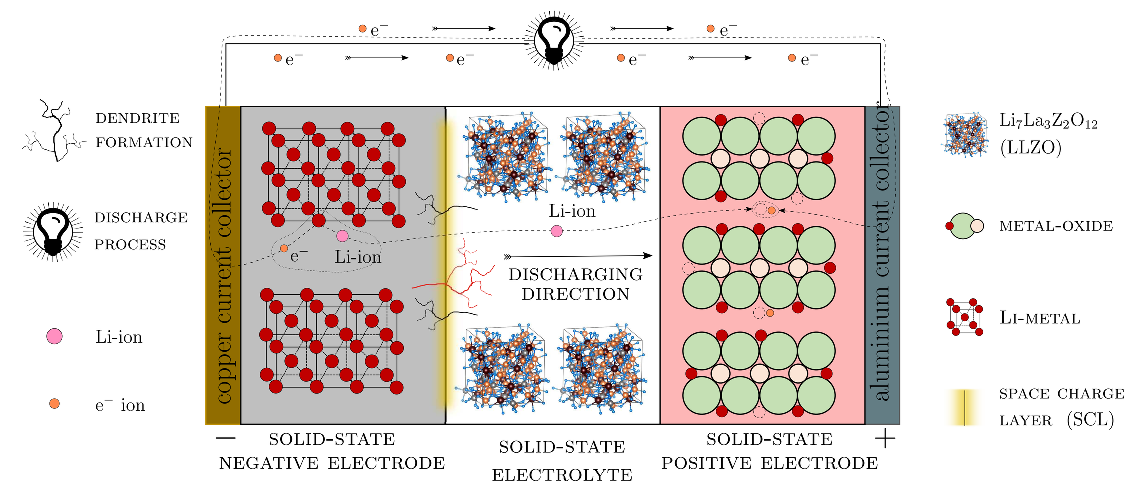
where $V_e : \mathbb{R}^3 \to \mathbb{R}$ is the electric potential applied globally on ASSB. Due to nature setting of ASSB taking the form (SE|SSE|SE) the electric potential becomes uniform. Additionally, $\boldsymbol{u}$ is the displacement field, θ temperature field, a crevice length, λ, μ Lamé constants,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



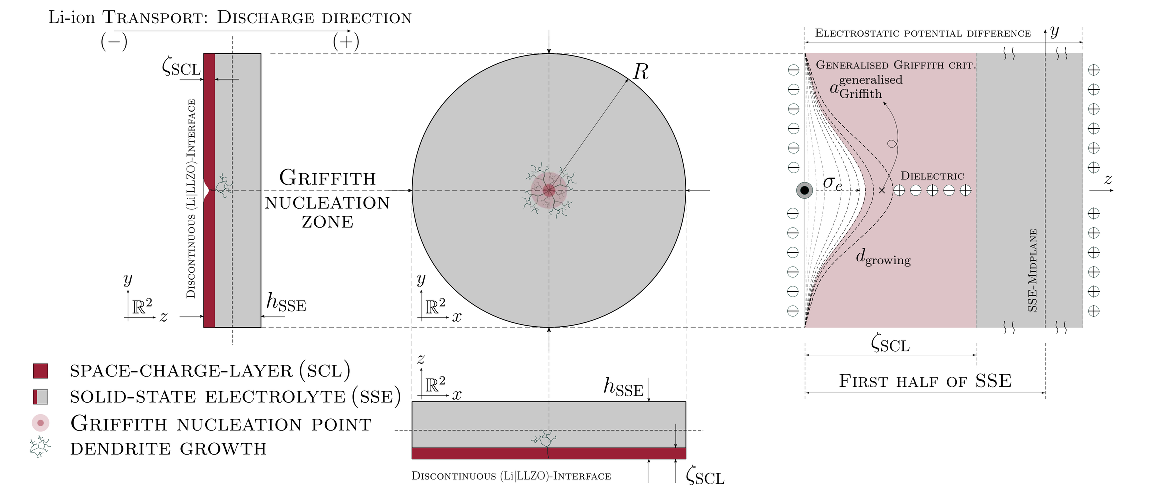
Next-generation All-solid-state battery

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



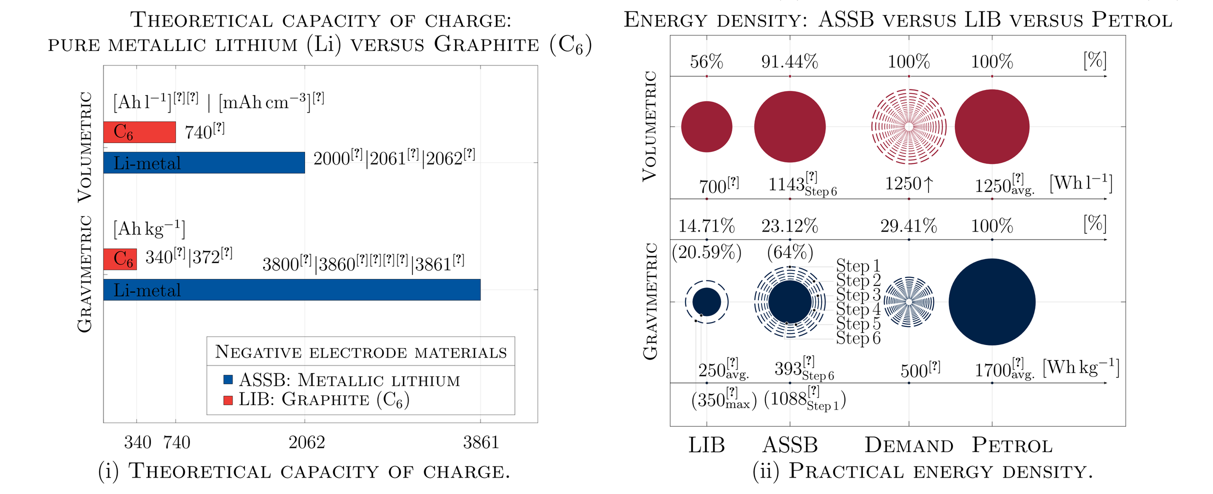
Space-charge Layer

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



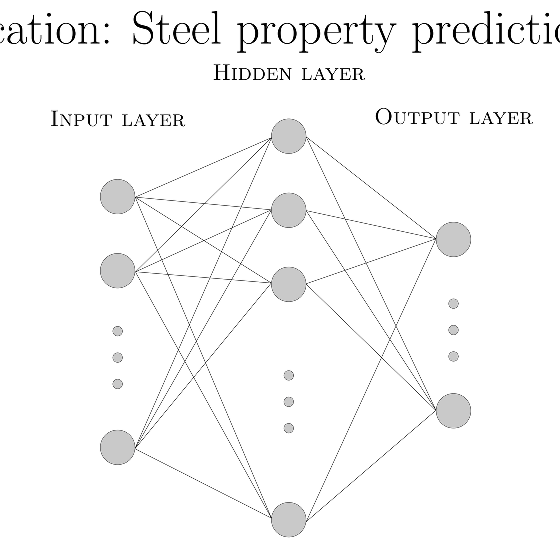
Energy density landscape

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



Artificial Neural Networks

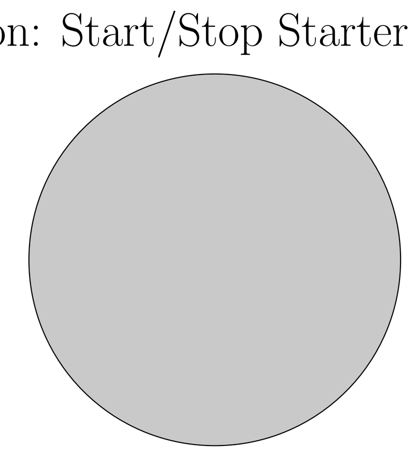
Application: Steel property prediction.



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;

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

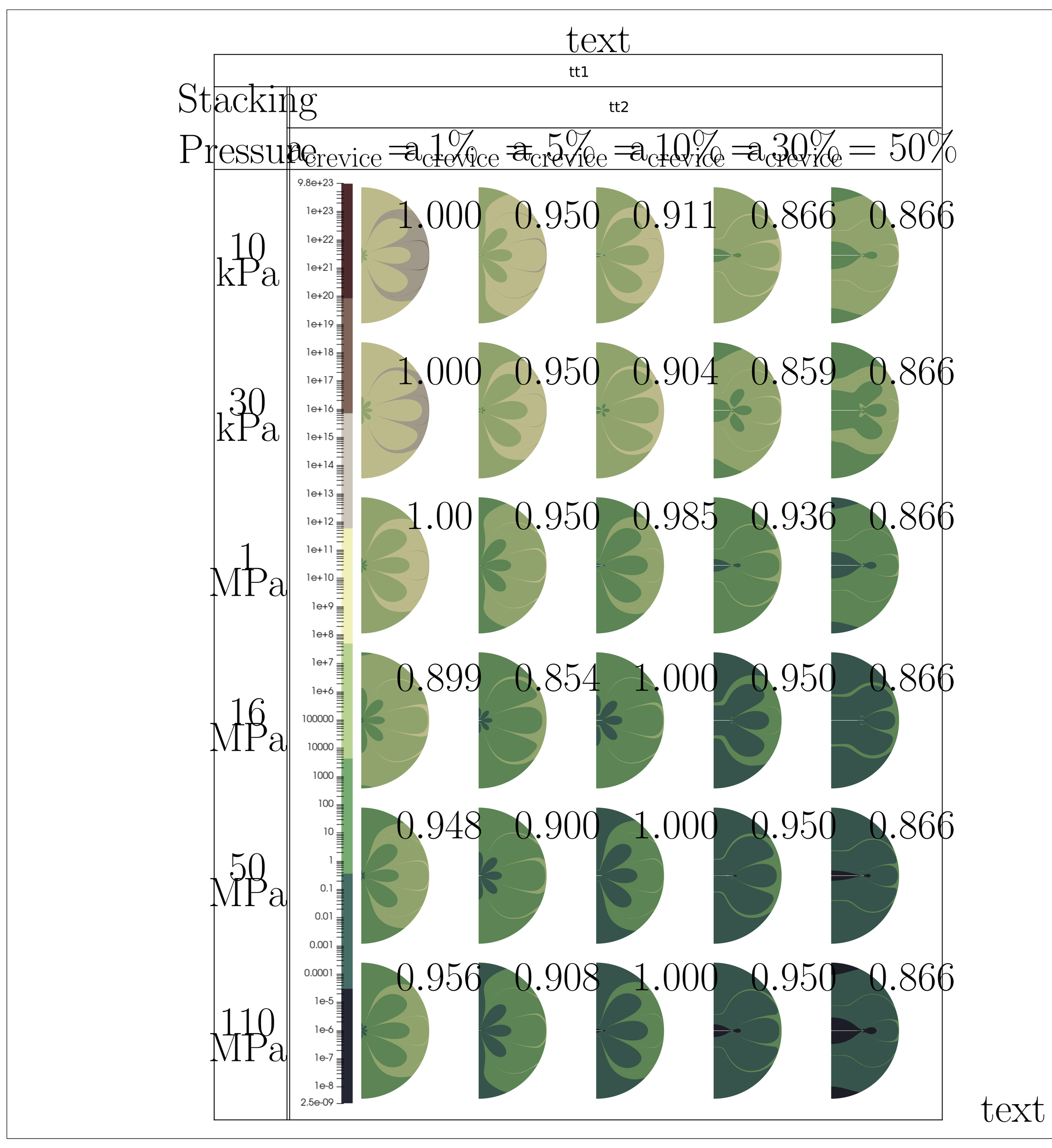
Governing conservation equations used to describe balance of mass, conservation of linear momentum, conservation of angular momentum, and conservation of energy with $\rho(\boldsymbol{x},t)$ is mass density per unit volume (puv); $\boldsymbol{b}(\boldsymbol{x},t)$ body force puv; $\boldsymbol{v}(\boldsymbol{x},t)$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

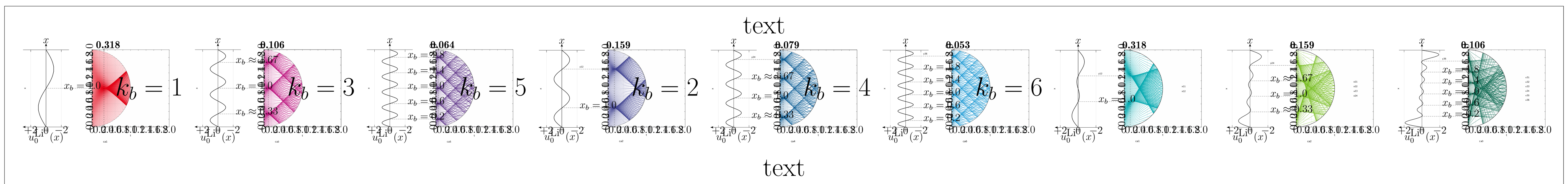
Strain energy is based on the deformation of SSE due to dendrite formation at (SE|SSE)-interface

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

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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