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].

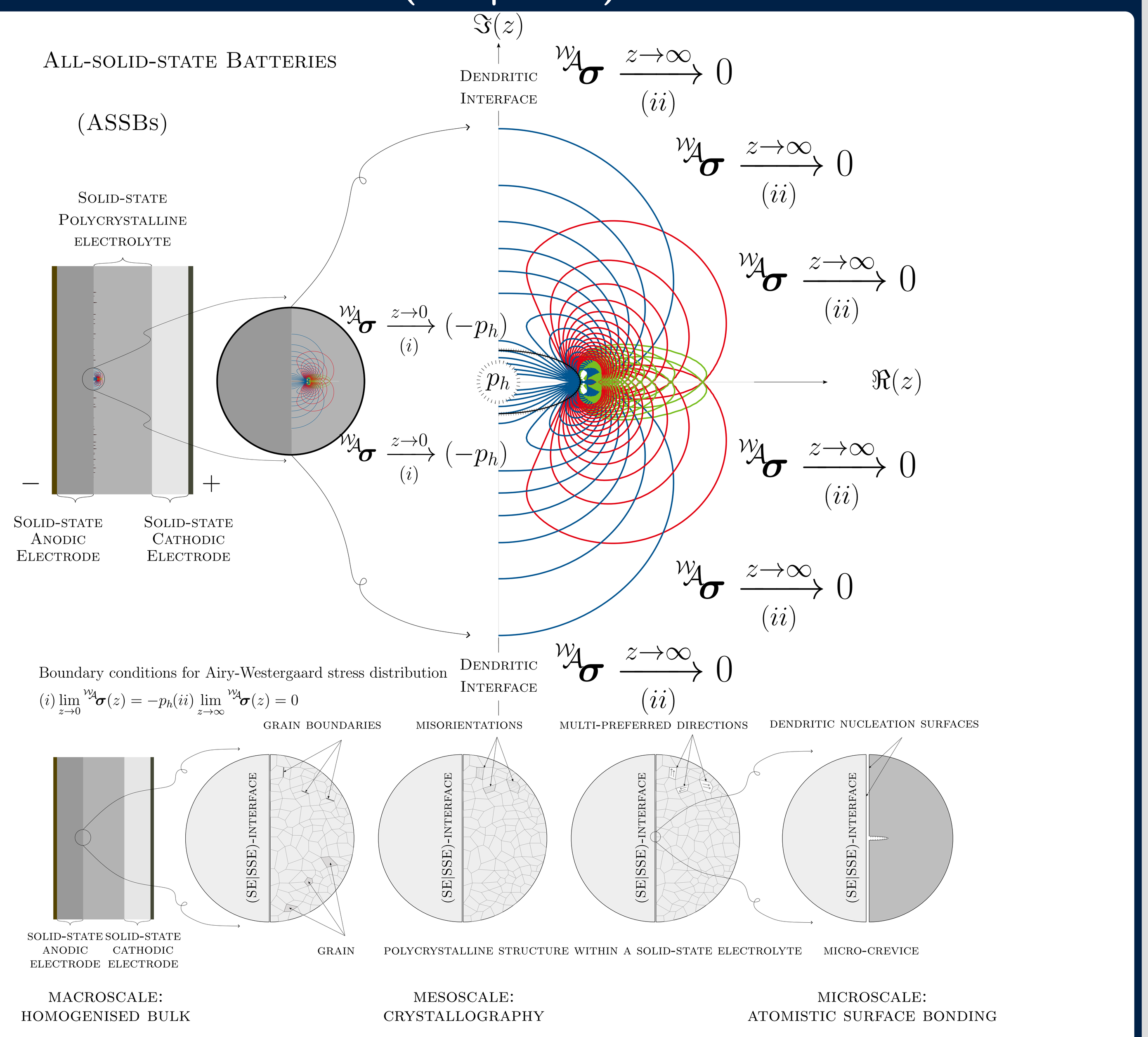
Next-generation All-solid-state battery (ng-ASSB) with a consideration of nucleation criterion defined by

$$\rho_{\text{SCL}}\frac{D^2\boldsymbol{u}_{\text{SCL}}}{Dt^2} + \nabla\cdot\Big(\mathbb{C}(\lambda,\mu) : \nabla\boldsymbol{u}^{(s)}_{\text{SCL}}\Big) + \rho_{\text{SCL}}\,\boldsymbol{b} = -\rho_{\text{SCL}}\,V_e, \tag{1}$$

$$\text{s.t.}\quad a^{\text{generalised}}_{\text{Griffith}} := a^* = \arg\{\min_{a\in\mathcal{V}} \iiint_\Omega f(a_{\text{crevice}}, \boldsymbol{u}_{\text{SCL}}, \theta_{\text{SCL}}, n^{\text{Li}^+}; \lambda, \mu, \boldsymbol{d}_{\text{SCL}}\otimes\boldsymbol{d}_{\text{SCL}})\,d\Omega - \iint_\Gamma f(a_{\text{crevice}}; \gamma_s)\,d\Gamma\}, \tag{2}$$

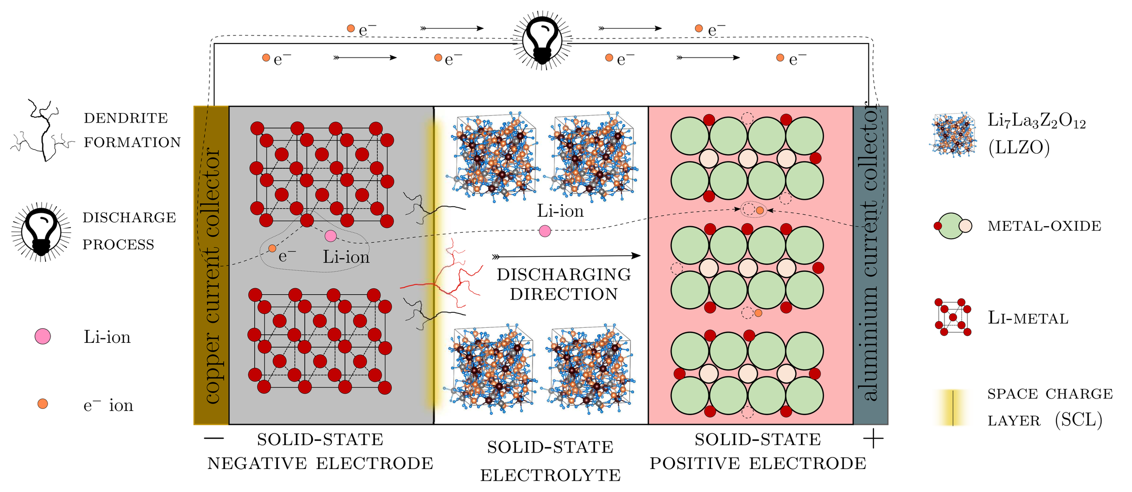
hold for $\forall a \in \mathcal{V}$. Here, $V_e : \mathbb{R}^3 \to \mathbb{R}$ is the electric potential applied globally on ASSB. Due to nature setting of ASSB taking the form (SE|SSE|SE) the electric potential becomes uniform. Additionally, $\boldsymbol{u}$ is the displacement field, θ temperature field, a crevice length, λ, μ Lamé constants, $\boldsymbol{d}\otimes\boldsymbol{d}$ embedded misorientation SCL structural tensor, and γ_s 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.



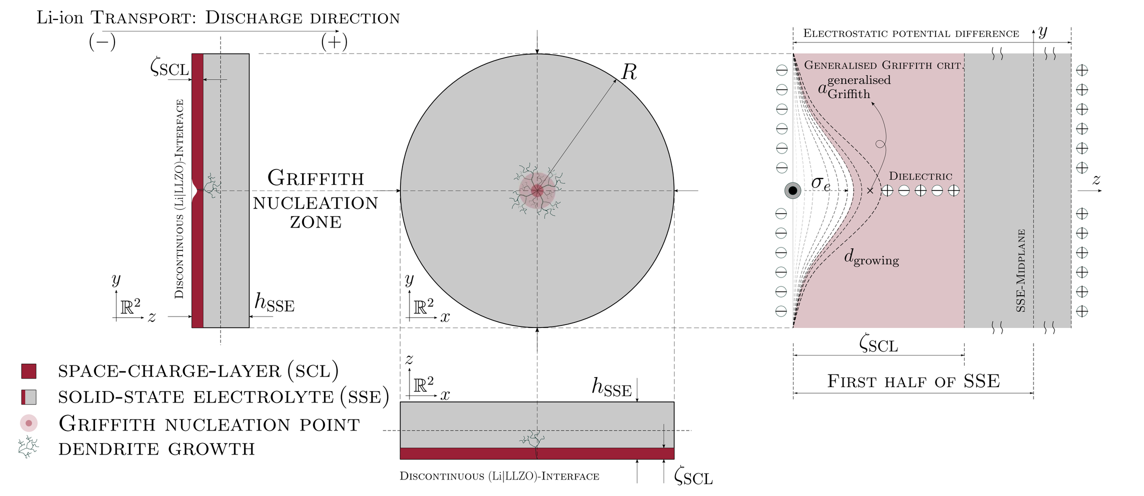
Next-generation All-solid-state battery

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



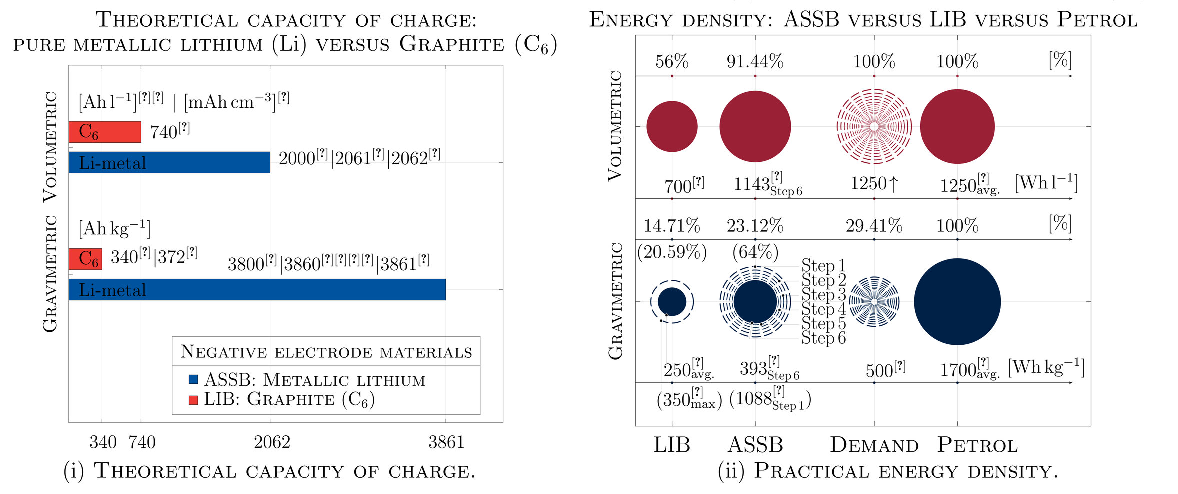
Observation: Space-charge Layer

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



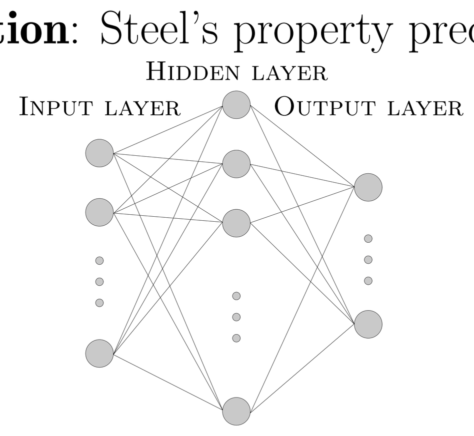
Motivation: Energy density landscape

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



Artificial Neural Networks

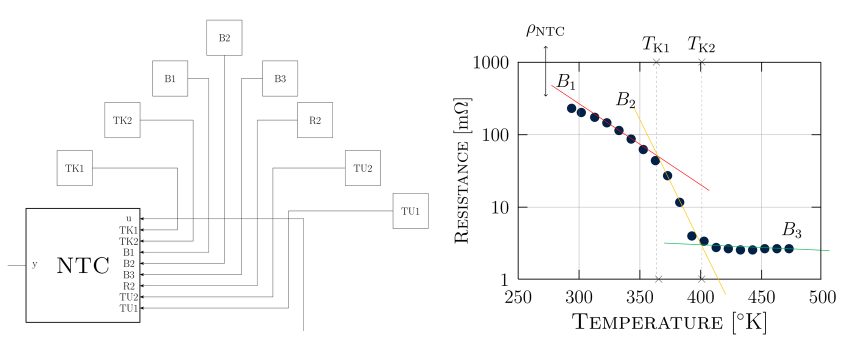
Application: Steel's property prediction.



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)

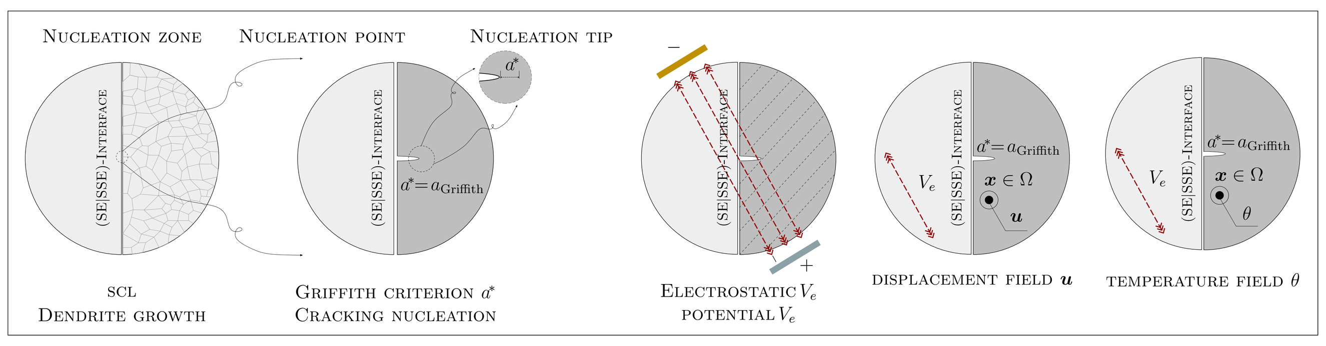


Nd/Gd Negative-Temperature Coefficient (NTC) semiconductor model validated [7].

Lithium-ion battery

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

State-of-the-art: Nucleation interface taking place at the unstable (SE|SSE)-Discontinuity



Coupled fields are Displacement field $\boldsymbol{u}$ and Temperature field θ:

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

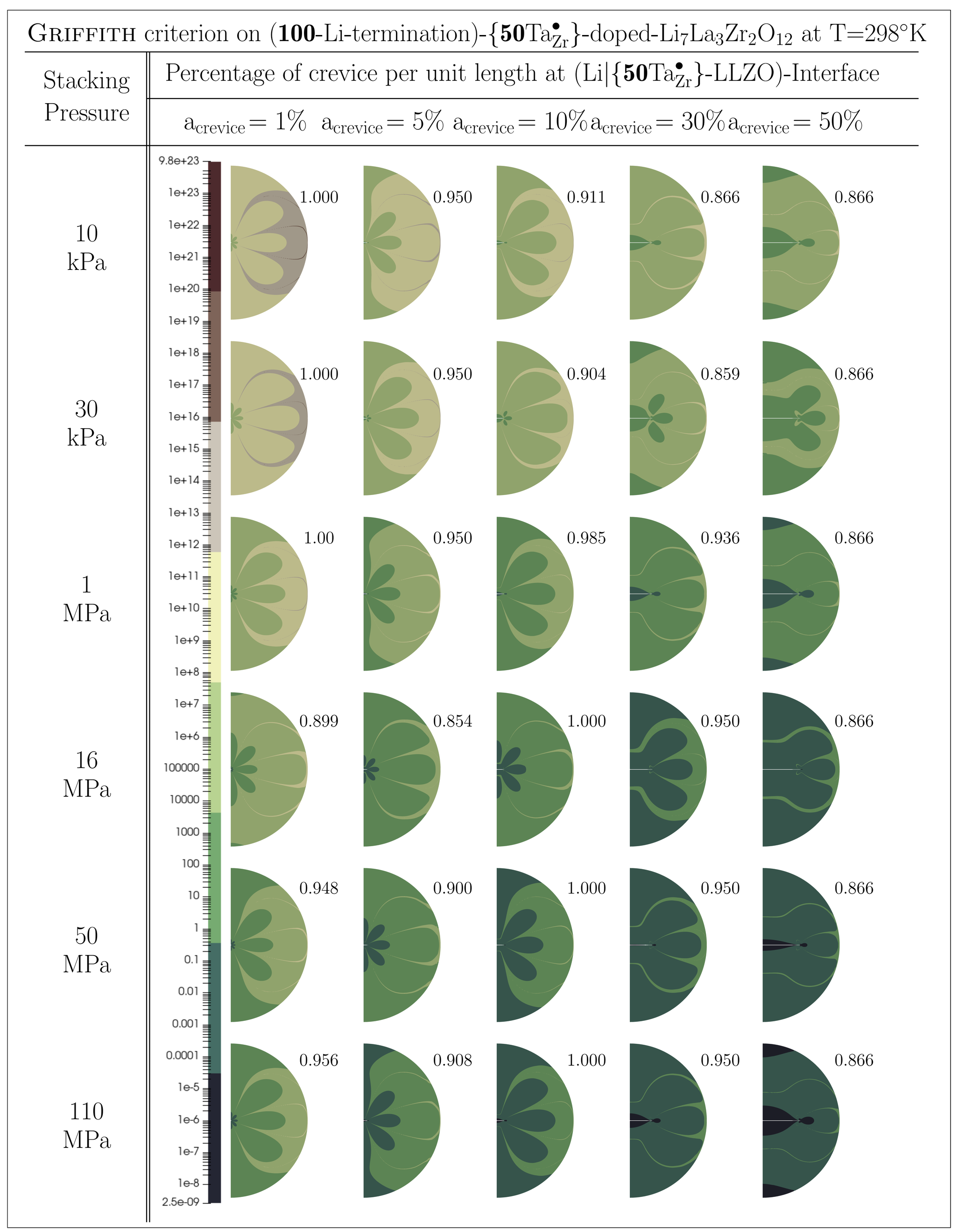
Governing conservation equations account for mass balance, linear and angular momentum, and energy conservation. These equations include variables such as mass density $\rho(\boldsymbol{x},t)$, body force $\boldsymbol{b}(\boldsymbol{x},t)$, velocity $\boldsymbol{v}(\boldsymbol{x},t)$, internal energy $e(\boldsymbol{x},t)$, heat flux $\boldsymbol{q}(\boldsymbol{x},t)$, heat source $r(\boldsymbol{x},t)$, Cauchy stress $\boldsymbol{\sigma}$, and infinitesimal strain $\boldsymbol{\varepsilon}$ per unit volume.

Strain energy (E_{st}) is derived from the SSE deformation due to dendrite formation at the unstable (SE|SSE)-Interface:

$$E_{\text{st}} := \iiint_\Omega f(a, \boldsymbol{u}; \lambda, \mu, \boldsymbol{d}\otimes\boldsymbol{d})\,d\Omega$$

Surface energy (E_{sf}) is assessed through the analysis of crevices at the (SE|SSE)-Interface under specific pressure conditions:

$$E_{\text{sf}} := \iint_\Gamma f(a;\gamma)\,d\Gamma$$

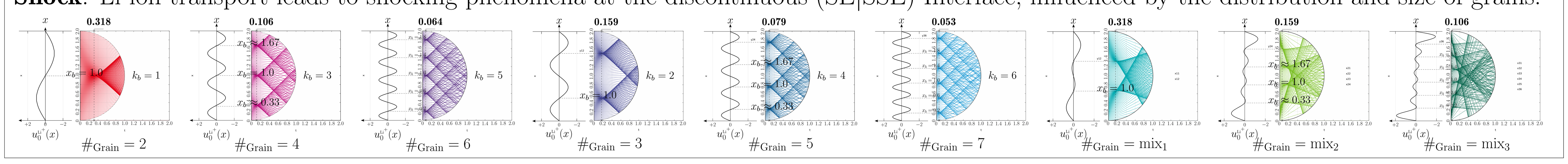


Solution: Analysing system of PDEs in (1) and (2) results in a simplified Griffith nucleation criterion, which incorporates Cauchy stress tensor denoted by σ, Young's elastic modulus E_Y, and experimentally-derived surface energy γ_s. Here, σ is calculated using FVM based on OpenFOAM library [1][2][3][4].

Griffith criterion:

$$a^{\text{simplified}}_{\text{Griffith}} = \sqrt{\frac{2\,E_Y\,\gamma_s}{\pi\,\sigma}}$$

Shock: Li-ion transport leads to shocking phenomena at the discontinuous (SE|SSE)-Interface, influenced by the distribution and size of grains.



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