

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].

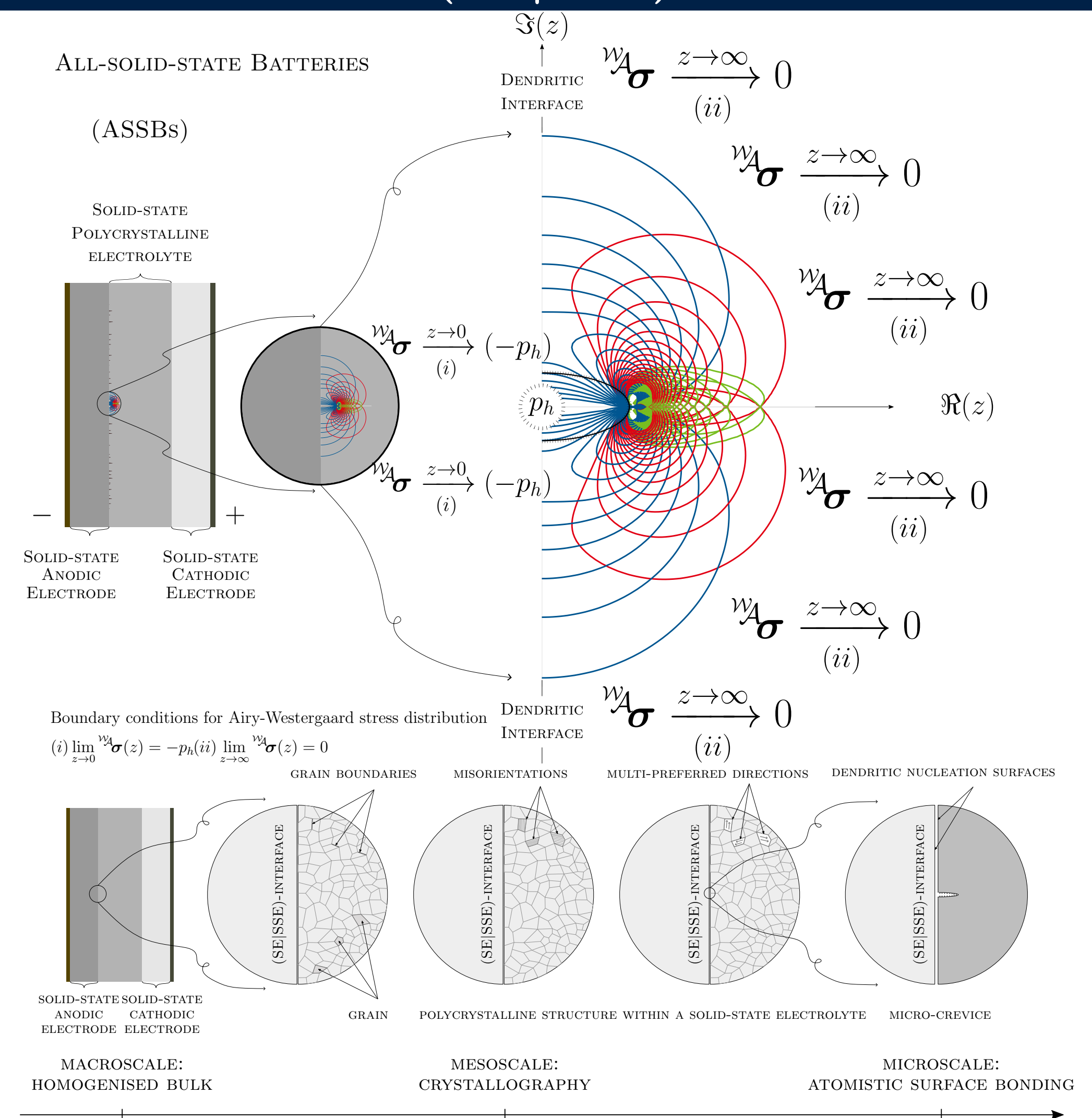
Next-generation All-solid-state battery (ng-ASSB) with a consideration of **nucleation criterion** defined by

$$\partial_t \mathbf{u} + \nabla \cdot \left(\mathbf{C}^{\text{fallocation}}(\lambda, \mu, \mathbf{d}_{G,i}^R, i=1, \dots, N, \mathbf{d}^E; \mathbf{x}) : \nabla \mathbf{u}^{(s)} \right) + \rho \mathbf{b} = -\rho \nabla V_e, \quad (1)$$

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

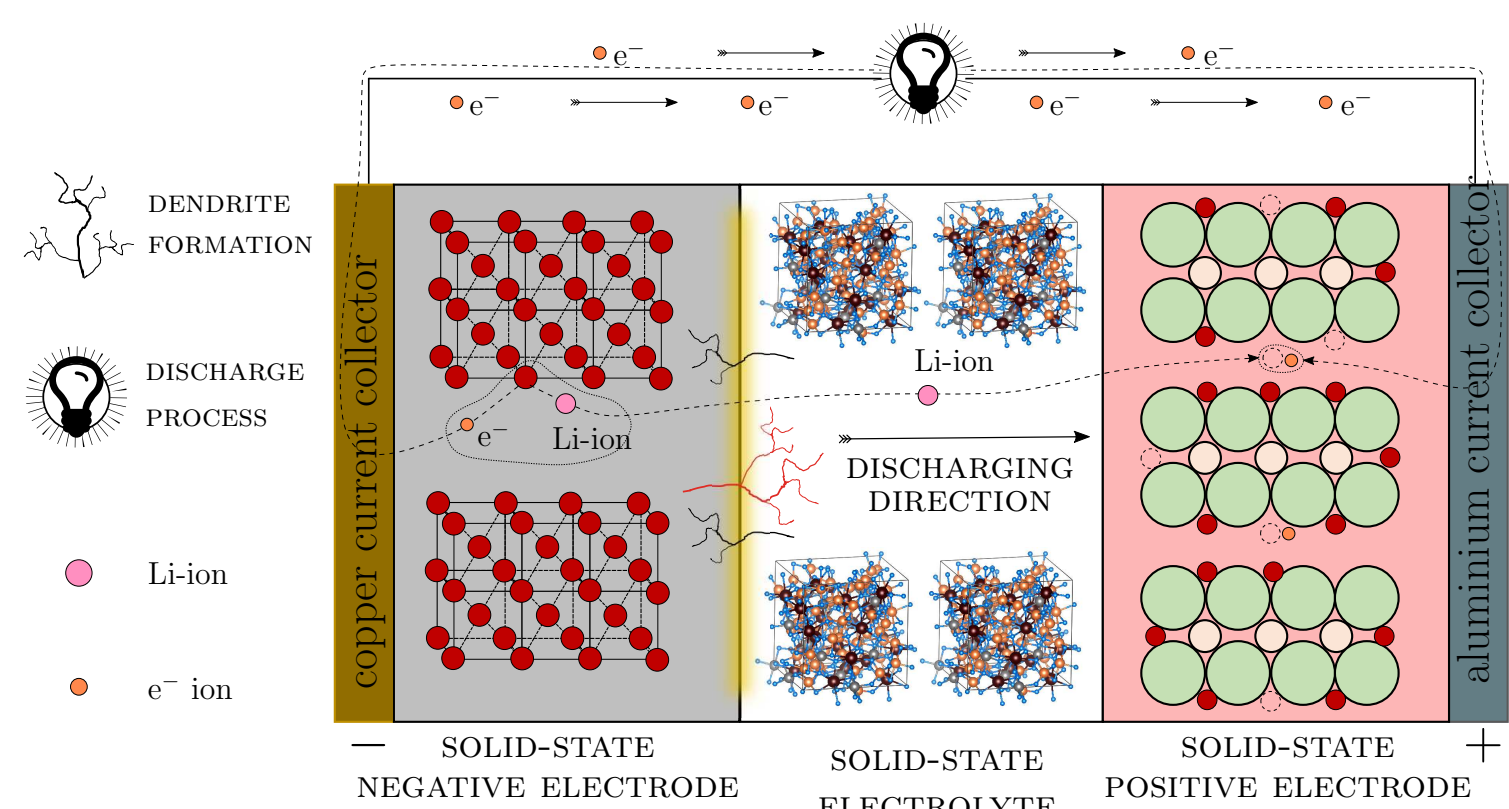
where $V_e : \mathbb{R}^3 \rightarrow \mathbb{R}$ is the electric potential applied globally on ASSB. Due to nature setting of ASSB taking the form (SE|SSE|SE) the electric potential becomes uniform. Additionally, \mathbf{u} is the displacement field, θ temperature field, a crevice length, λ, μ Lamé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



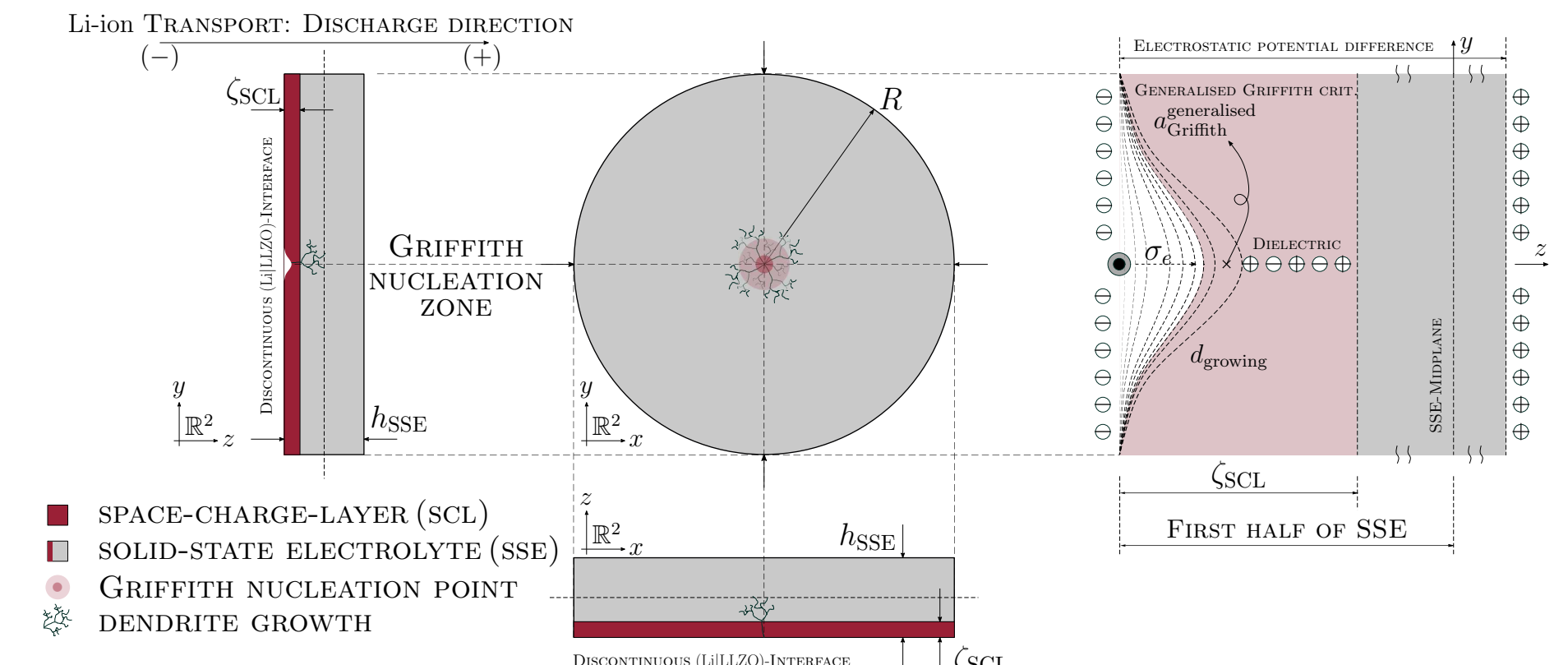
Next-generation All-solid-state battery

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



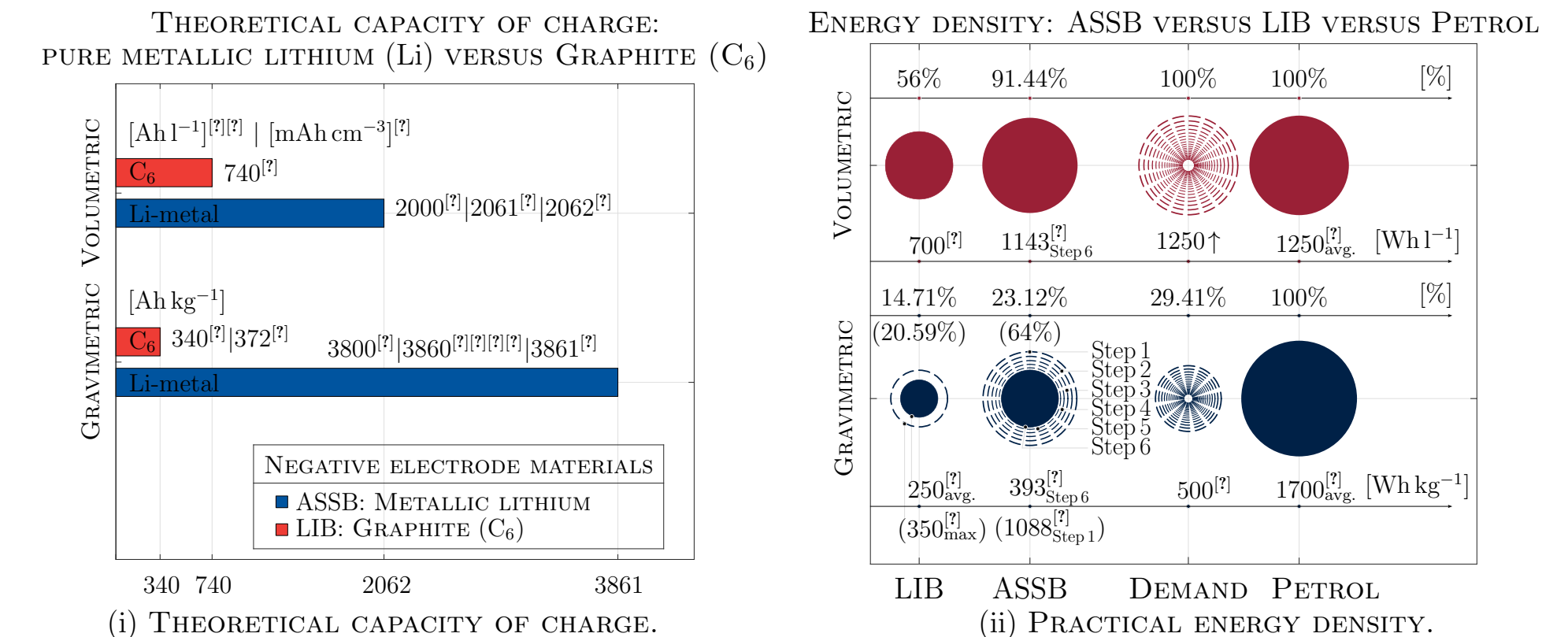
Observation: Space-charge Layer

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



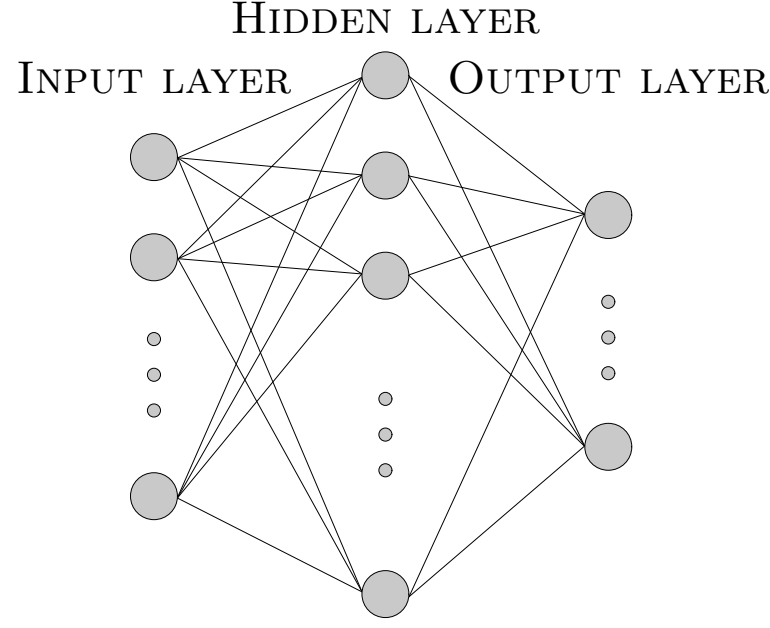
Motivation: Energy density landscape

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



Artificial Neural Networks

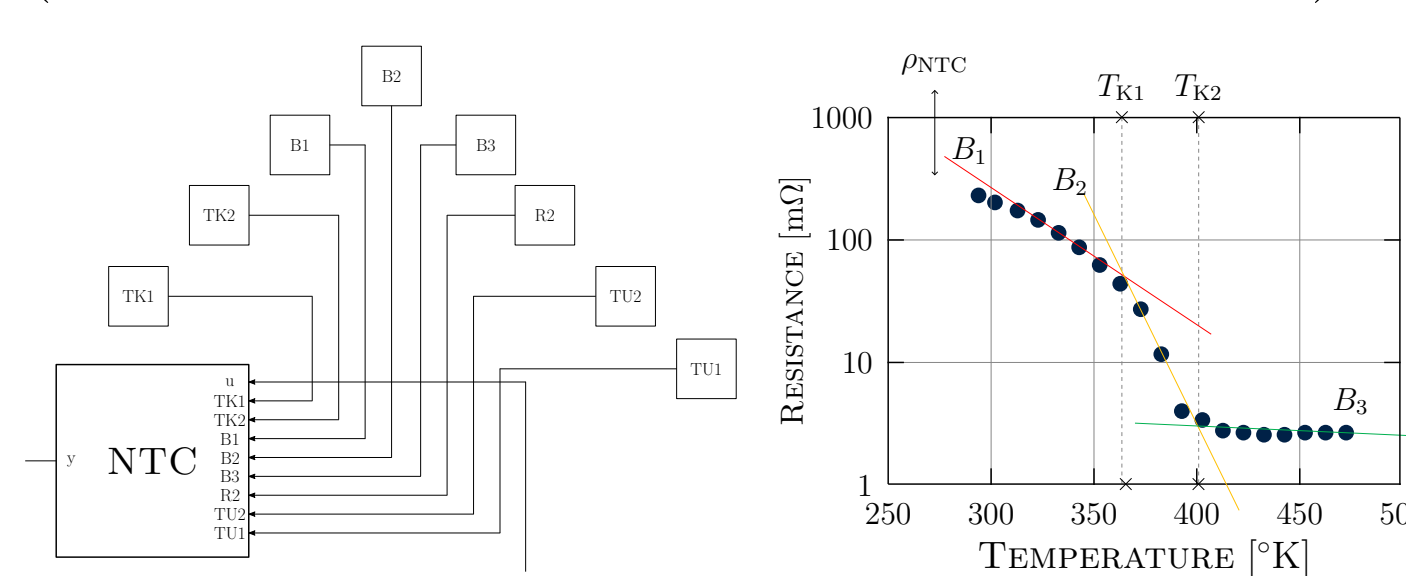
Application: Steel's property prediction.



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)

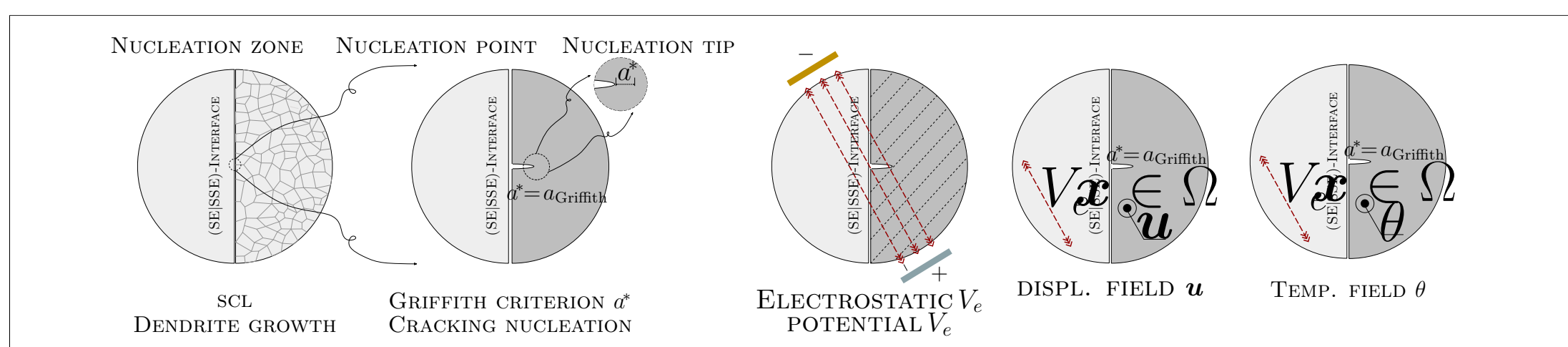


Negative-temp. Coefficient (NTC) Nd/Gd semiconductor is modelled and validated [7].

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 \mathbf{u} and temperature field θ ;

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

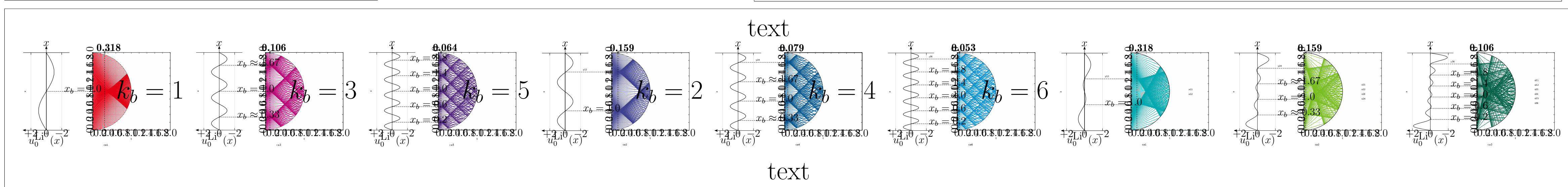
Governing conservation equations used to describe balance of mass, conservation of linear momentum, conservation of angular momentum, and conservation of energy with $\rho(\mathbf{x}, t)$ is mass density per unit volume (puv); $\mathbf{b}(\mathbf{x}, t)$ body force puv; $\mathbf{v}(\mathbf{x}, t)$ velocity;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

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

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

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

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



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