

# MATHEMATICAL MODELLING FOR ALL-SOLID-STATE BATTERY: SPACE-CHARGE LAYER

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## Mathematical modelling for the next-generation All-solid-state batteries: Nucleation (SE|SSE)<sup>(\*)</sup>-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].

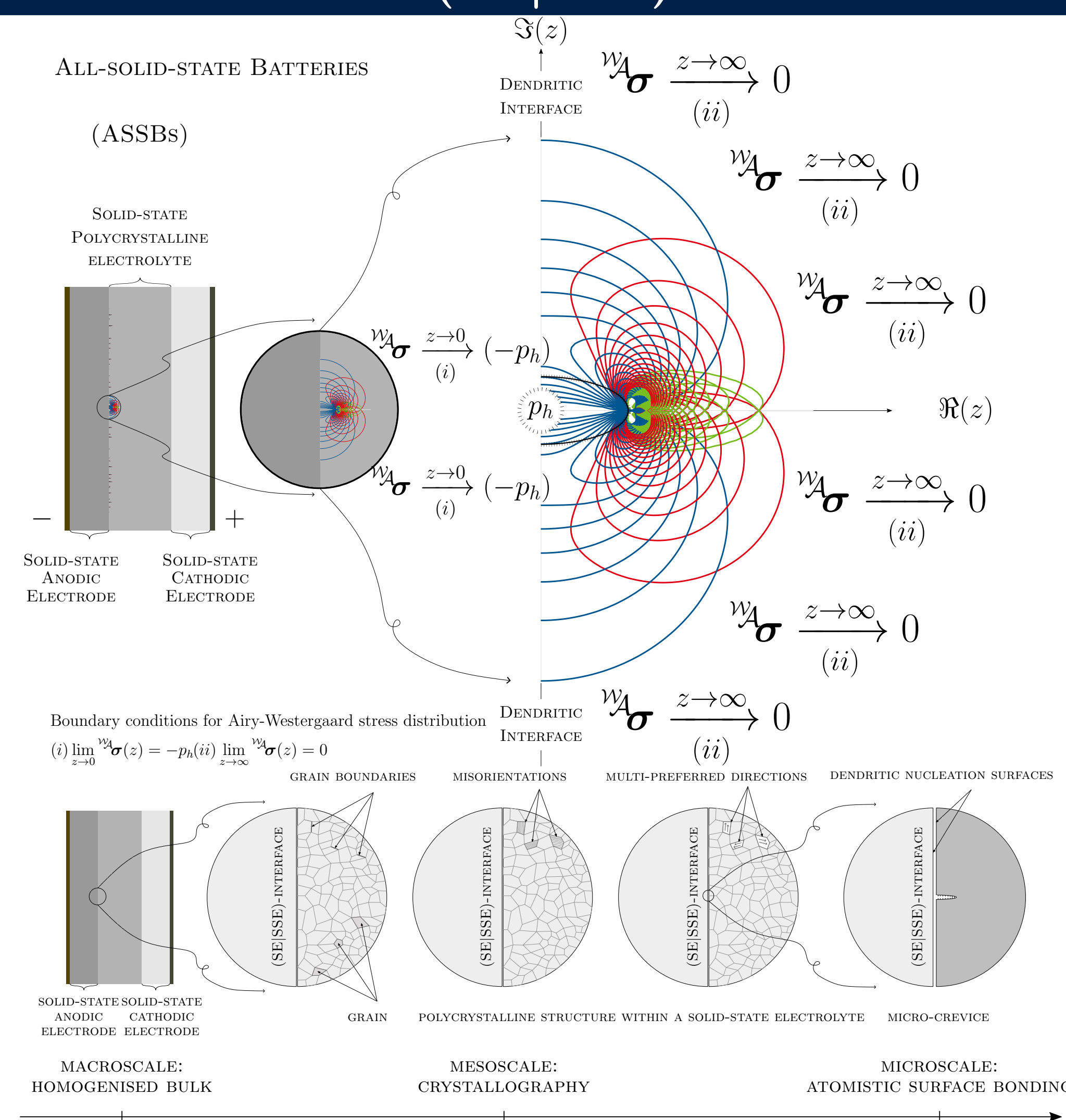
**Next-generation All-solid-state battery** (ng-ASSB) with a consideration of **nucleation criterion** defined by

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

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

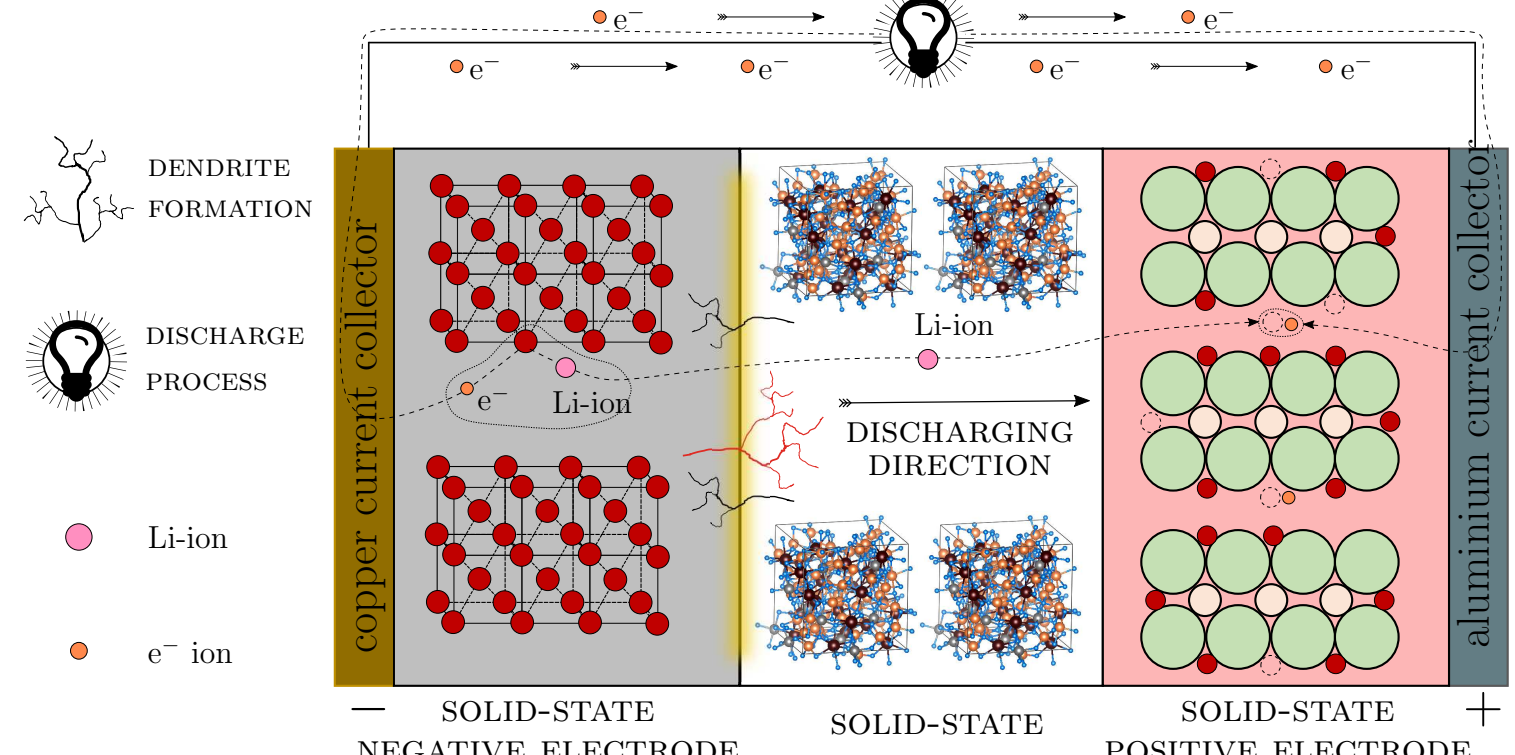
hold for  $\forall a \in \mathcal{V}$ . Here,  $V_e : \mathbb{R}^3 \rightarrow \mathbb{R}$  is the electric potential applied globally on ASSB. Due to nature setting of ASSB taking the form (SE|SSE|SE) the electric potential becomes uniform. Additionally,  $\mathbf{u}$  is the displacement field,  $\theta$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



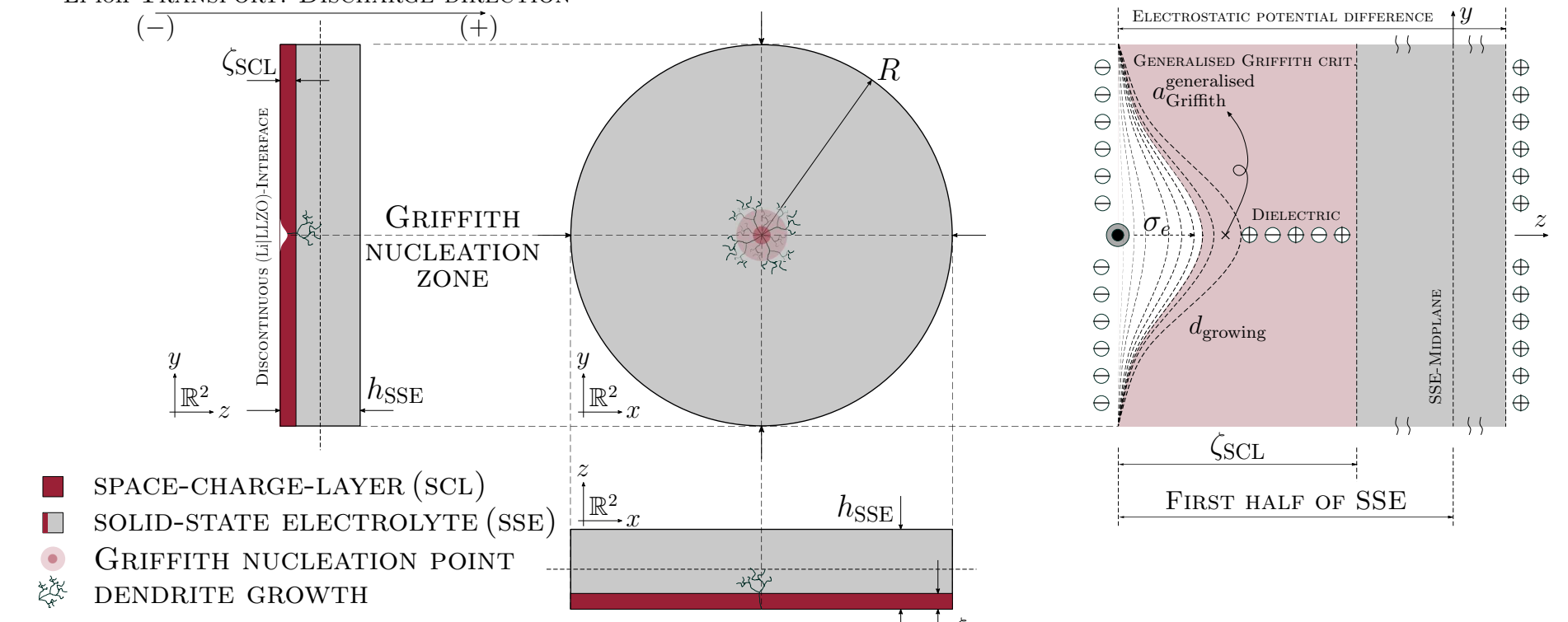
## Next-generation All-solid-state battery

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



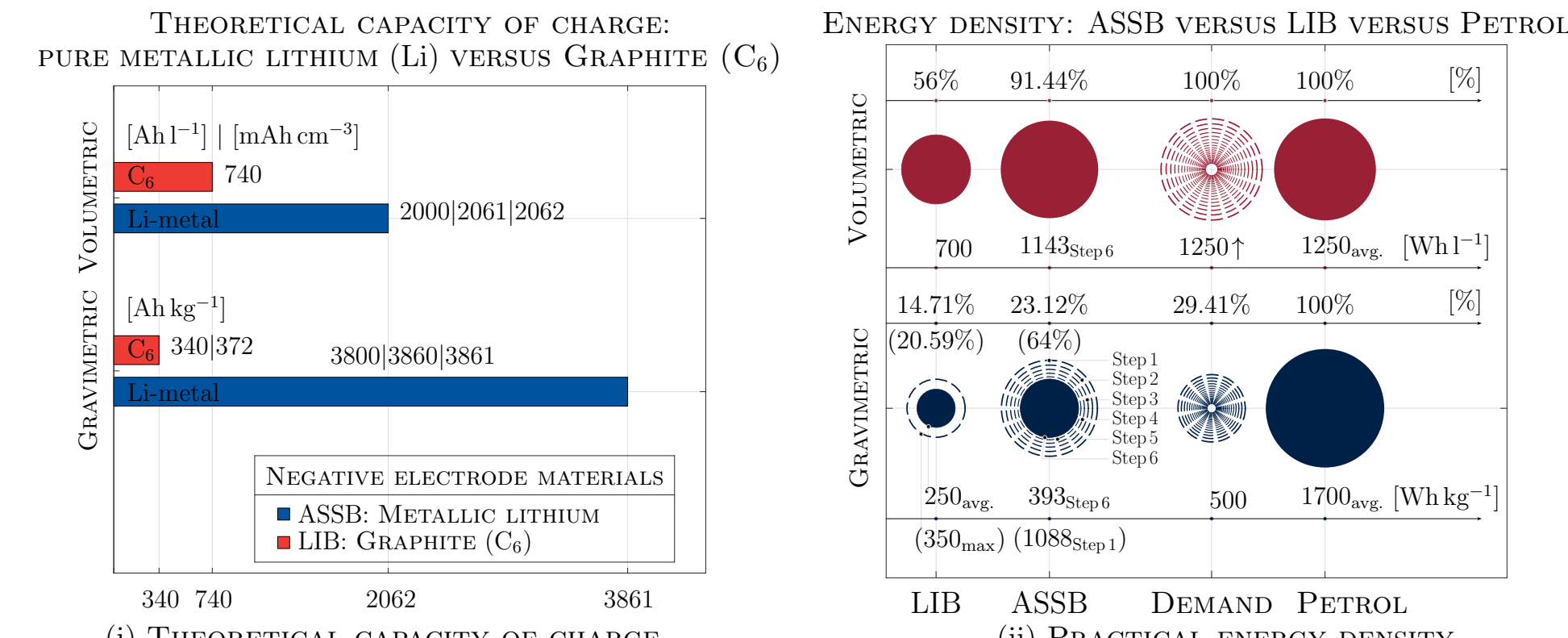
## Observation: Space-charge Layer

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



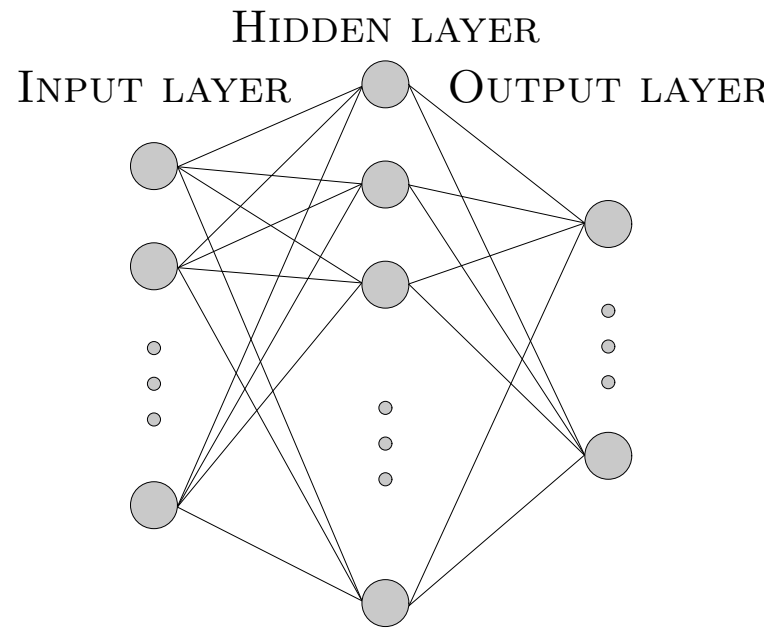
## Motivation: Energy density landscape

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



## Artificial Neural Networks

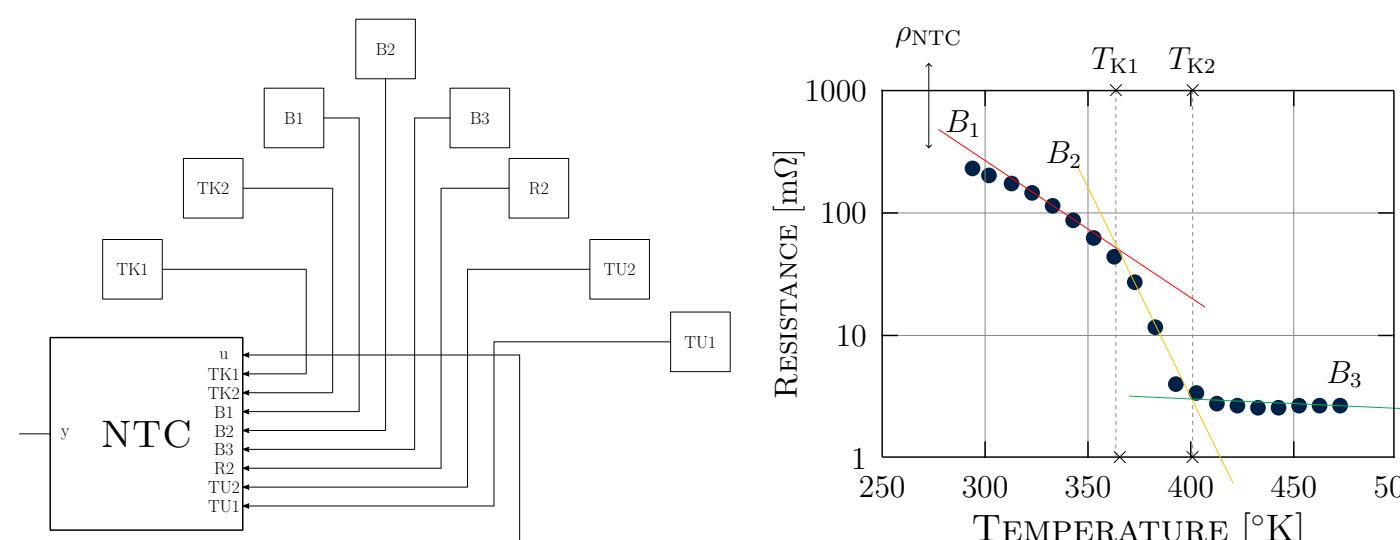
**Application:** Steel's property prediction.



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)

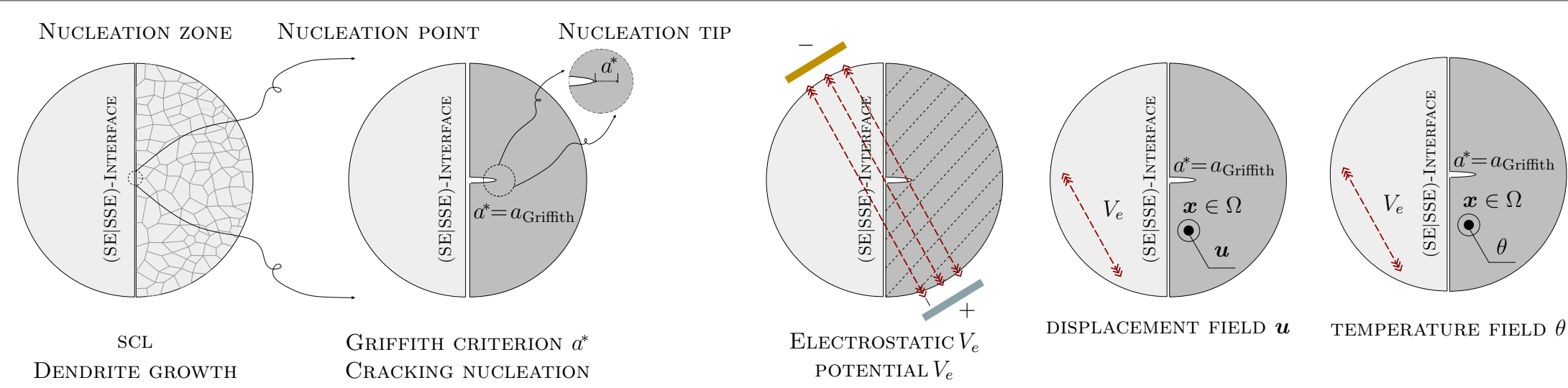


Nd/Gd Negative-Temperature Coefficient (NTC) semiconductor model validated [7].

## 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  $\mathbf{u}$  and Temperature field  $\theta$ :

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

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

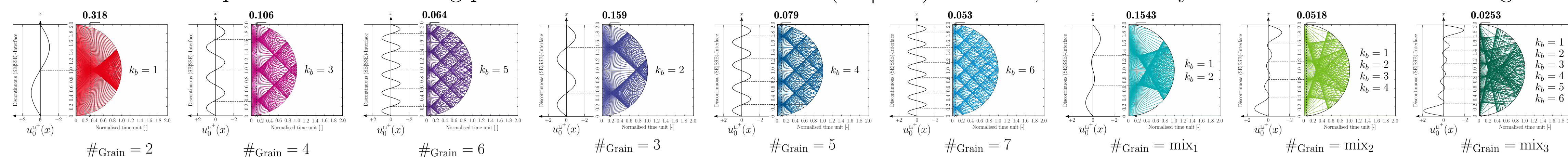
**Strain energy** ( $E_{\text{st}}$ ) is derived from the SSE deformation due to dendrite formation at the unstable (SE|SSE)-Interface:

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

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

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

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



### Solution:

Analysing system of PDEs arising in (1) and (2) results in a simplified Griffith nucleation criterion, including the Cauchy stress tensor denoted by  $\boldsymbol{\sigma}$ , Young's elastic modulus  $E_Y$ , and experimentally-derived surface energy  $\gamma_s$ . Here, the  $\boldsymbol{\sigma}$  is computed using FVM based on OpenFOAM library [1][2][3][4].

Griffith criterion:

$$\sigma_{\text{Griffith}}^{\text{simplified}} = \sqrt{\frac{2 E_Y \gamma_s}{\pi a_{\text{crevice}}}}$$

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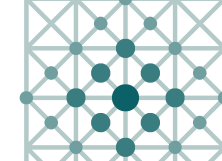
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