

# MATHEMATICAL MODELLING FOR ALL-SOLID-STATE BATTERY

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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.

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

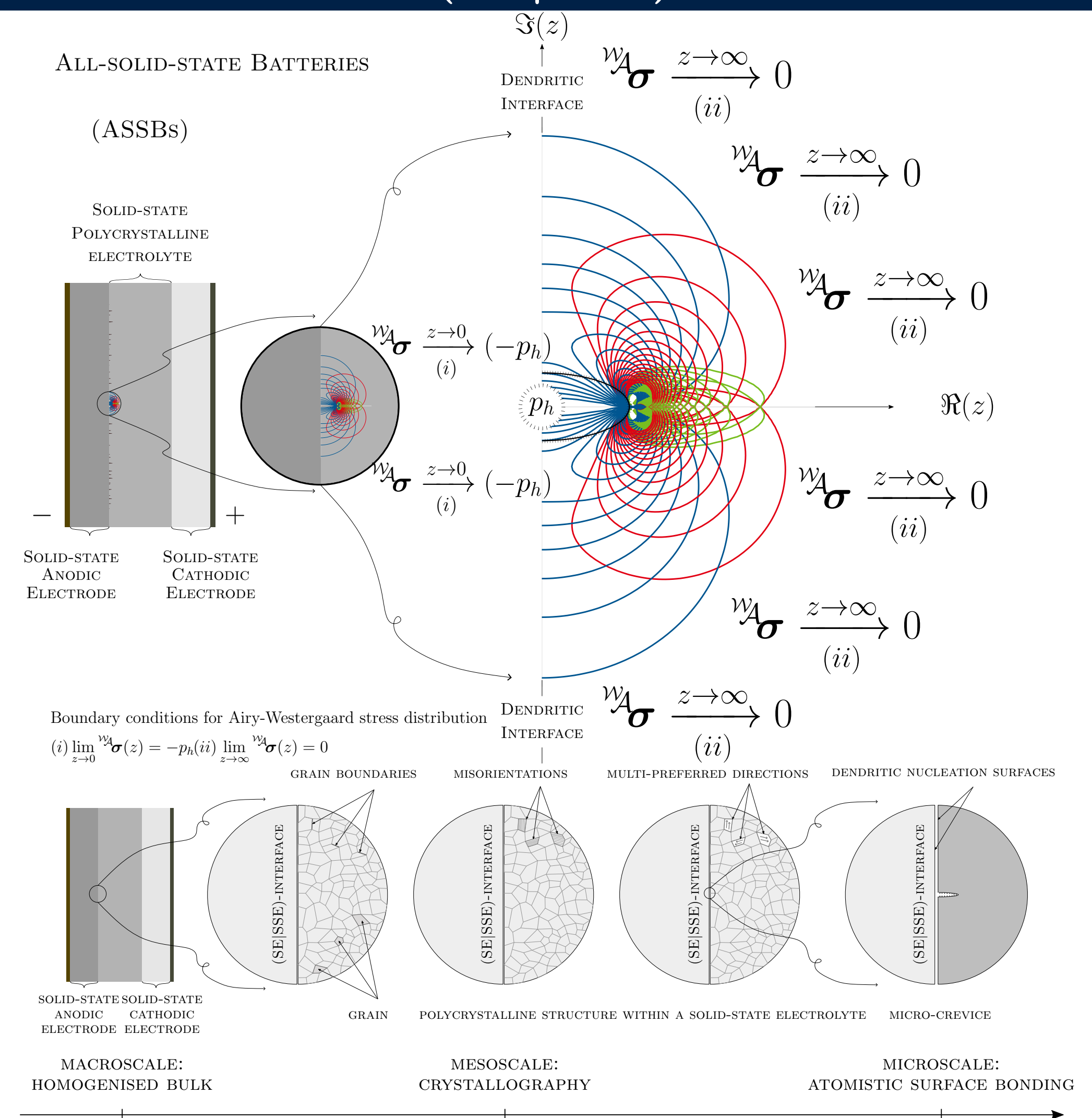
$$\partial_t \mathbf{u} + \nabla \cdot \left( \mathbf{C}^{\text{fallocation}}(\lambda, \mu, \mathbf{d}_{G,i,i=1,\dots,N}^R, \mathbf{d}^E; \mathbf{x}) : \nabla \mathbf{u}^{(s)} \right) + \rho \mathbf{b} = -\rho \nabla V_e, \quad (1)$$

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

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,  $\theta$  temperature field,  $a$  crevice length,  $\lambda, \mu$  Lamé constants,  $\mathbf{d}^{(*)} \otimes \mathbf{d}^{(*)}$  embedded misorientation structural tensor, and  $\gamma$  cracking-surface energy density, can help to improve ASSB performance [1][2].

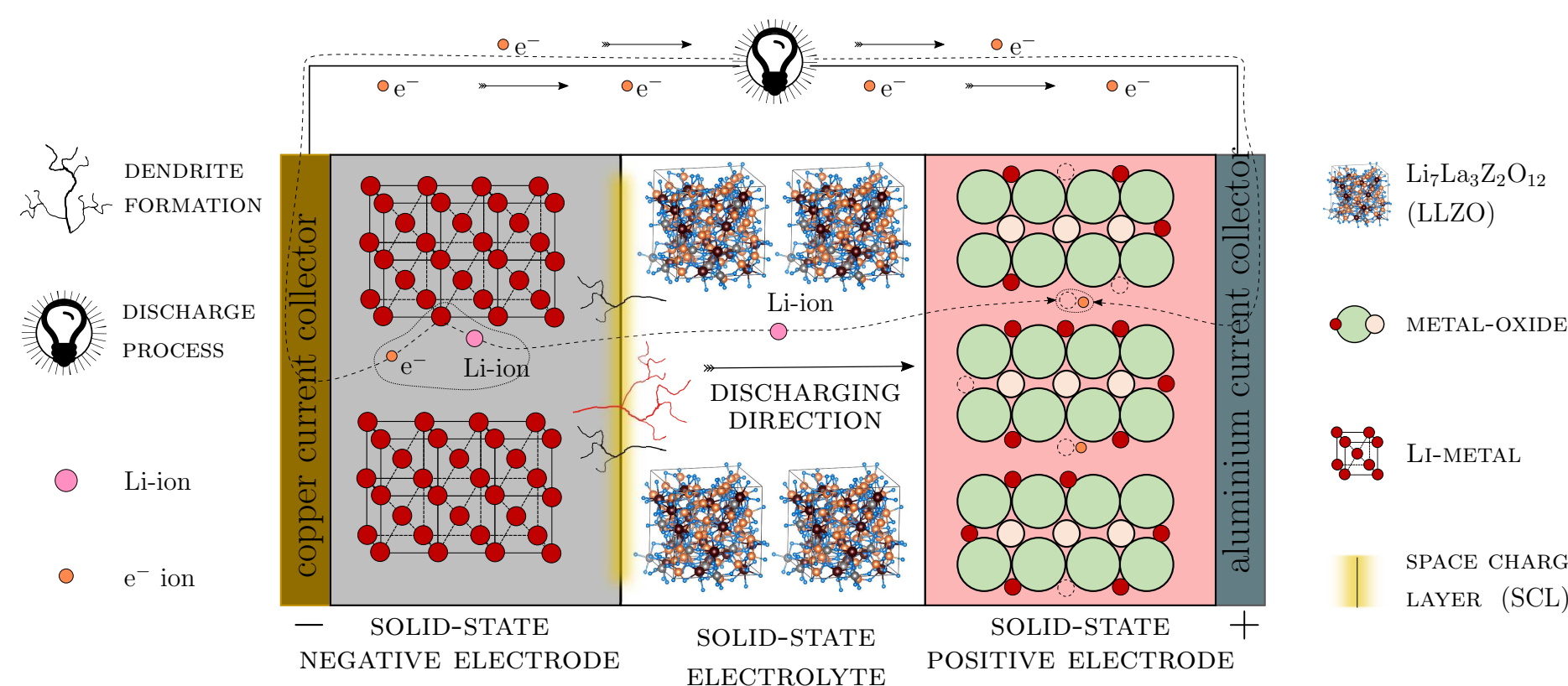
**Aim:** The study is with the purpose of gaining a better insight into dendrite nucleation and formation in ASSB.

**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].



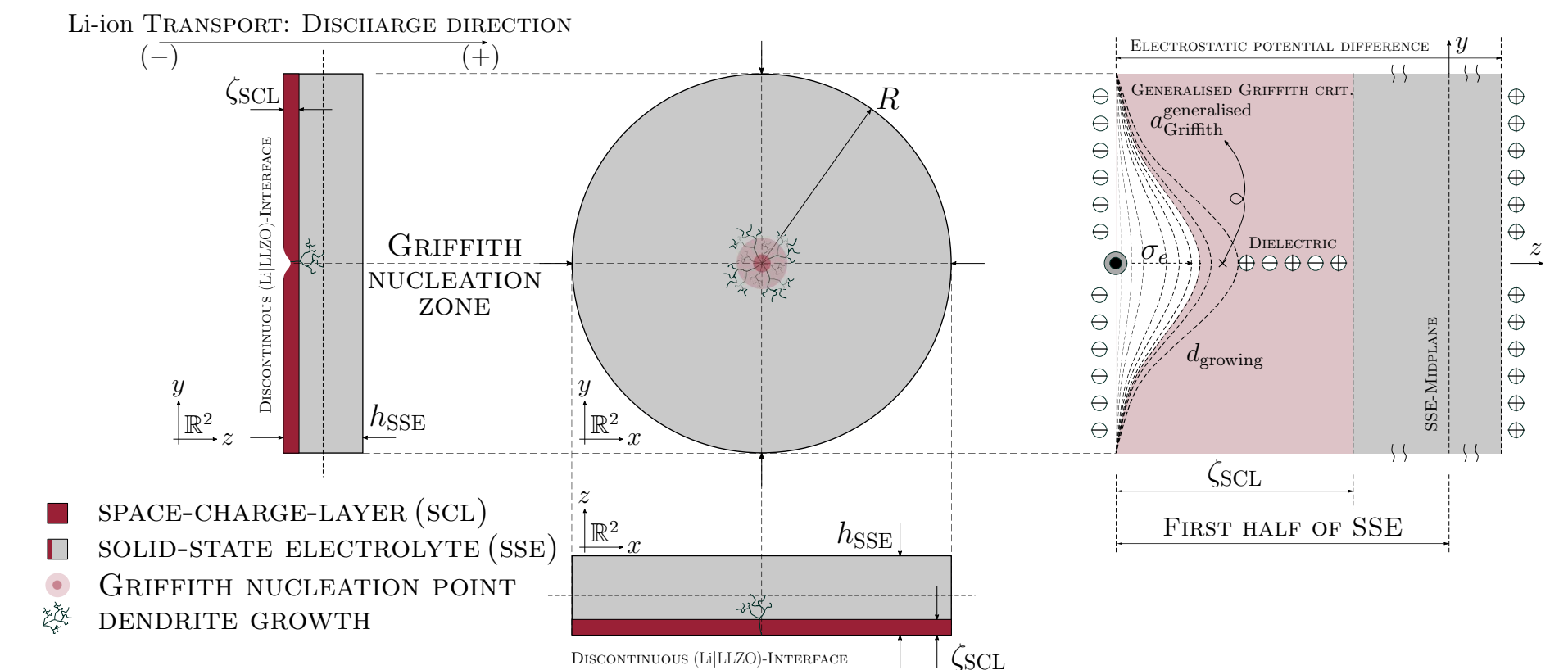
## Next-generation All-solid-state battery

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



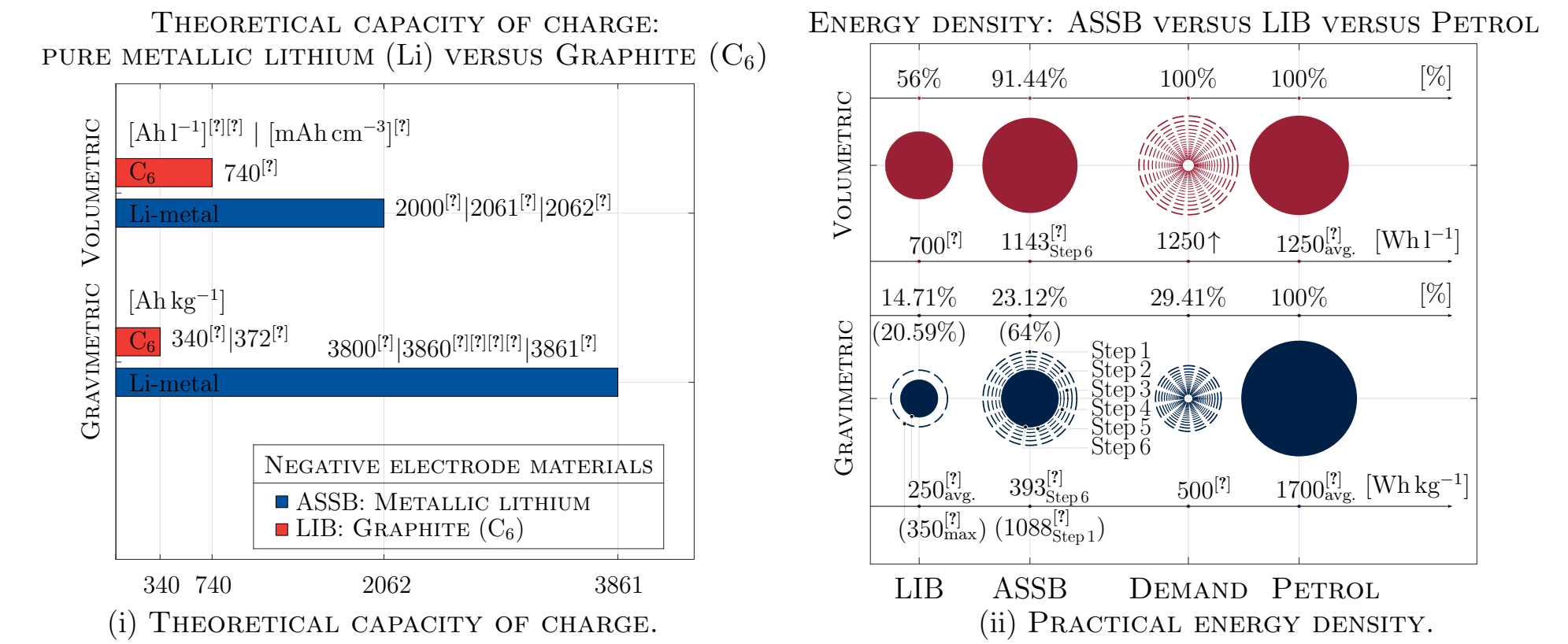
## Space-charge Layer

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



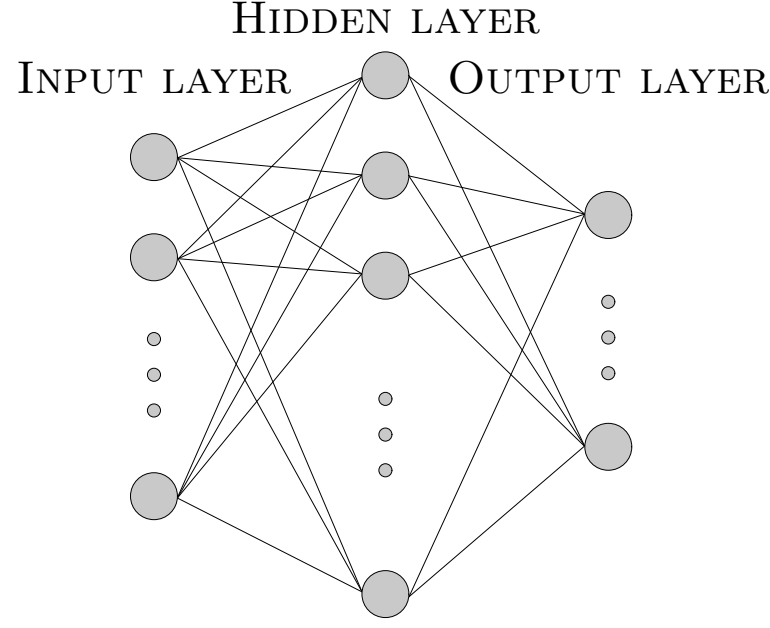
## Motivation: Energy density landscape

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



## Artificial Neural Networks

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



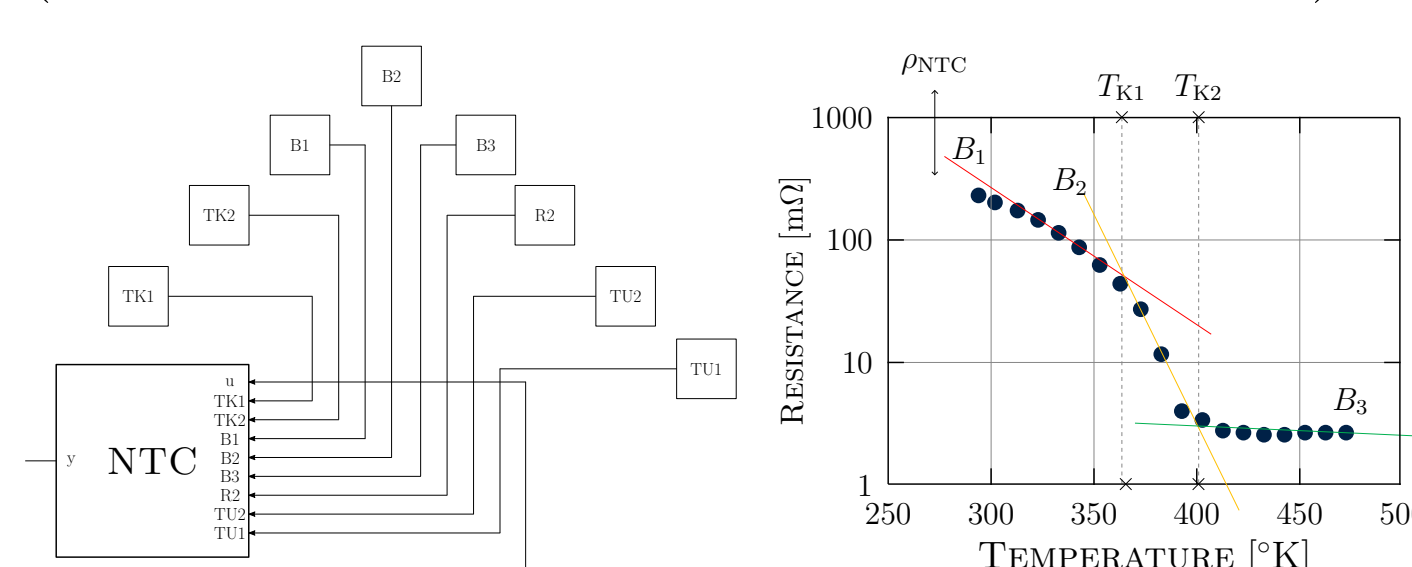
The ANNs scheme enhances bainitic trafo. temperature prediction, validated by [9].

## 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  $\theta$ ;

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

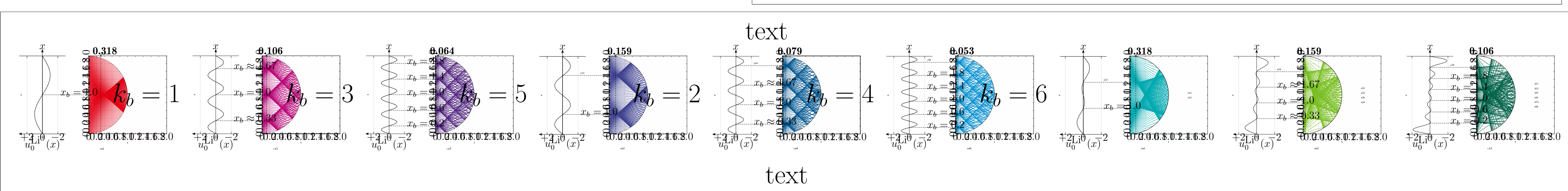
Governing conservation equations used to describe balance of mass, conservation of linear momentum, conservation of angular momentum, and conservation of energy with  $\rho(\mathbf{x}, t)$  is mass density per unit volume (puv);  $\mathbf{b}(\mathbf{x}, t)$  body force puv;  $\mathbf{v}(\mathbf{x}, t)$  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** is based on the deformation of SSE due to dendrite formation at (SE|SSE)-interface

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

**Surface energy** is analysed 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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Scan me

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## Acknowledgments

T. Vo expresses sincere gratitude to the JARA-CSD research project, led by Dr. S. Braun and Dr. C. Hüter, for their crucial support. Special thanks to Prof. Dr. R. Spatschek for hosting at IEK-2, FZ Jülich. Moreover, T. Vo's role as a teaching assistant in the courses of Mathematische Grundlagen I, II, III, IV, and NumPDE at Computational Engineering Science (CES), RWTH Aachen University (2019-2023), was accomplished and enriched thanks to the guidance and mentorship of Prof. Dr. M. Torrilhon, Prof. Dr. M. Schlottke-Lakemper, Dr. R. Speck, Prof. Dr. B. Berkels, Dr. S. Braun, Prof. Dr. J. Kowalski, Dr. A. Jha, Prof. Dr. B. Stamm, Dr. A. Litvinenko, and Dr. M. Kirchhart.