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].

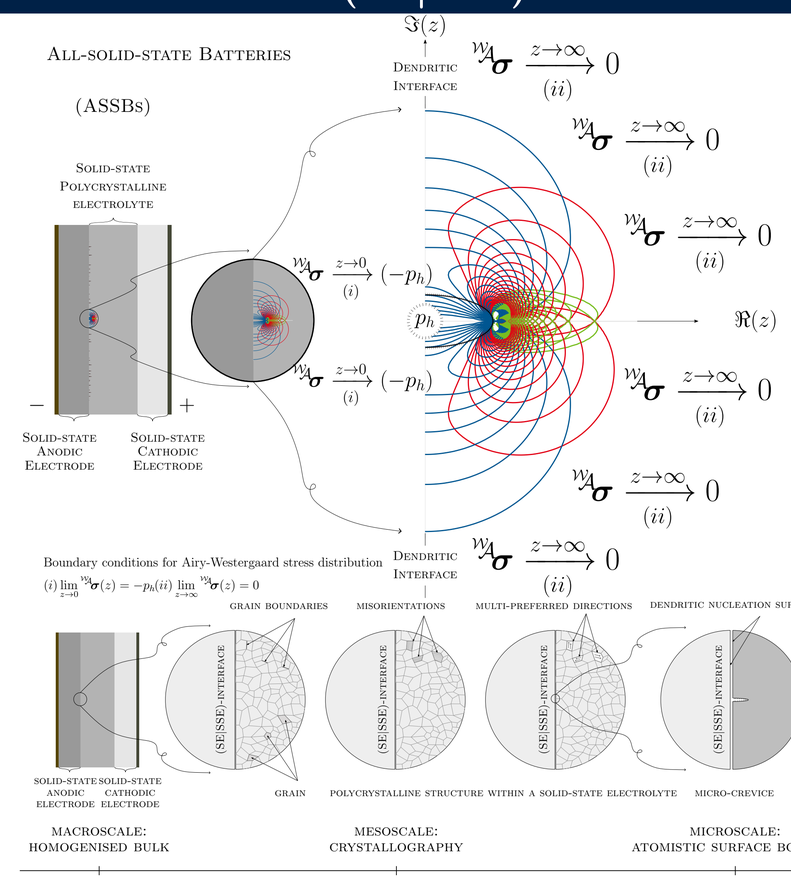
Next-generation All-solid-state battery (ng-ASSB) with a consideration of nucleation criterion defined by

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

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

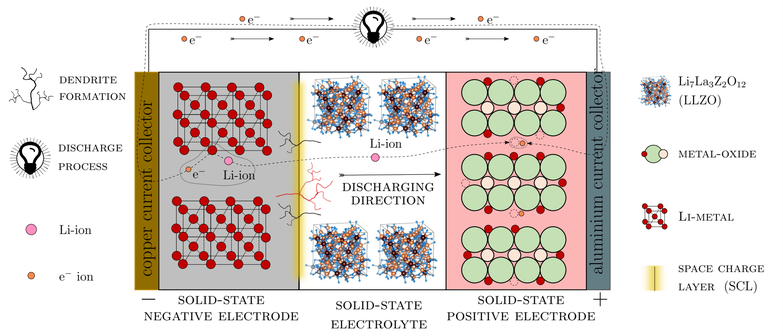
hold for $\forall\, a\in\mathcal{V}$. Here, $V_e:\mathbb{R}^3\to\mathbb{R}$ is the electric potential applied globally on ASSB. Due to nature setting of ASSB taking the form (SE|SSE|SE) the electric potential becomes uniform. Additionally, $\boldsymbol{u}$ is the displacement field, θ temperature field, 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.



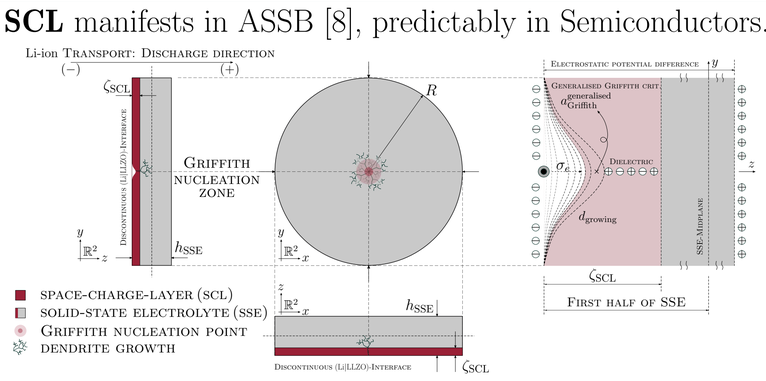
Next-generation All-solid-state battery

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



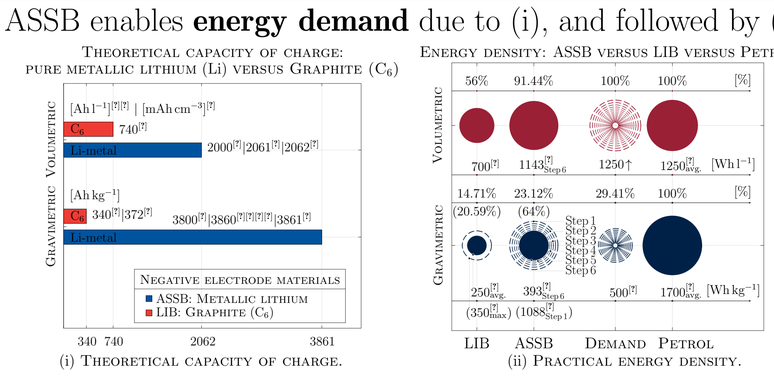
Observation: Space-charge Layer

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



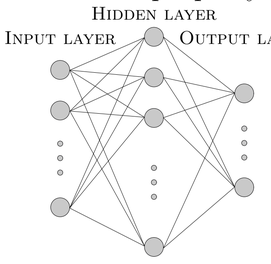
Motivation: Energy density landscape

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



Artificial Neural Networks

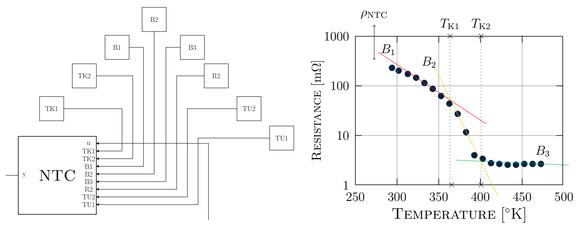
Application: Steel's property prediction.



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)

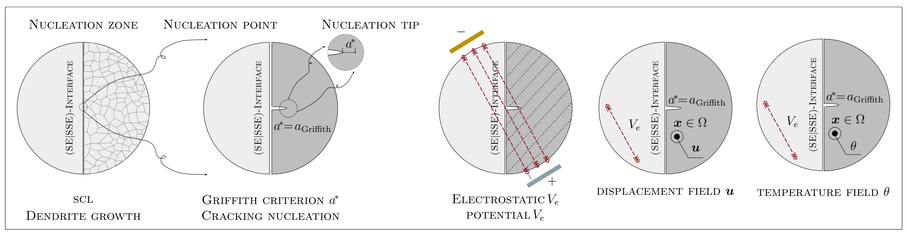


Nd/Gd Negative-Temperature Coefficient (NTC) semiconductor model validated [7].

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:

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

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

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

Griffith criterion on (**100**-Li-termination)-{**50**$Ta^{\bullet}_{Zr}$}-doped-$Li_7La_3Zr_2O_{12}$ at T=298°K

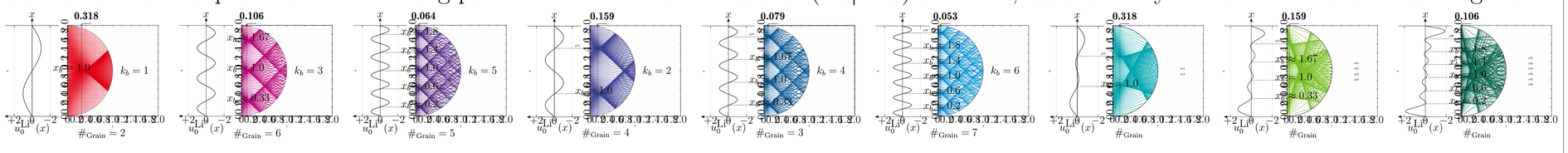
Stacking Pressure	Percentage of crevice per unit length at (Li|{**50**$Ta^{\bullet}_{Zr}$}-LLZO)-Interface				
	$a_{crevice}=1\%$	$a_{crevice}=5\%$	$a_{crevice}=10\%$	$a_{crevice}=30\%$	$a_{crevice}=50\%$
10 kPa	1.000	0.950	0.911	0.866	0.866
30 kPa	1.000	0.950	0.904	0.859	0.866
1 MPa	1.00	0.950	0.985	0.936	0.866
16 MPa	0.899	0.854	1.000	0.950	0.866
50 MPa	0.948	0.900	1.000	0.950	0.866
110 MPa	0.956	0.908	1.000	0.950	0.866

Solution: Analysing equations (1) and (2) yields a simplified Griffith nucleation criterion, incorporating Cauchy stress σ, Young's modulus E_Y, and experimentally-derived surface energy γ_s, with σ calculated using the OpenFOAM library.

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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