Next-generation 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 [1]. 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. This bottleneck is mainly due to liquid-based electrolyte 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, metallic Li-dendrite triggered at (SE|SSE)-interface is the main drawback as these dendritic threads extrapolate into grain boundary network of SSE, causing crevice, degradation of ionic conductivity, and the probability of short-circuit.

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

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

where, can help to improve ASSB performance.
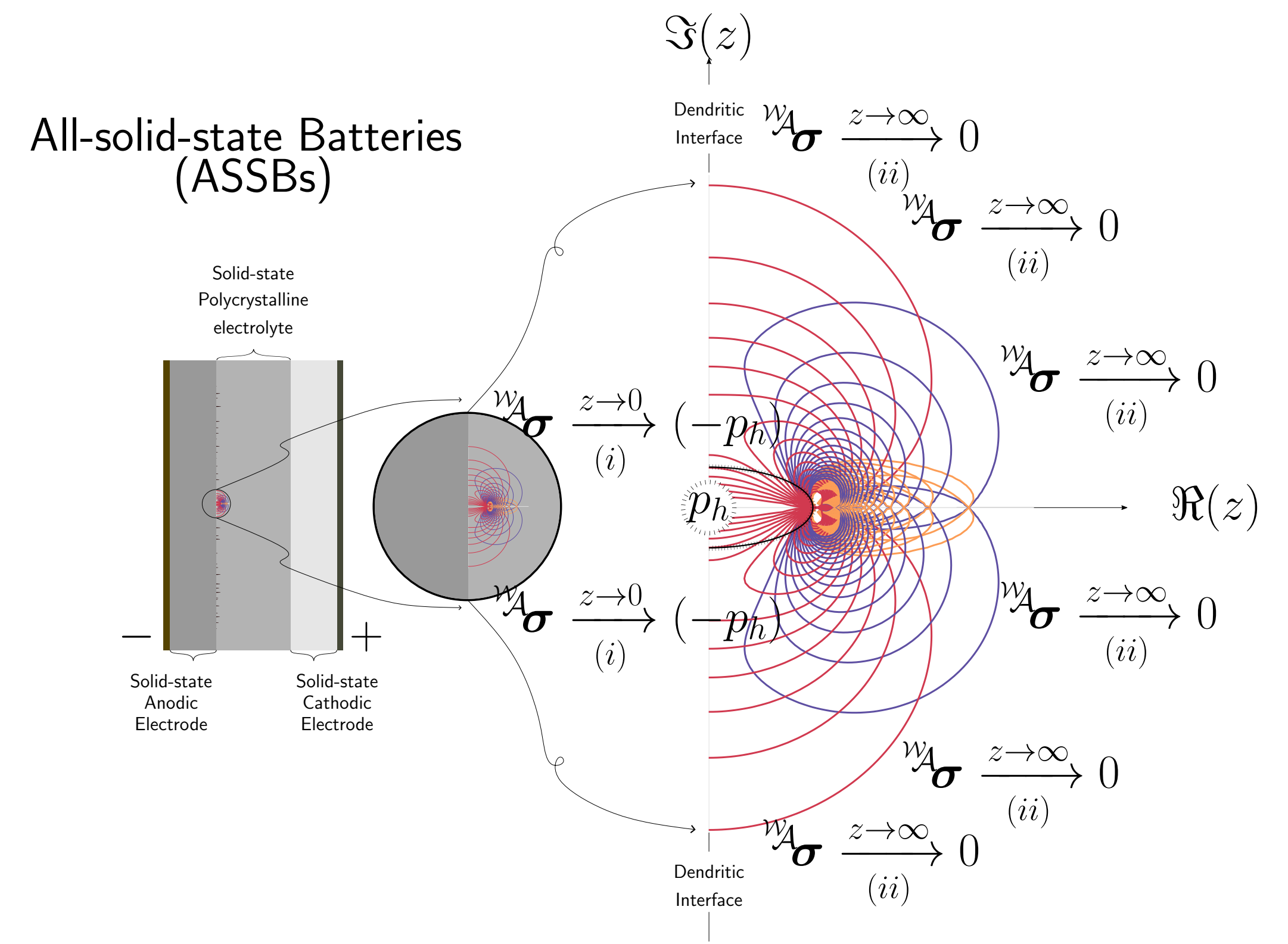
Interface

Interface between solid electrode and solid-state electrolyte (SE|SSE) taking place at space charge layer (SCL) [2] found in ASSBs critically exhibits mechanical and electrochemical instability [3]. This evidence points directly to the fact that the soft metallic li anode is erroneously prone to triggering dendrites, under cycles of electric charge & discharge [4].
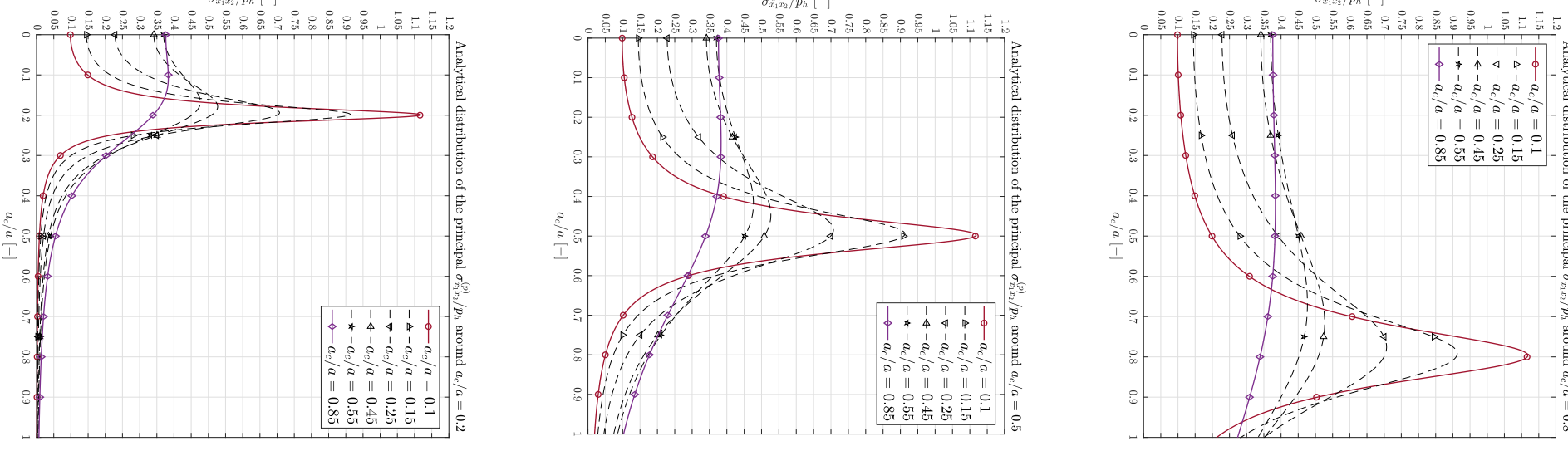
Distribution: ana. max. shear stress $^{w_A}\sigma^\Pi_{x_1 x_2}$ around crack tip a_c.

## Next-generation All-solid-state battery

Nucleation taking place at critical dendritic (SE|SSE)-interface
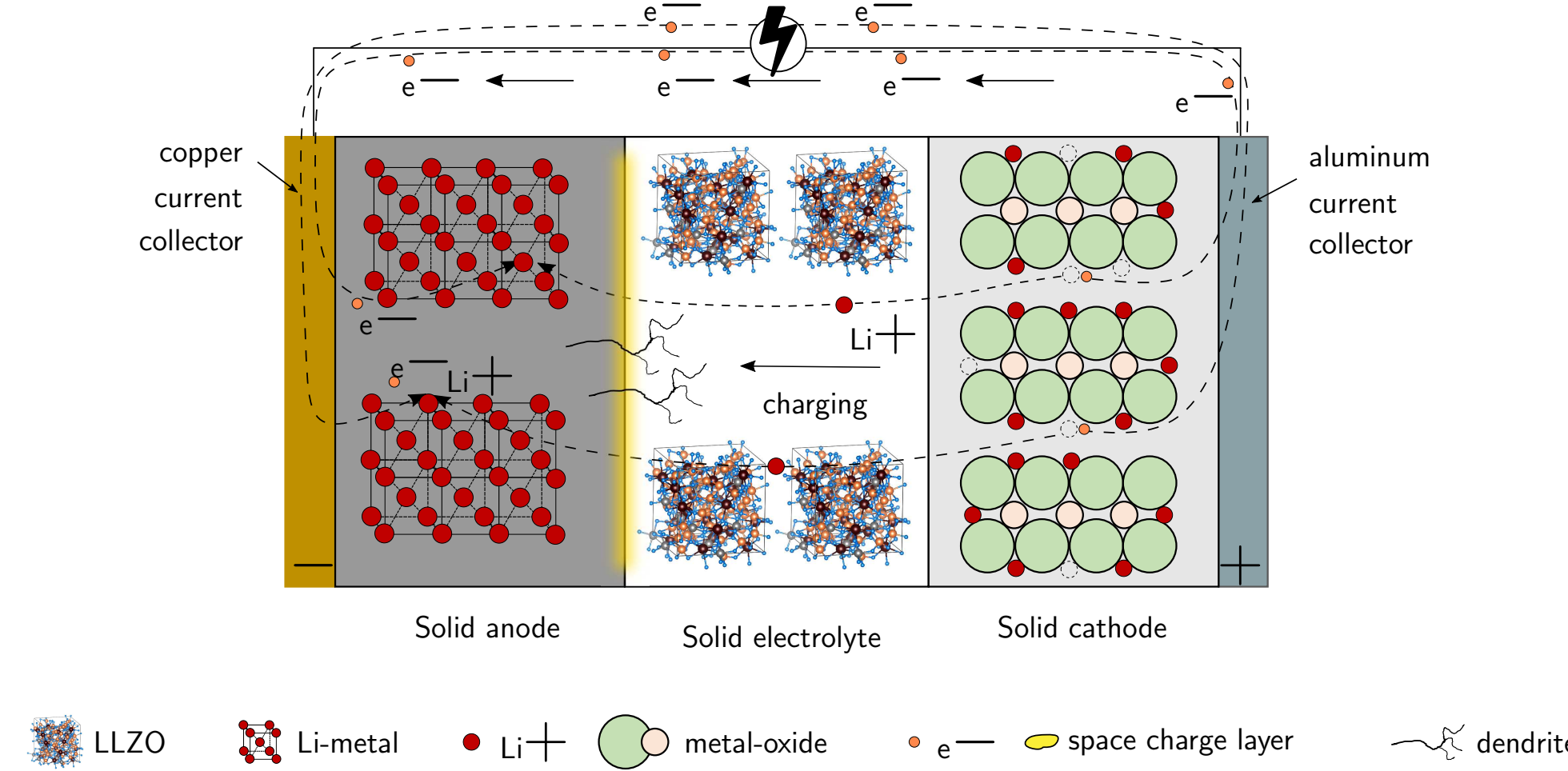
Nucleation taking place at critical dendritic (SE|SSE)-interface
Nucleation taking place at critical dendritic (SE|SSE)-interface

Embedded structural-tensor SSE

Polycrystalline garnet-typed SSE such as LLZO exhibit grain boundaries and various sizes and shapes of grains under microscopic observation. Therefore, this type of microstructure distinctively leads to nuance destruction of ceramic-like materials.
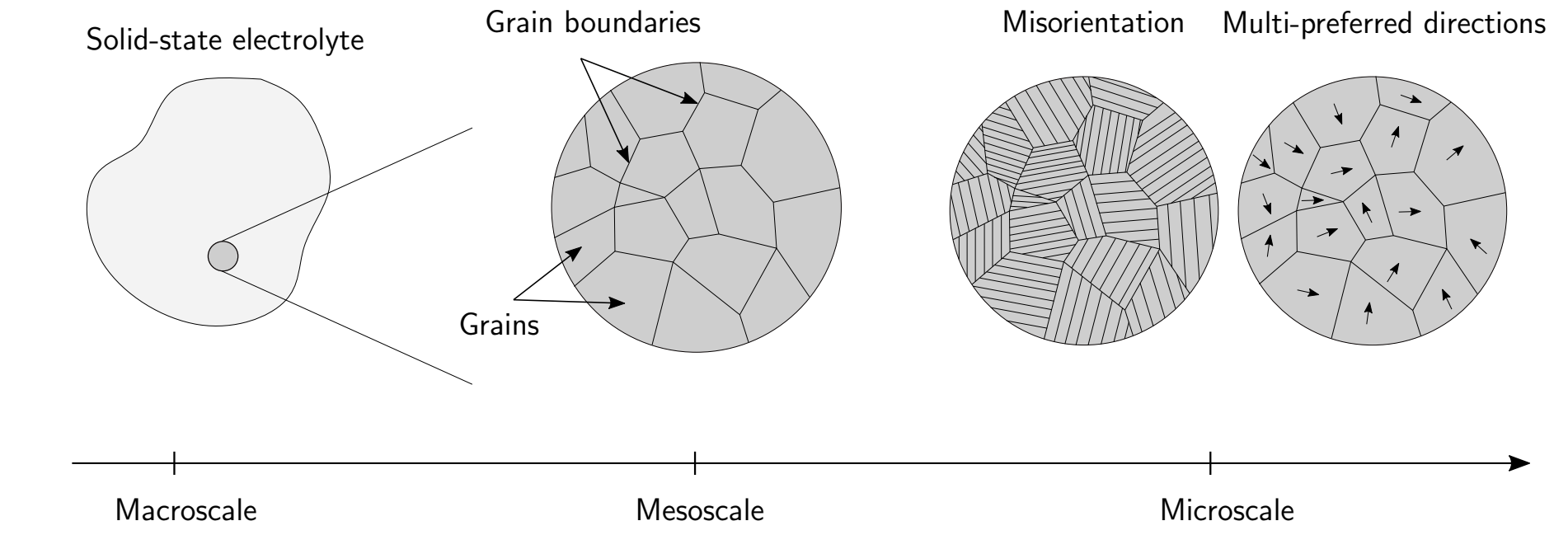
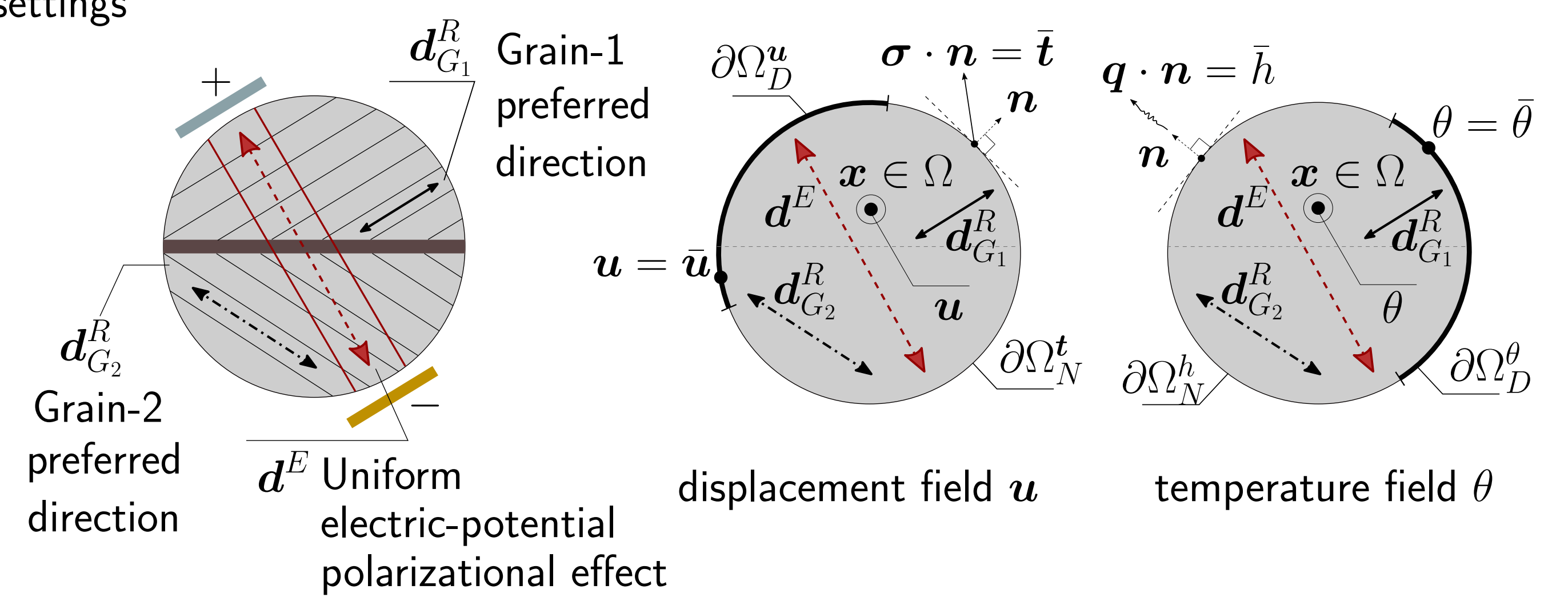Consequentially, dendrites contribute to degradation of ionic conductivity and trace along grain boundaries in SSE.

Nucleation interface: Taking place at the critical dendritic interface

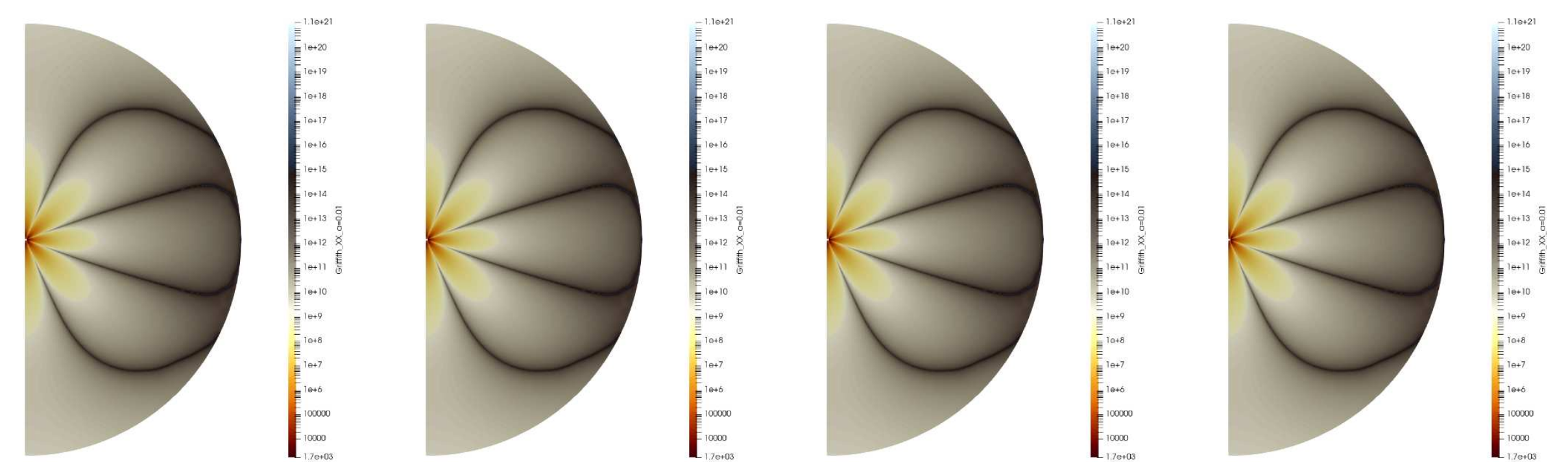$$\rho\, \partial_{t^2}^2 \boldsymbol{u}^{(s)} + \nabla \cdot \left(\overset{4}{\mathbb{C}} f^{\mathbb{D}(\Omega)}_{(\lambda,\mu)} : \nabla \boldsymbol{u}^{(s)} \right) + \rho \nabla V_e = \boldsymbol{0},$$

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

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Therefore
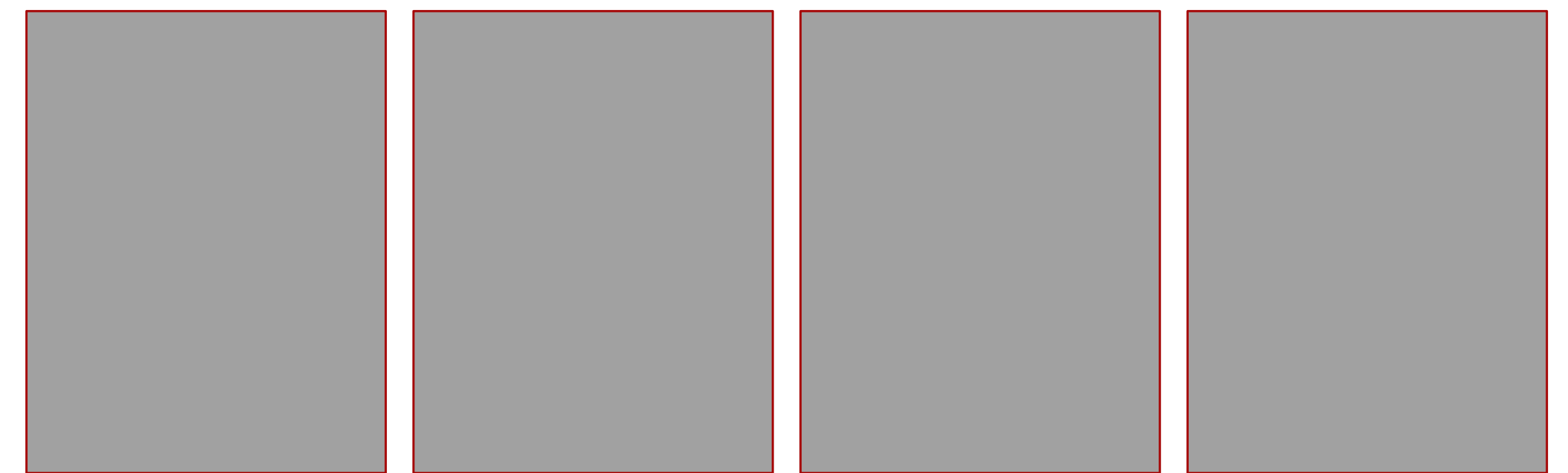
$$\therefore\, a_{\text{Griffith}} := a^* = \arg\min_{a \in \mathbb{R}} \iiint_\Omega f(a, \boldsymbol{u}; \lambda, \mu, \boldsymbol{d} \otimes \boldsymbol{d})\, d\Omega - \iint_\Gamma f(a; \gamma)\, d\Gamma \Big|_{\boldsymbol{u}^{(s)}}$$

Boundary settings

Grain-1 preferred direction
Grain-2 preferred direction
$\boldsymbol{d}^E$ Uniform electric-potential polarizational effect

displacement field $\boldsymbol{u}$

temperature field θ

The set of boundary conditions is likewise the path of the pressure-centric dendritic crack.

Comparison: Analytical vs. Numerical solutions

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