

Solid state battery formulation

1. Formulation

State variables

$$\mathcal{S} = \{\boldsymbol{\varphi}, c_\alpha, \Phi\}. \quad (1)$$

Generalized velocities

$$\mathcal{V} = \{\dot{\boldsymbol{\varphi}}, \dot{\mathbf{F}}, \dot{c}_\alpha, \nabla \dot{c}_\alpha, \nabla \dot{\Phi}\}. \quad (2)$$

Rate of the total potential is defined as

$$\dot{\Pi} = \int_{\Omega} \left(\dot{\psi} + \delta^* \right) dV - \mathcal{P}, \quad (3)$$

$$\psi = \psi^m(\mathbf{F}, c_\alpha) + \sum_{\alpha} \psi_{\alpha}^c(\mathbf{F}, c_\alpha, \nabla c_\alpha) + \psi^e(\mathbf{F}, \nabla \Phi), \quad (4)$$

$$\delta^* = \psi^{m*}(\dot{\mathbf{F}}) + \sum_{\alpha} \psi_{\alpha}^{c*}(\dot{c}_\alpha, \nabla \dot{c}_\alpha) + \psi^{e*}(\nabla \dot{\Phi}). \quad (5)$$

Thermodynamic forces

$$\mathcal{F} = \{\mathbf{P}, \mu_\alpha, \mathbf{J}_\alpha, \mathbf{D}\}, \quad (6)$$

with (from Coleman-Noll)

$$\mathbf{P} = \mathbf{P}^{\text{eq}} + \mathbf{P}^{\text{vis}}, \quad \mu_\alpha = \mu_\alpha^{\text{eq}} + \mu_\alpha^{\text{vis}}, \quad \mathbf{J}_\alpha = \mathbf{J}_\alpha^{\text{eq}} + \mathbf{J}_\alpha^{\text{vis}}, \quad \mathbf{D} = \mathbf{D}^{\text{eq}} + \mathbf{D}^{\text{vis}}, \quad (7a)$$

$$\mathbf{P}^{\text{eq}} = \psi_{,\mathbf{F}}, \quad \mu_\alpha^{\text{eq}} = \psi_{,c_\alpha}, \quad \mathbf{J}_\alpha^{\text{eq}} = \psi_{,\nabla c_\alpha}, \quad \mathbf{D}^{\text{eq}} = \psi_{,\nabla \Phi}, \quad (7b)$$

$$\mathbf{P}^{\text{vis}} = \delta_{,\dot{\mathbf{F}}}^*, \quad \mu_\alpha^{\text{vis}} = \delta_{,\dot{c}_\alpha}^*, \quad \mathbf{J}_\alpha^{\text{vis}} = \delta_{,\nabla \dot{c}_\alpha}^*, \quad \mathbf{D}^{\text{vis}} = \delta_{,\nabla \dot{\Phi}}^*. \quad (7c)$$

Balance laws are

$$-\nabla \cdot \mathbf{P} - \mathbf{b} = \mathbf{0}, \quad (8a)$$

$$-\nabla \cdot \mathbf{J}_\alpha + \mu_\alpha = 0, \quad (8b)$$

$$-\nabla \cdot \mathbf{D} + \rho_q = 0. \quad (8c)$$

2. Constitutive models

Yellow ones are kinematical quantities.

Blue ones are energetics.

Red ones are dissipations.

Multiplicative decomposition for swelling and thermal eigenstrains:

$$\mathbf{F} = \mathbf{F}^e \mathbf{F}^s. \quad (9)$$

Relevant derivatives:

$$\mathbf{F}_{,\mathbf{F}}^e = \delta_{ik} F_{lj}^{s-1}, \quad (10a)$$

$$\mathbf{F}_{,\mathbf{F}^s}^e = -F_{ik}^e F_{lj}^{s-1}. \quad (10b)$$

Swelling:

$$\mathbf{F}^s = (J^s)^{\frac{1}{3}} \mathbf{I}, \quad J^s = 1 + \beta^s \sum_{\alpha} \Omega_{\alpha} (c_{\alpha} - c_{\alpha}^0). \quad (11)$$

Relevant derivatives

$$\mathbf{F}_{,c_{\alpha}}^s = \frac{1}{3} (J^s)^{-\frac{2}{3}} \beta^s \Omega_{\alpha} \mathbf{I}. \quad (12)$$

Neo-Hookean:

$$\psi^m = \frac{1}{2} \lambda \ln^2(I_3) + \frac{1}{2} G [I_1 - 2 \ln(I_3) - 3], \quad I_1 = \text{tr}(\mathbf{F}^{eT} \mathbf{F}^e), \quad I_3 = \det(\mathbf{F}^e). \quad (13)$$

Relevant derivatives:

$$\psi_{,\mathbf{F}^e}^m = \lambda \ln(I_3) \mathbf{F}^{e-T} + G (\mathbf{F}^e - \mathbf{F}^{e-T}), \quad (14a)$$

$$\psi_{,\mathbf{F}}^m = \psi_{,\mathbf{F}^e}^m : \mathbf{F}_{,\mathbf{F}}^e, \quad (14b)$$

$$\psi_{,c}^m = \psi_{,\mathbf{F}^e}^m : \mathbf{F}_{,\mathbf{F}^s}^e : \mathbf{F}_{,c_{\alpha}}^s. \quad (14c)$$

Fick's first law of mass transport:

$$\psi_{\alpha}^c = \frac{1}{2} D_{\alpha} \nabla c_{\alpha} \cdot \nabla c_{\alpha}. \quad (15)$$

Relevant derivatives:

$$\psi_{\alpha, \nabla c_{\alpha}}^c = D_{\alpha} \nabla c_{\alpha}. \quad (16)$$

Mass transport viscosity:

$$\psi_{\alpha}^{c*} = \frac{1}{2} \eta_{\alpha} \dot{c}_{\alpha}^2. \quad (17)$$

Relevant derivatives:

$$\psi_{\alpha, \dot{c}}^{c*} = \eta_{\alpha} \dot{c}_{\alpha}. \quad (18)$$

Polarization:

$$\psi^e = \frac{1}{2} J \varepsilon_0 \varepsilon_r \mathbf{e} \cdot \mathbf{e}, \quad \mathbf{e} = \mathbf{F}^{-T} \nabla \Phi. \quad (19)$$

Relevant derivatives:

$$\psi^e_{,\nabla\Phi} = J \varepsilon_0 \varepsilon_r \mathbf{C}^{-1} \nabla \Phi, \quad (20a)$$

$$\psi^e_{,\mathbf{F}} = J \varepsilon_0 \varepsilon_r \left[\frac{1}{2} (\mathbf{e} \cdot \mathbf{e}) \mathbf{F}^{-T} - \mathbf{e} \otimes \mathbf{e} \right]. \quad (20b)$$