Battery Simulation Study Group 2018

Model #1

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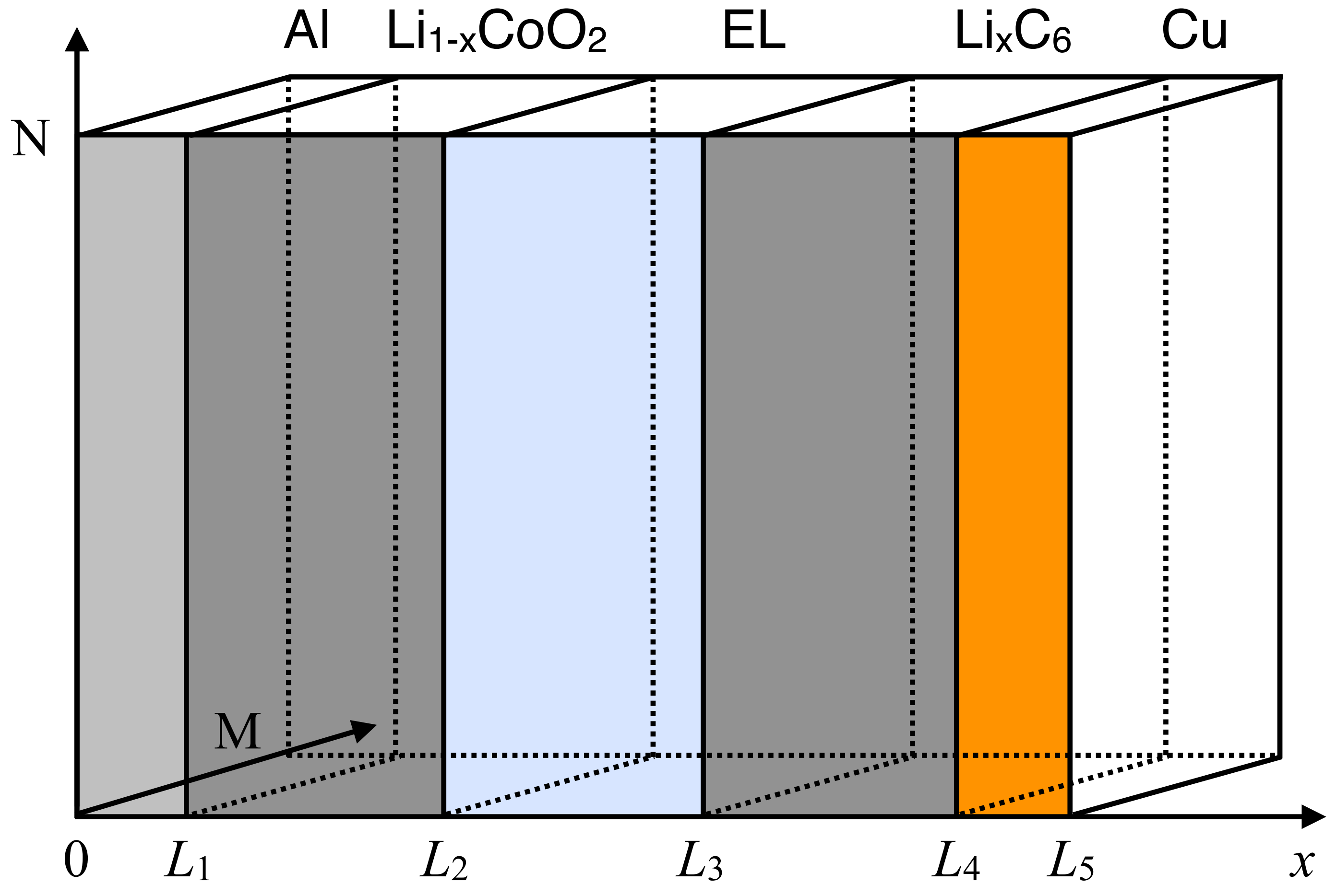
Model#1

Precondition

- Diffusion resistance of Li ion in electrolyte is 0.
- Diffusion resistance of Li ion in electrode is 0.
- Direction of current is along with x-axis.
- Temperature is 298 K



$$LiCoO_2 \rightleftharpoons xLi^+ + Li_{1-x}CoO_2 \qquad LiC_6 \rightleftharpoons xLi^+ + Li_{1-x}C_6$$

Metal electrical resistivity(Linear approximation)

$$\rho(T) = \rho_0[1 + \alpha(T - T_0)]$$

Butler-Volmer equation

$$j = j_0 \cdot \left\{ \exp\left[\frac{\alpha_a zF\eta}{RT}\right] - \exp\left[-\frac{\alpha_c zF\eta}{RT}\right] \right\}$$

Model#1: Butler–Volmer equation

Butler-Volmer equation

$$j = j_0 \cdot \left\{ \exp\left[\frac{\alpha_a z F \eta}{RT}\right] - \exp\left[-\frac{\alpha_c z F \eta}{RT}\right] \right\}$$

where:

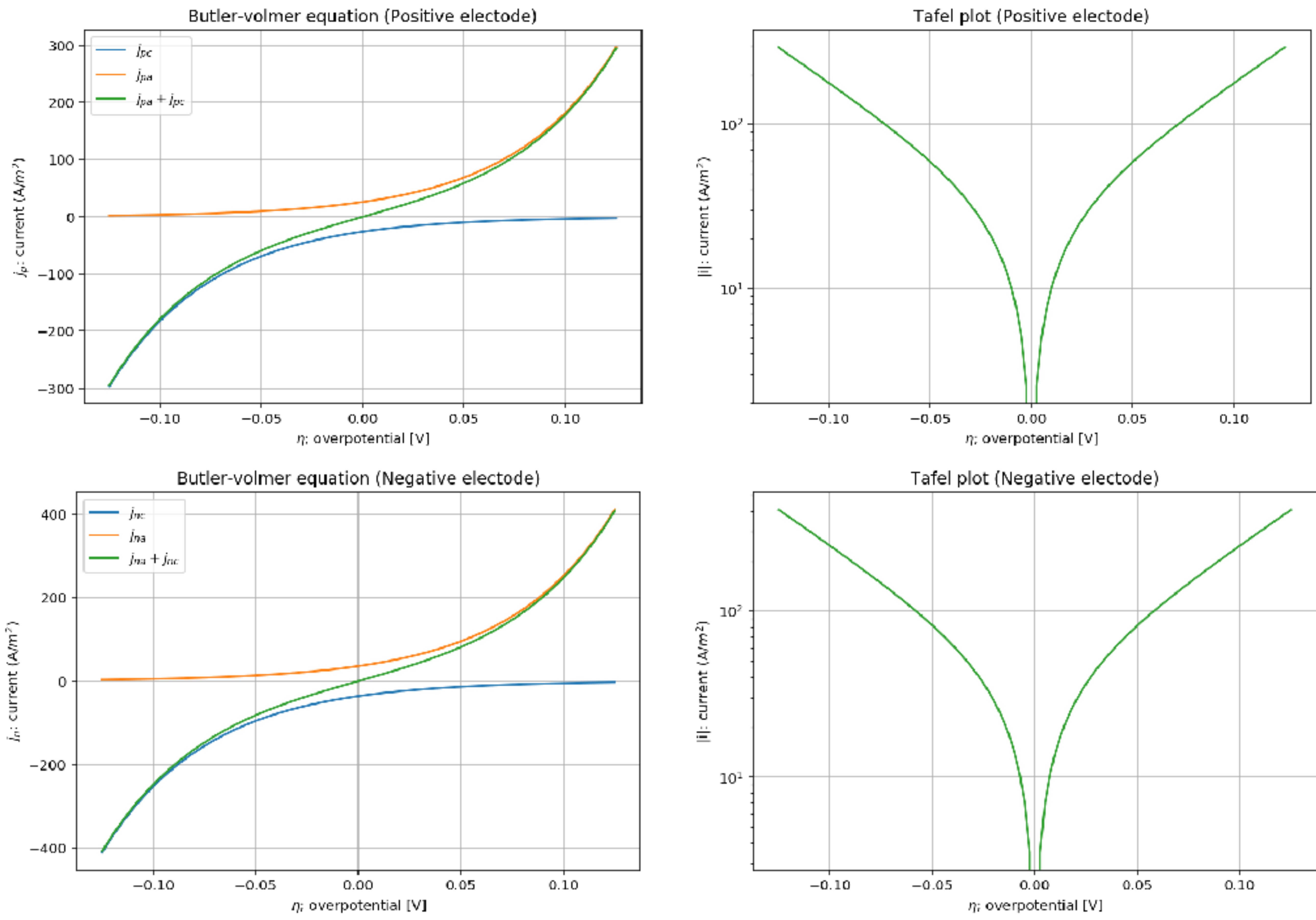
- j: electrode current density, A/m^2 (defined as $i = I/A$)
- j_o: exchange current density, A/m^2
- E: electrode potential, V
- E_{eq}: equilibrium potential, V
- T: absolute temperature, K
- z: number of electrons involved in the electrode reaction
- F: Faraday constant
- R: universal gas constant
- α_c: so-called cathodic charge transfer coefficient, dimensionless
- α_a: so-called anodic charge transfer coefficient, dimensionless
- η: activation overpotential (defined as $\eta = E - E_{eq}$).

F = 96485.33289(59) [C/mol]
R = 8.3144598(48) [J/(mol · K)]
z = 1

https://en.wikipedia.org/wiki/Butler–Volmer_equation

	$Li_{1-x}CoO_2$	Li_xC_6
j_0 (A/cm^2)	2.6 x 10^{-3}	3.6 x 10^{-3}
α_c, α_a (-)	0.5, 0.5	0.5, 0.5

K. Smith et al., Journal of Power Sources 161 (2006) 628–639



Model#1: Butler–Volmer equation

Butler-Volmer equation

$$j = j_0 \cdot \left\{ \exp\left[\frac{\alpha_a z F \eta}{RT}\right] - \exp\left[-\frac{\alpha_c z F \eta}{RT}\right] \right\}$$

If $\alpha_a = \alpha_c$

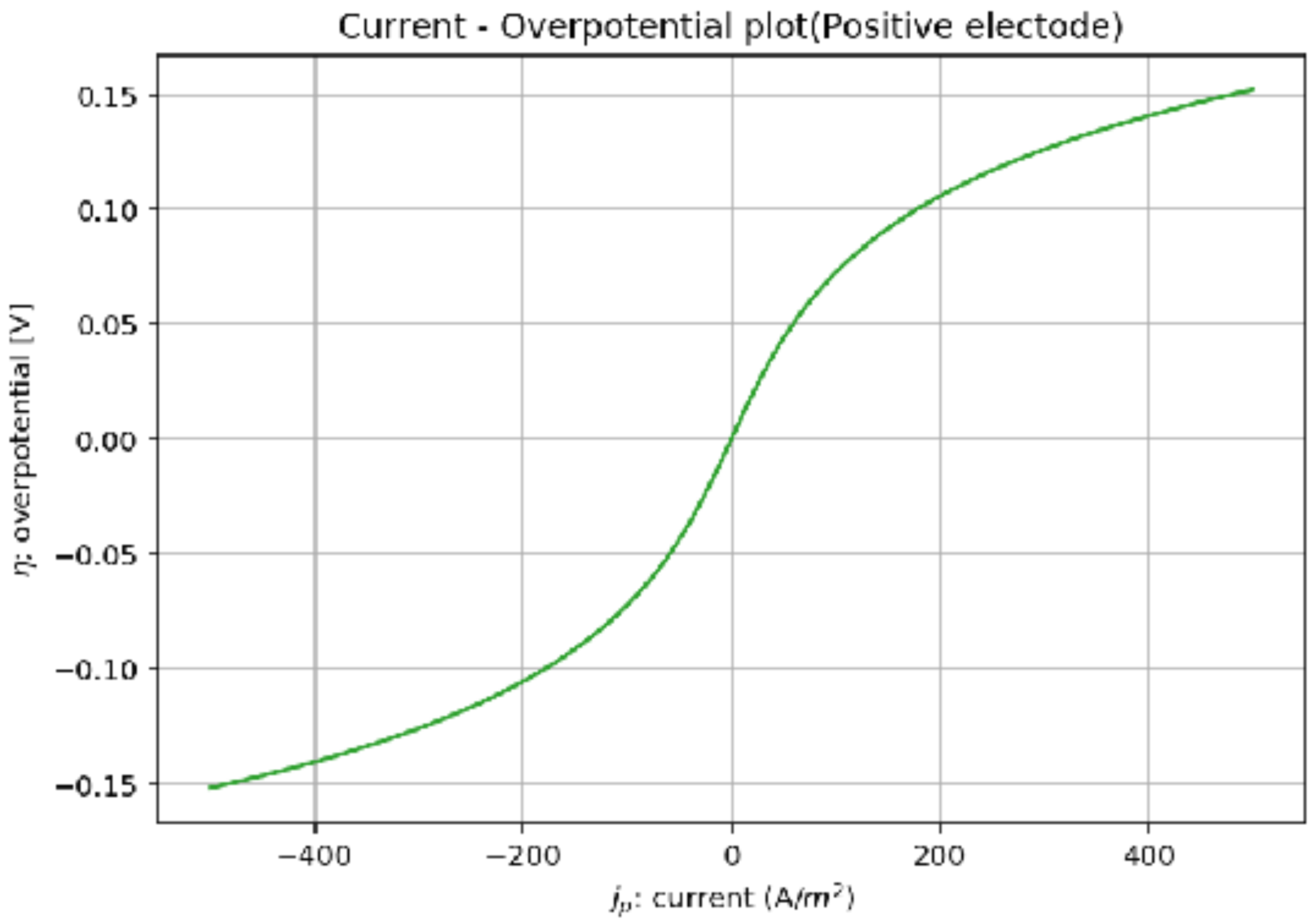
$$j = j_0\{\exp(\frac{\alpha z F \eta}{RT}) - \exp(-\frac{\alpha z F \eta}{RT})\}$$

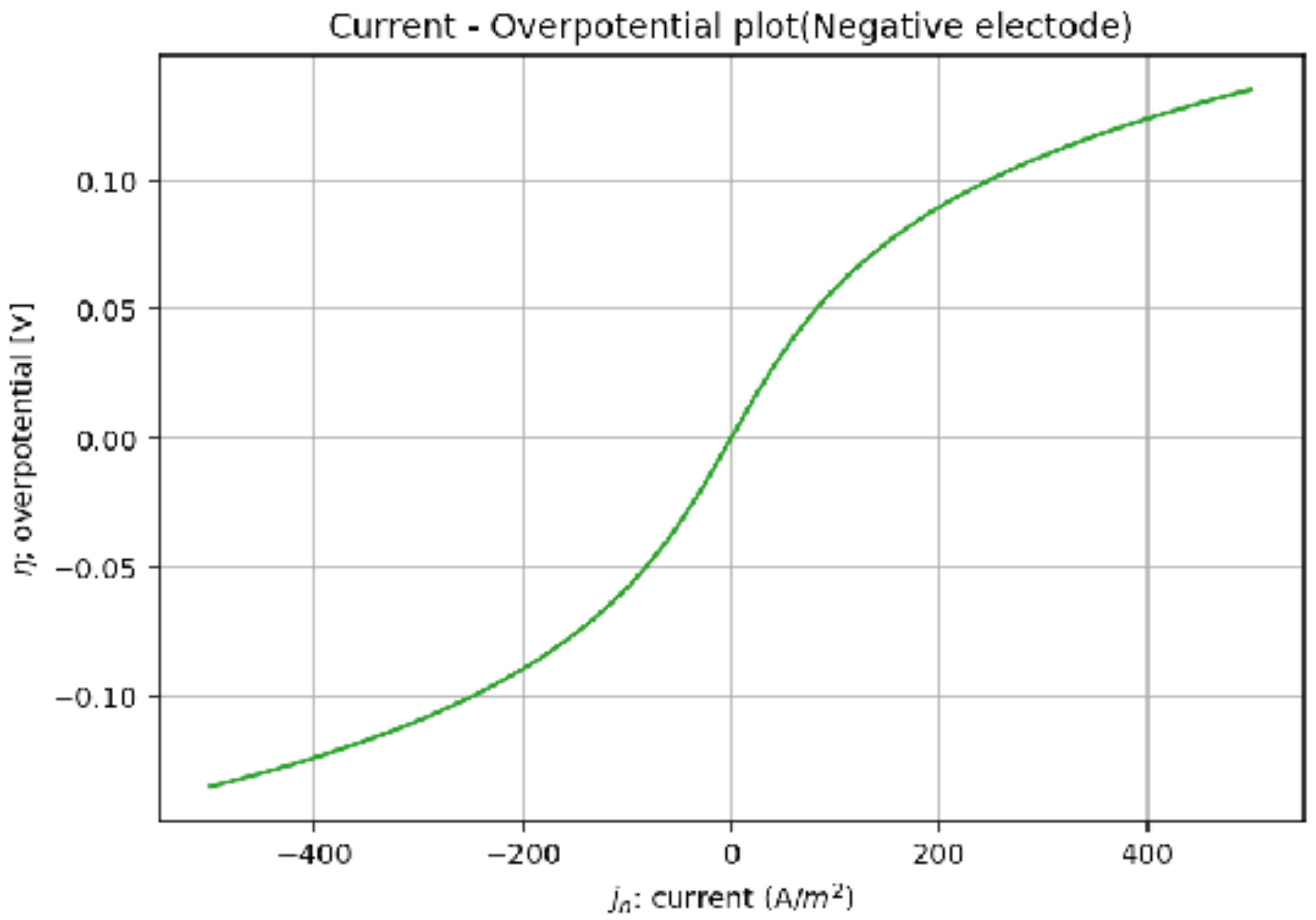
$$j = 2 j_0 \sinh \frac{\alpha z F \eta}{RT}$$

$$\eta = \frac{RT}{\alpha z F} \sinh^{-1}\left(\frac{j}{2 j_0}\right)$$

$$\eta = \frac{RT}{\alpha z F} \ln\left(\frac{j}{2 j_0} + \sqrt{\left(\frac{j}{2 j_0}\right)^2 + 1}\right)$$

https://ocw.mit.edu/courses/chemical-engineering/10-626-electrochemical-energy-systems-spring-2014/lecture-notes/MIT10_626S14_S11lec13.pdf





Model#1: Metal electrical resistivity

Metal electrical resistivity(Linear approximation)

$$\rho(T) = \rho_0[1 + \alpha(T - T_0)]$$

where α is called the *temperature coefficient of resistivity*, T_0 is a fixed reference temperature (usually room temperature), and ρ_0 is the resistivity at temperature T_0. The parameter α is an empirical parameter fitted from

$$\rho = R\frac{A}{\ell},$$

where

R is the electrical resistance of a uniform specimen of the material

ℓ is the length of the specimen

A is the cross-sectional area of the specimen

https://en.wikipedia.org/wiki/Electrical_resistivity_and_conductivity

	Al	Cu
ρ_0 (ohm・m) at 293.15K	2.82×10^{-8}	1.68×10^{-8}
α (/K)	0.0039	0.003862

https://ja.wikipedia.org/wiki/電気抵抗率の比較