Imperial College London

Department of Mechanical Engineering

PhD Thesis

Multiphysical Modelling and Experimental Parameterisation of Solid-State Lithium-Metal Batteries

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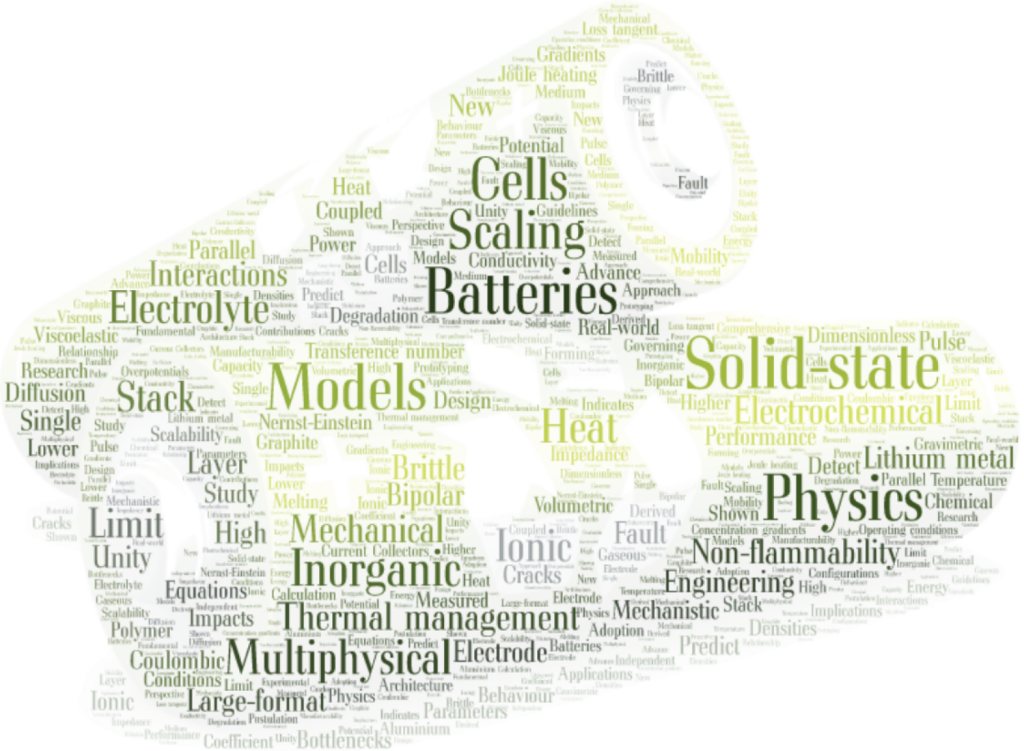
Abstract

Owing to the non-flammability and the potential to replace graphite negative electrodes with lithium metals, solid-state lithium-metal batteries show promise to be next-generation batteries. However, several critical bottlenecks such as a high impedance, a low ionic conductivity of the solid electrolyte, the scalability and manufacturability of large-format solid-state batteries limit the widespread adoption of these batteries for real-world applications.

In this thesis, an in-depth review of the possible multiphysical interactions affecting the performance and degradation of solid-state batteries is first presented. The behaviour of solid-state batteries under a wide range of operating conditions are intrinsically multiphysical, where solid-state electrochemistry and chemical degradations are often coupled to the thermal gradients and mechanical cracks. A comprehensive summary of different multi-physics mechanisms is especially relevant to detect potential fault behaviours before a complete failure in the future development of solid-state batteries. The impacts of solid-state physics on cell architecture engineering were also highlighted. Here, this research discusses how lithium metal's low melting temperature could limit the manufacturability of solid-state lithium-metal batteries and pave a new research direction towards using cell configurations without negative electrodes.

Based on a near-unity transference number due to negligible concentration overpotentials across the solid electrolyte, electrochemical models were developed to predict solid-state lithium-metal cells' performance under pulse operating conditions. A model-based approach was proposed to upscale the single-layer cell to forming large-format solid-state bipolar and parallel stacks by determining the scaling factor from dimensionless governing equations. Here, the model predicts how the choice of current collectors and volumetric change of lithium metal could limit the gravimetric and volumetric densities of large-format solid-state lithium-metal batteries. A bipolar aluminium solid-state cell stack is shown to have higher power and energy densities than a parallel lithium solid-state cell stack. Nevertheless, the performance of bipolar stacks is limited by their lower Coulombic stack capacity. This limitation indicates that an advanced electrode design is required for the future development of a bipolar stack. The stack model was further extended to study the impacts of heat generation, where the temperature-dependent model parameters were estimated based on different measurements of a single-layer cell. Although the model predictions show that heat generations due to Joule heating are insignificant for bipolar solid-state cell stacks, the Joule heating contributions cannot be neglected for parallel solid-state cell stacks. A good thermal management system is required for parallel solid-state cell stacks to mitigate adverse implications due to dominant heat generations. The thermally-coupled solid-state stack models proposed in this thesis can be used as design guidelines to advance large-format solid-state batteries' future prototyping.

For a wide range of electrolytes, including liquid and solid polymer electrolytes, an independent measurement or calculation of both electrolyte conductivity and diffusion coefficient is often time-consuming and challenging. As a result, Nernst-Einstein's relation has been used to relate the ionic conductivity to ionic diffusivity after determining either parameter. Although Nernst-Einstein's relation has been used for different electrolytes, the short perspective in this thesis demonstrates that this relation is not directly transferable to describe the ionic mobility in an inorganic solid electrolyte. The fundamental physics of Nernst-Einstein's relation shows that the relationship between the diffusion coefficient and electrolyte conductivity is derived for ionic mobility in a viscous or a gaseous medium. This postulation contradicts state-of-the-art experimental studies measuring the mechanical behaviour of inorganic solid electrolytes, showing that inorganic solid electrolytes are usually brittle rather than viscoelastic at ambient room temperature. The measurement of loss tangent is required to justify the use of Nernst-Einstein's relation. The outcome of such measurement has two implications. First, if the loss tangent of inorganic solid electrolytes is less than unity in the range of batteries operating temperatures, the impacts of using Nernst-Einstein's relation in modelling the ionic mobility should be quantified. Secondly, if the measured loss tangent is comparable to that of solid polymers and lithium metal, inorganic solid electrolytes may behave in a viscoelastic manner instead of the brittle behaviour usually suggested.


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Impacts
Polymer
Coulombic
Multiphysical
Electrode

Thesis Dissemination

Publications

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Declaration of Authorship

The material presented in **Chapter 1** and **Appendices** has been partially reproduced in the Early Stage Assessment of this PhD.

The material presented in **Chapter 2** has been published in M.-C. Pang, K. Yang, R. Brugge, T. Zhang, X. Liu, F. Pan, S. Yang, A. Aguadero, B. Wu, M. Marinescu, H. Wang and G. J. Offer. Materials Today (2021).

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Part of the material presented in **Abstract** and **Conclusions** has been partially published in the journal articles of the respective chapters.

I hereby certify that all material in this dissertation, which is not my own work, has been properly acknowledged.

Mei-Chin Pang

Date: July 1, 2021

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Acronyms

Li^+ lithium-ions. 67

AEF Area Enhancement Factor. 57

ALD Atomic Layer Deposition. 57

AM Active Materials. 16, 20, 30, 32, 35, 38, 41, 47, 57, 59, 60, 62, 63

APU Auxiliary Power Unit. 1, 3, 4

ARC Accelerating Rate Calorimeter. 19, 44

ASI Area Specific Impedance. x, 7, 8

BV Butler-Volmer. 25, 51, 175, 176, 179, 181, 189

CCD Critical Current Density. 11, 15, 16, 23, 35, 39, 40, 42, 45

CEI Cathode Electrolyte Interphase. 38

CNLS Complex Non-Linear Least Squares. 78

CPE Constant Phase Element. 155, 156

CRSS Critical Resolved Shear Stress. 25, 33

CV Cyclic Voltammetry. 16, 44, 52

DEMS Differential Electrochemical Mass Spectrometry. 44

DFT Density Functional Theory. x, 12, 14–16, 18, 23, 36, 61

DRT Distribution Function of Relaxation Times. ix, xii, 75, 107, 157, 159–162, 165

DSC Differential Scanning Calorimetry. 20, 23, 44

EC/DMC Ethylene Carbonate/DiMethyl Carbonate. 4, 14

EDX Energy-Dispersive X-ray spectroscopy. 37

EELS Electron Energy Loss Spectroscopy. 32, 45, 133, 163

EIS Electrochemical Impedance Spectroscopy. 23, 44, 49, 52, 53, 60, 140, 141, 153, 165

FBV Frumkin-Butler-Volmer. 51

FIB-SEM Focussed-Ion-Beam Scanning Electron Microscopy. 58

FWHM Full Width at Half Maximum. 160

GEIS Galvanostatic Electrochemical Impedance Spectroscopy. 153

GITT Galvanostatic Intermittent Titration Technique. 54, 73, 74, 83, 108, 111

KK Kramers-Kronig. xii, 157–159

LAGP $Li_{1+x}Al_xGe_{2-x}(PO_4)_3$. 19, 20, 26, 29, 31

LATP $Li_{1.2}Al_{0.2}Ti_{1.8}(PO_4)_3$. 19, 20, 52

LCO $LiCoO_2$. xi, xii, xiv, 19, 22, 30, 32, 36–38, 47, 53, 54, 57, 59, 60, 63, 67, 70–72, 77, 82–84, 88, 90, 91, 95, 99, 105, 107, 109, 110, 112, 133, 138, 150, 156, 157, 163, 165, 166

LGPS $Li_{10}GeP_2S_{12}$. 16, 17, 34, 36, 38, 59, 63, 126

LiPON Lithium Phosphorus Oxynitride. xi, xii, 2, 4, 5, 13, 15, 17–19, 21, 23–25, 31, 32, 34, 48, 49, 57, 63, 68, 72, 103, 105, 126, 132–134, 137, 156, 157, 163, 165, 166

LLTO $Li_{3x}La_{2/3-x}TiO_3$. 19, 20

c-LLZO $Li_7La_3Zr_2O_{12}$. 2, 5, 13, 15–27, 34, 36, 37, 40–42, 48, 49, 52, 63, 126, 134, 137

LMO $LiMn_2O_4$. 31, 38, 53

LPS Li_2S-P_2S_5. 2, 13, 15, 17, 18, 20, 23, 25, 27, 31, 37, 38, 58, 59, 63, 126

LSS Li_4SnS_4. 20

MD Molecular Dynamics. x, 14, 15, 68

MTRM Modulated Thermoreflectance Microscopy. 23

NCA $LiNi_{1-x-y}Co_xAl_yO_2$. 30, 37

NDP Neutron Depth Profiling. 15, 30, 31, 44, 49, 53

NE Negative Electrode. xviii, 3–6, 15, 16, 21, 26, 28, 30, 31, 33–35, 37, 39, 41, 46–48, 50–52, 55, 61, 63, 67, 69, 72, 79, 81, 93, 94, 96, 97, 99, 103, 107, 112, 114–117, 119, 124, 156, 181

NLEIS Non-Linear Electrochemical Impedance Spectroscopy. 52, 63

NMC $LiNi_{1-x-y}Mn_xCo_yO_2$. 20, 22, 32, 36–38, 58–60

NMR Nuclear Magnetic Resonance. 45

OCP Open-Circuit Potential. 54, 55, 93, 108, 110, 165

OCV Open Circuit Voltage. 74

PC Propylene Carbonate. 6, 7, 78

PE Positive Electrode. vii, viii, xi, xv–xviii, 3, 4, 6, 14, 16, 19–22, 26, 28–30, 32, 33, 35, 37–39, 44, 46–62, 66, 67, 70–73, 77–80, 82–91, 93–97, 99, 103, 105, 107–109, 112–114, 117, 123, 124, 138, 156, 165, 182

PEIS Potentiostatic Electrochemical Impedance Spectroscopy. 54, 73, 91, 107, 111, 138, 153, 165

PGSE Pulse-Gradient Spin-Echo. xi, 129–131

PNP Poisson-Nernst-Planck. 67, 70

PUS Picosecond Ultrasonic Spectroscopy. 23

PVD Physical Vapour Deposition. 57

PWL Piece-Wise Linear. xii, 159, 160

RBF Radial Basis Function. xii, 159–161

RUS Resonant Ultrasound Spectroscopy. 23, 24

SE Solid Electrolyte. vii, x, xi, xiii, xvi, xviii, xix, 1–9, 11, 13–53, 55–73, 77, 78, 81, 84, 86–91, 93, 95–97, 103, 104, 107, 108, 112, 114, 122, 135, 138, 142, 145, 146, 164, 165, 170, 181, 182

SEI Solid Electrolyte Interphase. 37

SEM Scanning Electron Microscopy. 20, 24, 26, 44, 58

SIMS Secondary Ion Mass Spectrometry. 45

SOC State-of-Charge. 35, 44, 70, 73–76, 83, 85, 90, 108–110, 124

SRXTM Synchrotron Radiation X-ray Tomographic Microscopy. 31

STEM Scanning Transmission Electron Microscopy. 29, 32, 133

TEM Transmission Electron Microscopy. 20, 37, 45, 133, 163

ToF-SIMS Time of Flight - Secondary Ion Mass Spectrometry. 37, 38, 42

USV Ultrasonic Sound Velocity. 23

XCT X-ray Tomography. 29, 31, 41, 45, 58

XPS X-ray Photoelectron Spectroscopy. 18, 23, 29, 37, 38, 45

XRD X-ray Diffraction. 20, 45, 54, 59

List of Symbols

Greek Symbols

$\Delta\phi$	Interfacial potential drop	V
Δp_c	Critical pressure	kPa
ΔV	Potential difference	V
$\alpha_{ox/red}$	Oxidation/reduction charge transfer coefficient	–
α_T	Thermal expansion coefficient	K^{-1}
α_{neg}	Li-LiPON charge transfer coefficient	–
α_{pos}	LiPON-LCO charge transfer coefficient	–
β	Phase difference between the current and the voltage	°
ϵ	Strain	–
ϵ	Surface emissivity	–
ϵ_0	Absolute permittivity of the vacuum ($\epsilon_0 = 8.85 \times 10^{-12}$ F m^{-1})	
ϵ_r	Relative permittivity	–
ϵ_T	Thermal strain	–
η''	Dimensionless overpotential	–
η^{mt}	Mass-transport overpotential	V
η_{neg}	Overpotential at the NE and SE interface	V
η_{pos}	Overpotential at the PE and SE interface	V
η_{diff}	Overpotential due to solid diffusion	V
η_{ohm}	Overpotential due to ohmic drop	V

γ	Geometric factor of the surface crack shape	–
λ	Debye length	nm
ν	Poisson's ratio	–
ω	Radian frequency	Hz
ϕ	Electric potential	V
ϕ''_{k}	Dimensionless potential	–
ϕ_{s}	Solid electrode potential	V
ϕ_{elec}	Electrolyte potential	V
ϕ_{neg}	Negative electrode potential	V
ϕ_{pos}	Positive electrode potential	V
ρ	Material density	$\mathrm{kg\,m^{-3}}$
σ''_{elec}	Dimensionless electrolyte conductivity	–
σ_{BP}	Bipolar plate electronic conductivity	$\mathrm{S\,m^{-1}}$
$\sigma_{\mathrm{elec,ref}}$	Reference electrolyte conductivity	$\mathrm{S\,m^{-1}}$
σ_{neg}	Li electronic conductivity	$\mathrm{S\,m^{-1}}$
σ_{pos}	LCO electronic conductivity	$\mathrm{S\,m^{-1}}$
σ_{st}	Stress	$\mathrm{N\,m^{-2}}$
σ_{tab}	Tab electronic conductivity	$\mathrm{S\,m^{-1}}$
σ_{elec}	Electrolyte conductivity	$\mathrm{S\,m^{-1}}$
τ	Time constant	s
τ_{diff}	Time constant due to diffusion in the PE	s
θ_{v}	Volume strain	–

Latin Symbols

ΔS	Entropy change	$\mathrm{J\,mol^{-1}\,K^{-1}}$
ΔV_{s}	Steady-state voltage difference	V
ΔV_{t}	Transient voltage difference	V
$\partial U(x_{\mathrm{Li}})/\partial T$	Entropic heat coefficient	$\mathrm{mV\,K^{-1}}$

A_{BP}	Bipolar plate surface area	m^2
A_{c}	Cathodic Tafel's slope	mV
A_{f}	Footprint area of the cell on the substrate	cm^2
A_{int}	True internal surface area	cm^2
$A_{\mathrm{tab,cross}}$	Tab cross-sectional area	m^2
A_{elec}	Surface area of the SE	m^2
A_{pos}	Surface area of the PE	m^2
C_{int}	Interfacial capacitance	$\mu\mathrm{F\ cm}^{-2}$
C_{p}	specific heat capacity at constant pressure	$\mathrm{J\ kg}^{-1}\ \mathrm{K}^{-1}$
D_{Li}	Diffusion coefficient of Li^+	$\mathrm{m}^2\ \mathrm{s}^{-1}$
D_{Li^+}	Diffusion coefficient of Li^+ in the SE	$\mathrm{m}^2\ \mathrm{s}^{-1}$
E	Young's modulus	GPa
E_{A}	Activation energy	$\mathrm{J\ mol}^{-1}$
F	Faraday's constant ($F = 96485\ \mathrm{C\ mol}^{-1}$)	
F_{c}	Coulombic force	N
G	Shear modulus	GPa
H_{v}	Hardness	GPa
I^{s}	Steady-state currents	mA
I^0	Initial current	mA
K	Bulk modulus	GPa
K_{c}	Fracture toughness	$\mathrm{MPa\ m}^{1/2}$
$L_{\mathrm{tab,y}}$	Tab height	m
L_{z}	Total domain thickness	m
N_{BP}	Number of unit cells in a bipolar stack	–
N_{Par}	Number of unit cells in a parallel stack	–
N_i	Flux density of species Li^+	$\mathrm{mol\ m}^{-2}\ \mathrm{s}^{-1}$
P_{v}	Indentation force	N

Q	Charge of the bodies	C
Q_{conv}	Heat dissipation by convection	W
$Q_{\mathrm{gen,tot}}$	Total heat generation	W
Q_{irrev}	Irreversible heat generation	W
Q_{rad}	Heat dissipation by radiation	W
Q_{rev}	Reversible heat generation	W
R_1^{s}	Steady-state resistance	Ω
R_1^0	Initial resistance	Ω
R_{AM}	Active materials ohmic resistance	Ω
R_{BP}	Bipolar plate ohmic resistance	Ω
R_{CC}	Current collector ohmic resistance	Ω
R_{int}	Interfacial areal resistance	$\Omega\,\mathrm{cm}^2$
R_{tab}	Tab ohmic resistance	Ω
R_{gas}	Universal gas constant ($R_{\mathrm{gas}} = 8.314\,\mathrm{J\,mol^{-1}\,K^{-1}}$)	
R_{ohmic}	Ohmic resistance	Ω
$R_{\mathrm{ct,neg}}$	Charge transfer resistance	Ω
R_{elec}	Electrolyte resistance	Ω
Res	Real and imaginary impedance residuals	%
T	Temperature	K
T^+	Transference number	–
T_{amb}	Ambient temperature	K
T_{ref}	Reference temperature ($T_{\mathrm{ref}} = 298.15\,\mathrm{K}$)	K
U	Open-circuit Potential	V
V	Cell voltage	V
V_{BP}	Bipolar stack voltage	V
V_{cell}	Cell volume	m^3
V_{m}	Molar volume of the PE	$\mathrm{m^3\,mol^{-1}}$

Z	Impedance	Ω
Z_{pol}	Polarisation resistance	Ω
$\overline{c}_{\mathrm{Li}}$	Average Li concentration in the PE	$\mathrm{mol\,m^{-3}}$
a	Specific interfacial area	$\mathrm{m^{-1}}$
a_{c}	Flaw size	μm
a_{v}	Indentation length	m
c''_{Li}	PE dimensionless lithium concentration	–
c_{+}	Concentration of mobile cations	$\mathrm{mol\,m^{-3}}$
c_{v}	Crack length	nm
c_{Li}	Electrode lithium concentration	$\mathrm{mol\,m^{-3}}$
$c_{\mathrm{LCO,max}}$	LCO maximum lithium concentration	$\mathrm{mol\,m^{-3}}$
$c_{\mathrm{Li^+}}$	Concentration of $\mathrm{Li^+}$ in the SE	$\mathrm{mol\,m^{-3}}$
d_{BP}	Bipolar plate thickness	m
$d_{\mathrm{cell,BP}}$	Bipolar cell thickness	m
$d_{\mathrm{cell,Par}}$	Parallel cell thickness	m
d_{int}	Distance between the center of the charges	nm
d_{neg}	Thickness of the NE	m
d_{pouch}	Pouch thickness	m
d_{elec}	Thickness of the solid electrolyte	m
d_{pos}	Thickness of the positive electrode	m
f_{int}	Interfacial characteristic frequency	kHz
f_{c}	Characteristic frequency	Hz
h	heat transfer coefficient	$\mathrm{W\,m^{-1}\,K^{-1}}$
i	Current density	$\mathrm{A\,m^{-2}}$
i''	Dimensionless current	–
i''_0	Dimensionless exchange current density	–
$i_{0,\mathrm{neg/pos}}$	Exchange current densities	$\mathrm{mA\,cm^{-2}}$

i_0	Exchange current density	$\mathrm{A\,m^{-2}}$
i_{app}	Externally applied current density	$\mathrm{A\,m^{-2}}$
i_{cell}	Cell current density	$\mathrm{A\,m^{-2}}$
i_{ct}	Faradaic current due to charge-transfers at the interfaces	$\mathrm{mA\,cm^{-2}}$
i_{c}	Critical current density	$\mathrm{A\,m^{2}}$
i_{DL}	Double layers current	$\mathrm{mA\,cm^{-2}}$
i_{int}	Interfacial current	$\mathrm{mA\,cm^{-2}}$
i_{pulse}	Externally applied pulse current density	$\mathrm{A\,m^{-2}}$
i_{stack}	Stack current density	$\mathrm{A\,m^{-2}}$
$i_{0,\mathrm{neg}}$	Exchange current densities	$\mathrm{mAcm^{-2}}$
j	Flux	$\mathrm{mol\,m^{-2}\,s^{-1}}$
k_{BP}	Bipolar plate thermal conductivity	$\mathrm{W\,m^{-1}\,K^{-1}}$
k_{CC}	Current collector thermal conductivity	$\mathrm{W\,m^{-1}\,K^{-1}}$
k_{elec}	LiPON thermal conductivity	$\mathrm{W\,m^{-1}\,K^{-1}}$
k_{LCO}	LCO thermal conductivity	$\mathrm{W\,m^{-1}\,K^{-1}}$
$k_{\mathrm{ox/red}}$	Oxidation or reduction rate-constant	$\mathrm{mol\,m^{-2}\,s^{-1}}$
k_{pouch}	Pouch thermal conductivity	$\mathrm{W\,m^{-1}\,K^{-1}}$
$k_{\mathrm{x/y/z}}$	In-plane/cross-plane thermal conductivity	$\mathrm{W\,m^{-1}\,K^{-1}}$
k_{eff}	Effective thermal conductivity	$\mathrm{W\,m^{-1}\,K^{-1}}$
k_{pos}	Electrochemical rate constant	$\mathrm{mol\,m^{-2}\,s^{-1}}$
t''	Dimensionless time	–
$u_{\mathrm{Li^+}}$	Mobility of $\mathrm{Li^+}$ in the SE	$\mathrm{m^2\,mol\,J^{-1}\,s^{-1}}$
v	Bulk velocity of the SE	$\mathrm{m\,s^{-1}}$
z_{n}''	Dimensionless length	–
$z_{\mathrm{Li^+}}$	Number of proton charges carried by an ion	–

Dedicated to

my partner, mentors and best friends.

What good will it be for someone to gain the whole world, yet forfeit their soul? Or what can anyone give in exchange for their soul?

Matthew 16:26 (NIV)

Chapter 1

Introduction

A journey of a thousand miles begins
with a single step.
千里之行，始于足下。

Laozi | 老子

1.1 Lithium battery technology

Among all the storage technologies, electrochemical energy storage, particularly battery technology, plays a significant role in sectors ranging from portable electronics to high-duty applications such as delivering electric vehicles' power supply and Auxiliary Power Unit (APU) during ground and flight operations.[1] Figure 1.1 compares the specific energy and power of batteries to other storage technologies such as fuel cells, flywheels, capacitors and combustion engines. While batteries have high theoretical specific energy, they lag in power densities when compared to internal combustion engines.[2] Many works have been dedicated to enhancing the performance characteristics of batteries *via* an array of experimental and computational modelling techniques. For instance, Zhao *et al.*[3] modelled the impacts of thermal gradients induced by tab and surface cooling on Li-ion cell performance using empirical equivalent circuit networks models. Finegan *et al.*[4] used *in-operando* tomography to study the behaviour of Li-ion batteries during thermal runaway. This thesis focuses on the multiphysical modelling and experimental characterisation of next-generation batteries by replacing the liquid electrolytes in conventional Li-ion batteries with inorganic Solid Electrolyte (SE).

The Faraday Institution[5] has outlined eight research challenges and goals to be achieved by 2035 (Figure 1.2). Future batteries should achieve 2/3 in cost reduction as well as two times the current energy densities and four times the current power density. The battery packs should be inherently safe from thermal runaway, achieve a lifetime of 15 years in operations and 95%

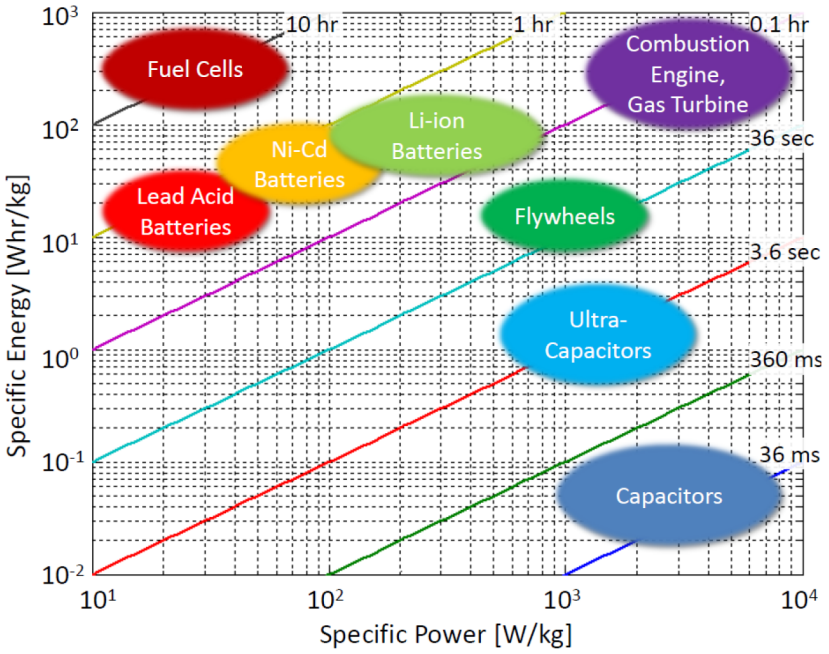


Figure 1.1 Performance characteristics of batteries in terms of specific energy and power compared to fuel cells, flywheels, capacitors and combustion engines. Reproduced with permission from Ref. 2, Copyright (2010), IEEE.

of recyclability. Compared to current cells, which usually have an operating temperature limit between −20 °C and 60 °C, a 50% increase in the operating temperature range is expected by 2035. In terms of models development, the Faraday Institution has also set out to achieve complete predictability for battery performance and ageing.[5] Solid-state batteries show promise to meet these targets in energy density, power density, safety and lifetime.

1.2 Solid electrolyte versus liquid electrolyte

One of the primary differentiations between solid-state Li metal batteries and conventional Li-ion batteries is the electrolyte.

While liquid electrolytes such as Propylene Carbonate (PC) or DiMethyl Carbonate (DMC) are used as a medium to transport lithium-ions in conventional batteries,[6,7] a typical solid-state Li metal battery uses inorganic SE such as Lithium Phosphorus Oxynitride (LiPON), cubic phase $Li_7La_3Zr_2O_{12}$ (c-LLZO) or Li_2S-P_2S_5 (LPS) as the ionic conductor and mechanical separator. Figure 1.3 illustrates the architectures of a conventional Li-ion cell compared to a solid-state Li metal cell and a solid-state Li-ion cell.

In general, a conventional Li-ion cell consists of a porous Negative Electrode (NE) (typically made of graphite) and Positive Electrode (PE) (usually made of a layered transition metal

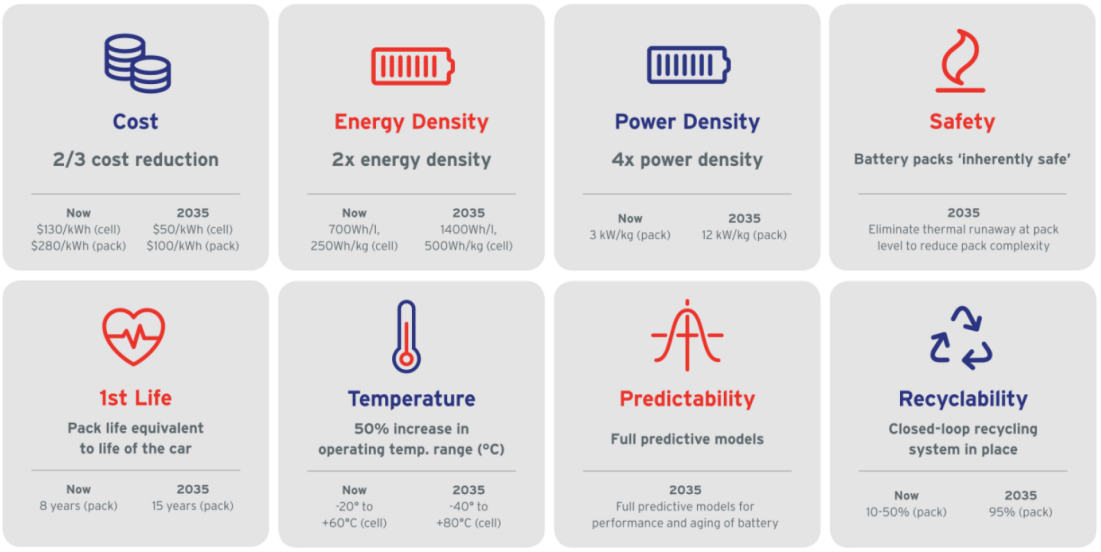


Figure 1.2 Battery challenges and goals outlined by the Faraday Institution in terms of cost, energy density, power density, safety, lifetime, operating temperature range, models predictability and recyclability. Reproduced with permission from Ref. 5, courtesy of the Faraday Institution.

oxide), and a liquid electrolyte that fills up the porous electrodes and the separator. As shown by Figure 1.3, replacing the liquid electrolyte with a SE yields two possible cell designs: (1) solid-state Li metal cell, where pure metallic Li is used as the NE or (2) solid-state Li-ion cell, where the liquid electrolyte in the porous NE and PE configurations is substituted by the SE to form composite solid electrodes.[8]

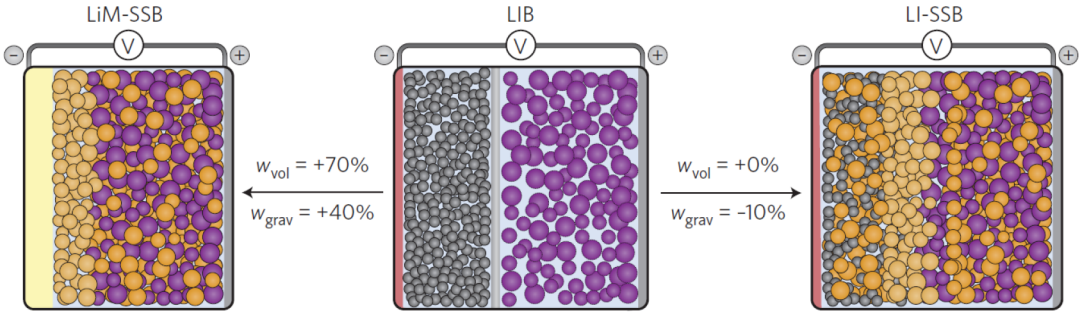


Figure 1.3 Distinction in the cell architecture of a conventional Li-ion battery and solid-state batteries: A conventional Li-ion battery consists of a porous PE (violet circles) and NE (grey circles), in which the liquid electrolyte (light blue) wets the electrodes and infiltrates the voids throughout the cell. In a solid-state Li-ion battery (right), the liquid electrolyte in both porous electrodes is substituted by SEs (dark orange) to form composite solid electrodes. In a solid-state Li metal battery (left), the porous NE can be replaced completely with a Li metal foil (light yellow). The light orange particles represent another type of SE, indicating that different SEs can be used for the composite electrodes and the electrolyte. Reproduced with permission from Ref. 8, Copyright (2016), Nature Energy.

1.2.1 Safety features and the lifetime performance of inorganic solid electrolytes

The non-flammability of inorganic SEs has been considered the paradigm shift toward making better next-generation batteries.[9,10] The liquid electrolytes in conventional high-voltage Li-ion batteries consist of flammable esters and ethers, which could cause electrolyte decomposition and subsequently fire hazards when operated beyond their voltage limits.[11]

A fire incident was reported in the APU battery of the Japan Airlines Boeing 787-8 on January 7, 2013.[12] Figure 1.4 shows the photograph of the Li-ion battery used in the 787 Main and APU before and after the thermal damage. The battery had eight individual Li-ion cells (Figure 1.4, left). The battery pack disassembly shows that cells 5 to 8 demonstrated the most severe thermal and mechanical damage. It was concluded that an internal short circuit had taken place in cell 5 or cell 6, which led to a cascading thermal runaway and subsequently the release of smoke and fire.[1,12] Replacing liquid electrolytes with inorganic SEs show promise to reduce the risk of flammability. As a result, critical safety control systems at system levels could be reduced, allowing solid-state battery packs to achieve even higher gravimetric and volumetric energy densities.[1,13]

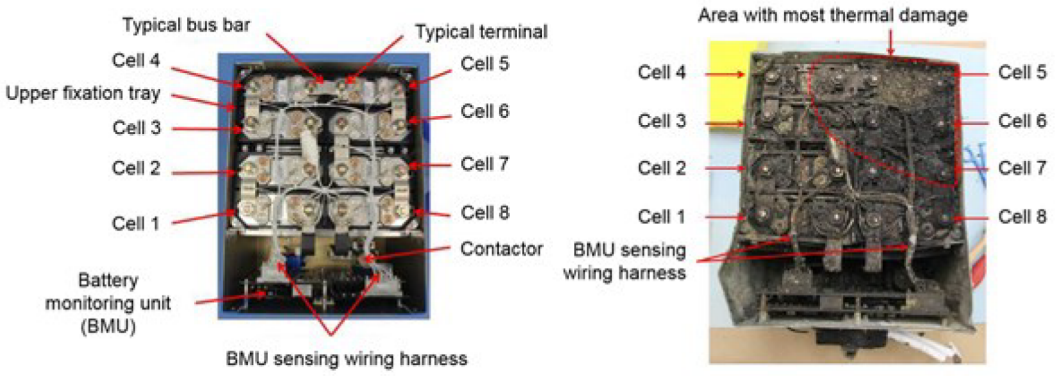


Figure 1.4 (Left) Battery used in the APU of Boeing 787-8. (Right) Damage occurred in the battery due to a cascading thermal runaway. Reproduced with permission from Ref. 12, Copyright (2013), National Transportation Safety Board (NTSB).

Besides a lower risk of flammability in a solid-state battery, Li *et al.*[11] have demonstrated in a long-term degradation study that a solid-state battery shows a better capacity retention over 10000 cycles compared to batteries using liquid electrolytes. Figure 1.5 shows the lifetime performance of a solids-state Li metal cell (Li|LiPON|$LiNi_{0.5}Mn_{1.5}O_4$) and four different conventional Li-ion cells using different volumes of liquid electrolytes (1.2 M $LiPF_6$ in Ethylene Carbonate/DiMethyl Carbonate (EC/DMC)). The liquid-based Li-ion cells used identical PEs and Li metal as NEs. The solid-state Li metal cell was shown to retain 90% of its initial capacity after 10000 cycles (Figure 1.5a), resulting in a high Couloumbic efficiency of 99.98% (Figure 1.5b) and a cumulative charge loss of only 7.9 mAh g^{-1} (Figure 1.5c).[11] In contrast, the capacity of the best-performance conventional liquid-based cell fades to 70% after

6000 cycles, achieving the Couloumbic efficiency below 99.5% with more than 900 mAh g^{-1} cumulative charge loss after 1000 cycles. This potential to obtain a long-term cycling stability becomes one of the major incentives in developing next-generation solid-state batteries.[11]

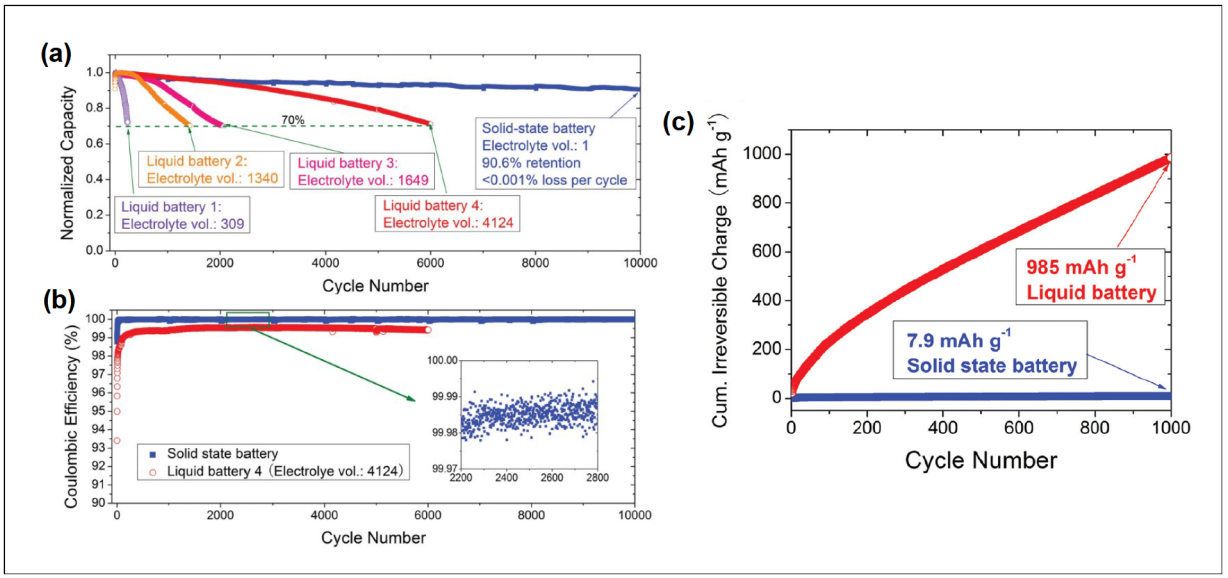


Figure 1.5 Lifetime performance of a solid-state Li metal cell and conventional Li-ion cells: (a) Comparison in terms of the capacity retention of four conventional Li-ion cells with different volumes of liquid electrolytes and a solid-state Li metal cell. (b) Coulombic efficiency of the solid-state Li metal cell and the best-performing conventional Li-ion cell. (c) Cumulative irreversible charge loss of both cells over 1000 cycles. Reproduced with permission from Ref. 11, Copyright (2015), John Wiley and Sons.

1.2.2 Lithium metal as the negative electrodes

In most Li-ion batteries, porous NEs with graphite are used as the host matrix. Due to the higher mechanical strength of a SE compared to a porous membrane in conventional Li-ion batteries, the use of inorganic SE could potentially prevent the dendrites penetration in solid-state batteries. In general, the term "dendrite" denotes the formation of a wide range of branched metal morphologies, which may not accurately describe the complex Li metal mechanisms observed in SEs.[14–16] Therefore, the term "Li filament" is used throughout this thesis to represent these Li metal features. The early modelling work by Monroe and Newman[17] suggested that the risks of Li filaments propagation could be prevented if a SE has a shear modulus at least two times larger than the shear modulus of Li metal. The shear modulus of Li metal is 4.25 GPa,[18] whereas SEs such as c-LLZO and LiPON have a shear modulus of $58-60$ GPa and 31 GPa, respectively.[16,18,19] As such, Li metal could substitute graphite as the NE. Table 1.1 outlines the physical properties of Li metal and graphite. Because of a lower density as well as a higher gravimetric and volumetric capacity of Li metal,[20] replacing graphite with Li metal could increase the volumetric energy density by 70% and gravimetric energy density by 40% (Figure 1.3).[8]

Table 1.1 Material properties of metallic Li and graphite (Reproduced with permission from Ref. 20, Copyright (2011), McGraw-Hill.)

	Metallic Li	Graphite
Atomic/molecular weight [g]	6.94	72.06
Standard reduction potential at 25 °C [V]	−3.01	−2.8
Density [$g\,cm^{-3}$]	0.54	2.25
Gravimetric capacity [$Ah\,g^{-1}$]	3.86	0.372
Volumetric capacity [$Ah\,cm^{-3}$]	2.06	0.837

Due to the differences between the gravimetric and volumetric capacity of Li metal and graphite NE, distinguishing the terminologies between a Li metal cell and a Li-ion cell becomes important. In this thesis, a Li metal cell denotes a cell using Li as the NE, whereas a Li-ion cell refers to a cell with both electrodes as the intercalation electrodes.[1] Figure 1.6 illustrates this difference for a conventional cell architecture based on liquid electrolytes.

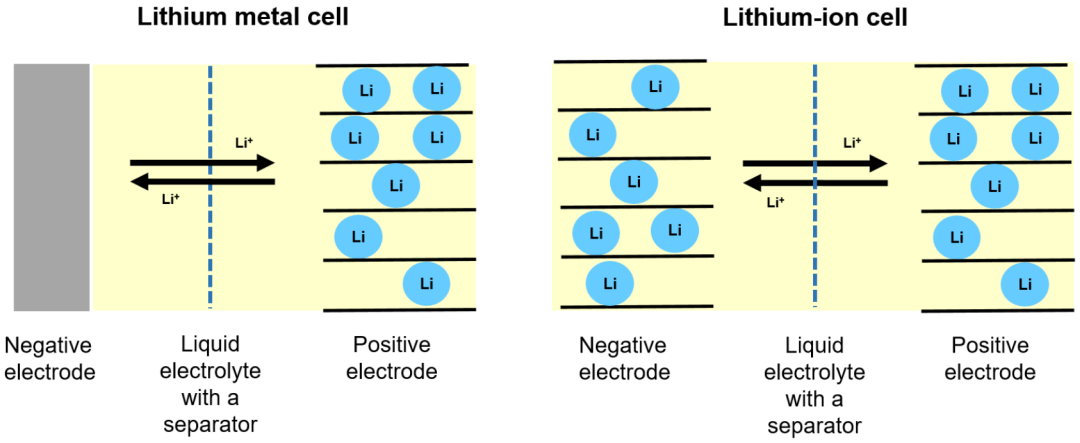


Figure 1.6 Distinction between a Li metal cell and a Li-ion cell: A Li metal cell has Li as the negative electrode, whereas a Li-ion cell uses a porous electrode for both PE and NE.[1]

One of the main reasons preventing the use of Li metal in conventional Li-ion batteries is the formation of dendrites or Li filaments, which could penetrate through the porous separator to induce an internal short-circuit (Figure 1.7a).[21] Under high C-rate charge or discharge, uneven Li dissolution and deposition could occur, leading to the formation of Li filaments.[6] Figure 1.7b shows the morphology of a single Li filament in the Propylene Carbonate (PC) electrolyte, and Figure 1.7c illustrates the mechanism of Li filaments formation due to non-uniform Li dissolution and deposition.[6]

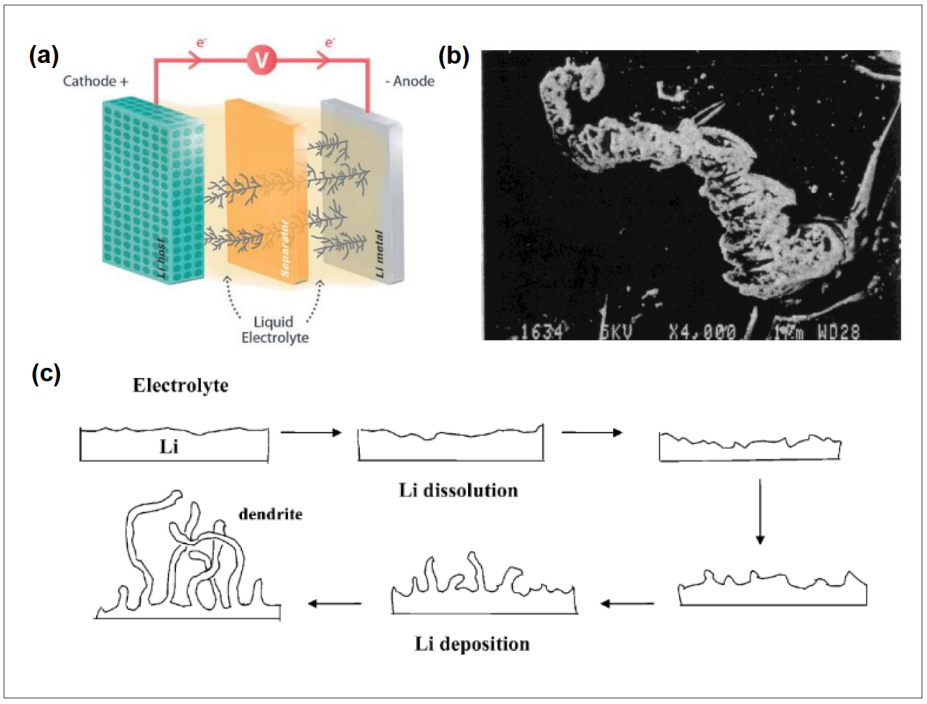


Figure 1.7 (a) A short-circuit scenario due to the Li filaments formation and penetration in conventional Li-ion cells. Reproduced with permission from Ref. 21, Copyright (2016), The Royal Society of Chemistry. (b) The micrograph of a single Li filament formation in the PC electrolyte. (c) The non-uniform dissolution and deposition of Li metal causes the formation of dendrites or Li filaments. Reproduced with permission from Ref. 6, Copyright (2004), American Chemical Society.

1.2.3 Limitations of solid-state lithium metal batteries

Despite the advantages of solid-state batteries discussed in Section 1.2.1 and Section 1.2.2, the commercial production of these batteries are still limited. One of the barriers inhibiting the development of solid-state batteries is its high Area Specific Impedance (ASI) compared to conventional batteries.[11] Figure 1.8a and Figure 1.8b compare the ASI of both solid-state and liquid-based cells over 4000 cycles.[11] While the conventional Li-ion cell with liquid electrolyte was shown to demonstrate an ASI less than 80 $\Omega\,cm^2$ and an absolute impedance of about 600 Ω after 4000 cycles, a Li metal solid-state cell had a consistent ASI of about 200 $\Omega\,cm^2$ and an absolute impedance up to 10000 Ω.[11] This magnitude of impedance results in a lower discharge capacity at both low and high C-rates, as shown by Figure 1.8c.[11] Various interdependent mechanisms such as low ionic conductivity, limited charge-transfer contact points, bulk solid diffusion, voids formation and grain boundaries resistance are at play to cause this high magnitude of impedance.[7,22–27]

1.3 Focus and aims of research

Based on the promising energy density and non-flammability of inorganic solid-state batteries, it is evident that replacing liquid electrolytes with inorganic SEs could achieve the required

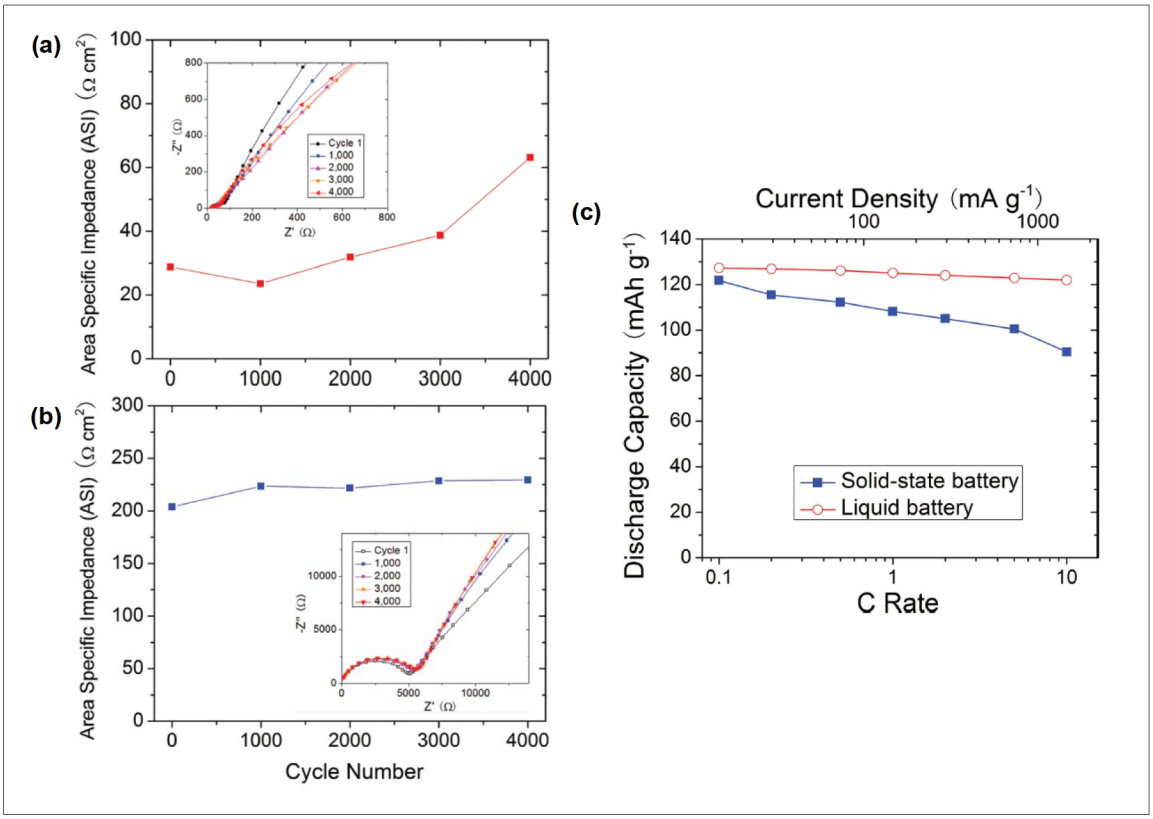


Figure 1.8 (a) Area Specific Impedance (ASI) of a conventional Li-ion cell and (b) a solid-state Li metal cell. The Nyquist plots were obtained at discharged state (3.5V). (c) The discharge capacity of both cell chemistries under low and high C-rates. Reproduced with permission from Ref. 11, Copyright (2015), John Wiley and Sons.

breakthrough to manufacture better next-generation batteries. However, the performance characteristics of solid-state batteries are still not comparable to conventional Li-ion batteries under high and low current loads.[11]

The main objective of the present research is to study the underlying multiphysical mechanisms governing the performance of solid-state batteries under different operating conditions. By understanding the performance-limiting mechanisms, guidelines for possible cell designs can be proposed. The research questions can be outlined as follows:

1. Which mechanisms are limiting the performance of solid-state Li metal batteries under pulse operating conditions?

2. How does upscaling of a single-layer cell affect the gravimetric and volumetric of large-format solid-state batteries?

3. What are the thermal behaviour of large-format solid-state batteries? How does a bipolar stack solid-state battery differ from a parallel stack in terms of heat generations and temperature gradients?

4. How do the mechanical properties of inorganic SEs affect the electrochemical transport across the SEs?

A combination of experimental and numerical methodologies are used to answer these research objectives. The last research question is answered by studying the mathematical derivations of the Nernst-Einstein's relation and linking its fundamental assumptions to the electrochemical performance of an inorganic SE.

1.4 Thesis outline

The structure of this thesis is organised as follows:

Chapter 2 (Literature review) surveys the works done by others on understanding the multiphysical interactions between different mechanisms that govern the overall performance of solid-state batteries. The multi-physics mechanisms are linked to the performance and degradation of solid-state batteries, and provides a framework in studying the mechanistic behaviour of solid-state Li metal batteries in this research.

Chapter 3 (Diffusion limitations under pulse-operating conditions) presents a simplified electrochemical model and the experimental procedures in estimating the required model parameters. The model is then used to explore the performance-limiting mechanisms under pulse operating conditions and propose possible cell designs for next-generation solid-state Li metal batteries.

Chapter 4 (Large-format solid-state bipolar and parallel stacks) outlines a model-based scaling approach to compare the performance characteristics of large-format solid-state bipolar and parallel stacks. The electrochemical stack models are coupled with two-dimensional thermal models to analyse how different operating temperatures affect the performance of both stack configurations.

Chapter 5 (Mechanical behaviour of inorganic solid electrolytes) discusses the impacts of inorganic SE mechanical properties on the choice of electrochemical models. Here, the fundamental assumptions underpinning the Nernst-Einstein's equations are studied and linked to the ionic transport across an inorganic SE.

Chapter 6 (Conclusions and future works) summarises the findings from this thesis and outlines suggestions for future works in this field.

Chapter 2

Literature review

Many signs of progress have been achieved in researching next-generation solid-state batteries by improving the ionic conductivity of the SE,[22,24,28] reducing the interfacial impedance by the use of coatings[25,29] and suppressing the Li filamentary growth.[15,26,30,31] Despite these advances, there is a lack of holistic understanding of the underlying interactions between different multiphysical mechanisms. A real solid-state cell has multiple components. The operations of solid-state batteries are inherently multiphysical, involving different electrochemical and chemical reactions coupled with unique thermal and mechanical behaviour. Little attention has been given to discussing how the interplay of these mechanisms affects overall cell performance and degradation behaviours under different operating conditions.

Different works focussing on sulfide-based SEs have been reported due to their high ionic conductivity approaching the conductivity of liquid electrolytes.[42–46] Whilst sulfide-based SEs have the highest ionic conductivity compared to other SEs, this class of SE also has other significant drawbacks such as the generation of toxic H_2S gas upon exposure to moisture and a higher risk of cell failure due to Li filaments propagation. A comparative analysis in terms of quantitative multiphysical properties between different classes of SEs and cell components has not been discussed in the literature. In the case of cell failure, such as excessive Li plating and stripping, the nucleation and propagation of Li filament in solid-state batteries depends strongly on the Critical Current Density (CCD). CCD can be defined as the current density, at which Li filaments propagate through the SE to cause an internal short-circuit and an immediate voltage drop.[30] As solid-state Li-metal cells can be cycled safely below the limit of CCD, this parameter reveals the capability of inorganic SEs to suppress the nucleation and propagation of Li filaments.[26,30] LiPON has the largest CCD ($> 10\,\mathrm{mA\,cm^{-2}}$) followed by LPS ($0.3 - 1.0\,\mathrm{mA\,cm^{-2}}$) and c-LLZO ($0.3 - 0.5\,\mathrm{mA\,cm^{-2}}$) (see Table 2.1).[23,29–31,47] Nevertheless,

Part of this chapter has been published in M.-C. Pang, K. Yang, R. Brugge, T. Zhang, X. Liu, F. Pan, S. Yang, A. Aguadero, B. Wu, M. Marinescu, H. Wang and G. J. Offer. Materials Today (2021). The journal policy for including the published article in a thesis can be found in Appendix I.

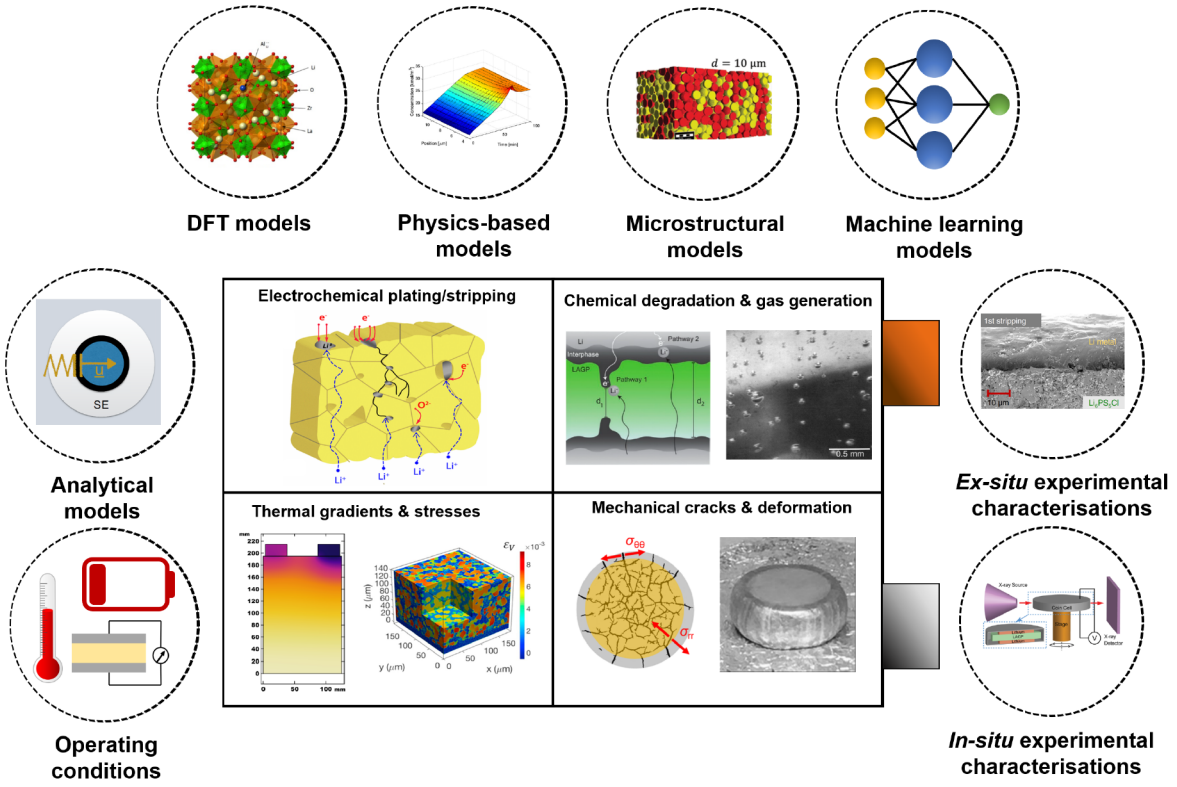


Figure 2.1 Schematic illustration of the multiphysical interactions between electrochemical (Reprinted with permission from Ref. 32), chemical (Reprinted with permission from Ref. 33 and Ref. 34), thermal (Reprinted with permission from Ref. 35 and Ref. 36) and mechanical mechanisms (Reprinted with permission from Ref. 37 and Ref. 38), and the effects of operating conditions on these mechanisms. Here, a combined review of state-of-the-art modelling approaches and experimental characterisation techniques is presented. The modelling techniques include analytical models (Reprinted with permission from Ref. 39), Density Functional Theory (DFT) models (Reprinted with permission from Ref. 18), physics-based models (Reprinted with permission from Ref. 40), microstructural models (Reprinted with permission from Ref. 41) and machine learning models. The right panel illustrates state-of-the-art characterisation categories reviewed in this work to understand the multiphysical interacting mechanisms in solid-state batteries (Reprinted with permission from Ref. 26 and Ref. 37)

the CCD is also a function of operating temperatures and critical pressures.[23,30,48,49] Therefore, effective prevention of excessive Li plating and stripping requires a combined understanding of solid-state electrochemistry, microstructure, mechanics, operating conditions, and their interactions.

This chapter aims to review the underlying multiphysical mechanisms governing the performance and degradation behaviour of solid-state batteries. The gaps in physics-based modelling of solid-state Li-metal batteries will be identified and further discussed in the subsequent chapters of this thesis. As shown by Figure 2.1, it is important to understand the multiphysical interactions between different mechanisms governing the overall performance of solid-state batteries. These interactions are reviewed *via* an array of modelling and characterisation techniques. Although interfacial stabilities play an essential role in determining cell performance, the importance of

a holistic mechanistic review of different cell components and their multiphysical interactions is highlighted. A comprehensive summary of different degradation mechanisms will be especially useful for future development of smart sensors for solid-state batteries, where the mechanistic understanding of different degradations and their trigger conditions is critical to detect potential fault behaviours before a complete failure. The individual aspects of cell performance, such as the interfacial phenomena, are only discussed briefly as these topics are covered in details by Cheng *et al.*,[50] Famprikis *et al.*,[51] Banerjee *et al.*[52] and Xiao *et al.*[53]

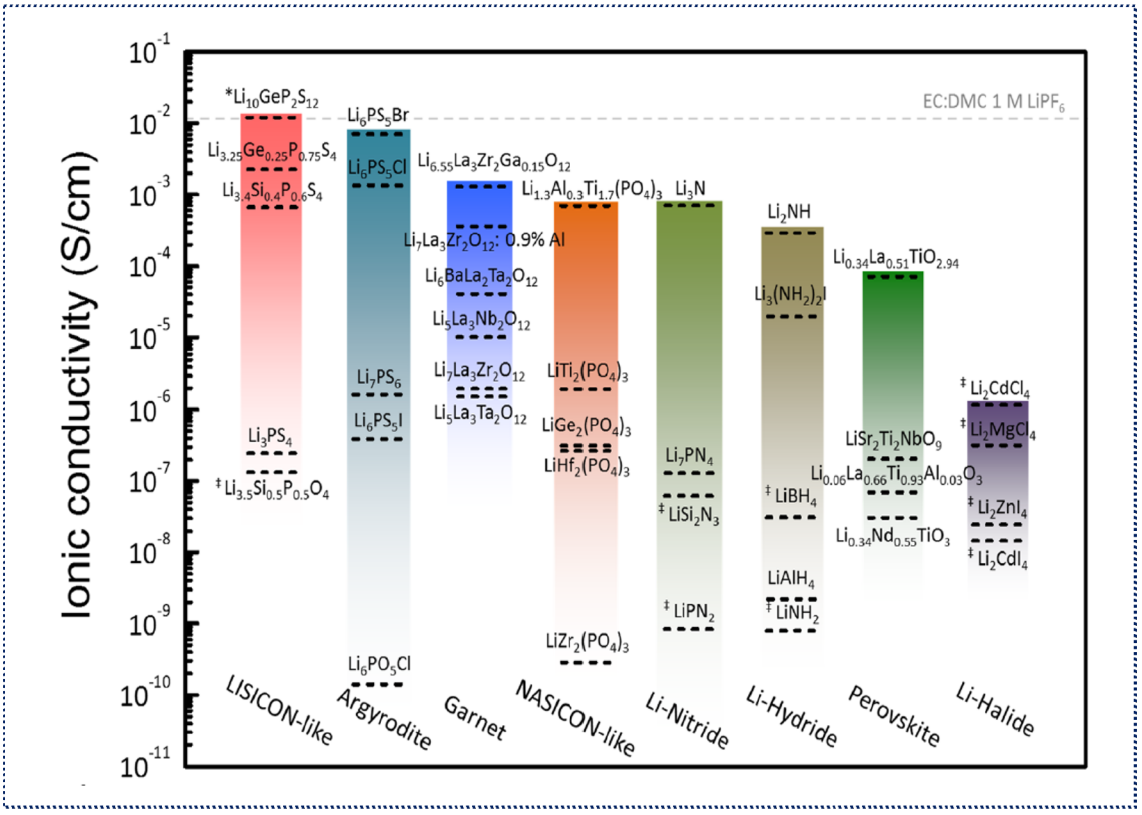


Figure 2.2 A comparison of total ionic conductivity for different classes of inorganic solid electrolytes such as LISICON, argyrodite, garnet, NASICON, Li-Nitride, Li-Hydride, perovskite and Li-halide. Reprinted with permission from Ref. 54, Copyright (2016), American Chemical Society.

2.1 Multiphysical properties of solid-state cells

The behaviour of solid-state batteries under a wide range of conditions is inherently multiphysical, involving electrochemical and chemical reactions as well as thermal and mechanical responses. Han *et al.* have compared the properties for three representative classes of inorganic SEs (LiPON, c-LLZO and LPS).[31] The works of Han *et al.*[31] are extended in this review to consider the multiphysical properties of inorganic SEs and interactions between different cell components, in order to illustrate the complex interplay between electrochemical, chemical, thermal and mechanical mechanisms.

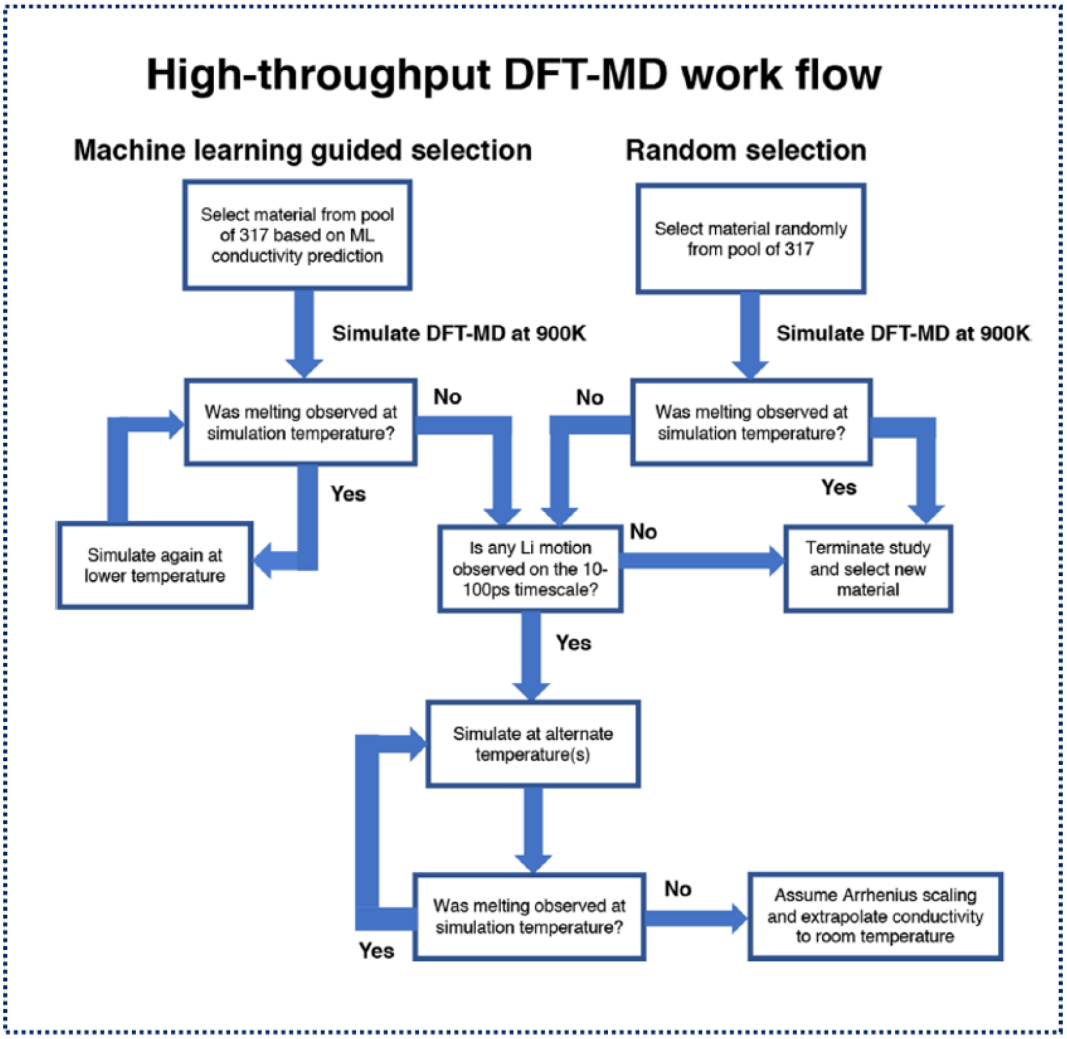


Figure 2.3 A combined machine learning and Density Functional Theory (DFT)-Molecular Dynamics (MD) work flow, where the materials are chosen for the DFT-MD simulations based on the predicted superionic conductivities from the logistic regression machine learning model. Reprinted with permission from Ref. 55, Copyright (2019), American Chemical Society.

2.1.1 Electrochemical and chemical properties

Ionic and electronic conductivity. An ideal SE should have a high ionic conductivity ($> 10^{-3}$ S cm^{-1}) and a low electronic conductivity ($< 10^{-9}$ S cm^{-1}).[22,31,54] Compared to the ASI of liquid electrolytes (in the range of mΩ cm^2 – Ω cm^2),[56–59] inorganic SEs usually have an ASI several orders of magnitude higher ($\gg 200\ \Omega$ cm^2) due to the low electrolyte conductivity.[22–24,47,60,61] The resistance of grain boundaries is often cited as a major reason causing the low ionic conductivity in inorganic SEs.[22,54] Various research efforts have been dedicated to reducing the electrolyte resistance *via* optimising the processing conditions, doping, reducing the electrolyte thickness and increasing the operating temperatures.[22,24,28,61–63] Among all the representative classes of inorganic SEs reviewed in this work, sulfide-based SEs have the highest ionic conductivity ($10^{-3} - 10^{-2}$ S cm^{-1}) comparable to that of the liquid electrolyte such as Ethylene Carbonate/DiMethyl Carbonate

(EC/DMC) 1M $LiPF_6$ (10^{-2} S cm^{-1}), as shown by Figure 2.2.[54] However, their stability against Li and PE is a challenge and limits their lifetime.

The experimental trial-and-error searches for promising new materials that satisfy a high-performance SE requirements are time and cost-consuming. Sendek *et al.*[64] have developed a data-driven ionic conductivity classification model using logistic regression machine learning algorithms to distinguish between potential solid electrolytes with superionic structures ($\sigma_{elec} \geqslant 10^{-4}$ S cm^{-1}) and non-superionic structures ($\sigma_{elec} < 10^{-4}$ S cm^{-1}).[64] They further performed Density Functional Theory (DFT)-Molecular Dynamics (MD) simulations on the most promising materials screened by machine learning models to study the structure-property relationships of these superionic solids.[55] Figure 2.3 illustrates the workflow of a combined machine learning and DFT-MD approaches.

Compared to the progress achieved in improving ionic conductivity, the research on the role of the electronic conductivity of inorganic SEs is often overlooked. Recently, Han and co-workers[31] demonstrated the critical role of the electronic conductivity in determining the growth of Li filaments. The current-time behaviour, from a potentiostatic hold, of Cu|c-LLZO|Cu and Cu|Li_3PS_4|Cu cells were measured and both SEs were shown to have electronic conductivities of 5.5×10^{-8} S cm^{-1} and 2.2×10^{-9} S cm^{-1} respectively, which is much higher than the electronic conductivity of LiPON (10^{-14} S cm^{-1}).[31,63] By correlating the electronic conductivity to the time-resolved Li concentration profiles of Li_3PS_4, c-LLZO and LiPON measured using *operando* Neutron Depth Profiling (NDP), they concluded that the high electronic conductivity of c-LLZO and Li_3PS_4 was the reason for promoting the formation of Li filaments within the SE. A high electronic conductivity lowers the critical overpotential of the SE and causes the reduction of Li^+ into Li within the bulk SE.[31]

Critical Current Density (CCD). The CCD could be further distinguished as the critical current for stripping and the critical current for plating. The stripping critical current denotes "the current density, above which Li is stripped faster than it is replenished at the Li/SE interface, resulting in void formation."[26] The rate of Li transport to the interface is governed predominantly by the diffusion of Li atoms within Li metal and Li metal creep.[26] In reality, the CCD for plating and stripping are interrelated: When the local current density at the NE-SE interface exceeds the CCD for stripping, the void formation will increase the local plating current density. As a result, more Li filaments will be formed until a short-circuit and cell failure occurs (see Section 2.2.5).[26]

The CCD is usually measured using galvanostatic cycling with stepped current densities on a non-blocking symmetrical cell.[23,29–31,47] Figure 2.4a shows the influence of temperature on applied current densities: the higher the operating temperature, the larger is the current density.[23,30,49] The high CCD of LiPON can be attributed to the more homogeneous film morphology with fewer grain boundaries and its lower electronic conductivity compared to c-LLZO and LPS SEs.[31,65] LiPON films are synthesised using the sputtering method, whereas

other inorganic SEs such as c-LLZO and LPS films are usually made *via* powder processing routes such as cold-pressing, hot-pressing, tape casting and sintering.[65] These powder processing methods result in the formation of grain boundaries, small intergranular pores and surface scratches due to polishing, which subsequently cause the SEs to be more susceptible to Li filaments propagation during operation.[65] It is worth noting that liquid electrolytes such as fluoroethylene carbonate (FEC)-based electrolytes can be cycled at 2 mA cm^{-2} for 1100 cycles without short-circuiting.[66] However, due to the large variability of reported CCD values in Li-metal solid-state cells, many factors could be at play influencing the reported value. Therefore, a standardised protocol in terms of cell architecture and operating conditions is urgently needed.

The CCD (i_c) was also shown to be a function of the critical pressure, Δp_c:‡[49]

$$i_c = 2\pi f_{int}\sqrt{6\epsilon_r|\Delta p_c|} = \frac{\sqrt{6\epsilon_r|\Delta p_c|}}{R_{int}C_{int}}, \tag{2.1}$$

where f_{int} is the interfacial characteristic frequency, Δp_c is the critical pressure, ϵ_r is the relative permittivity, R_{int} is the interfacial areal resistance and C_{int} is the interfacial capacitance. According to this model, filaments nucleate at the grain boundaries whenever the current induces a particular critical pressure described by the difference between the pressure in the electrolyte interior and its interface with the NE. Thus, the critical pressure is a material property containing information about the SE mechanical properties, grain structure, and Li-wetting energetics. Interfaces between conductive ceramics and Li are typically capacitive, and therefore sustain space-charge layers under pressure.[49]

Sakamoto and co-workers also highlighted the pressure-dependence of CCD,[70] in creating a new terminology – critical stack pressure. They showed that at low external stack pressures, the Li stripping rate is more dominant than the mechanical deformation at the interface, inducing the formation of voids and ultimately increasing resistance of the Li/c-LLZO interface.[70] However, the different processes occurring during plating and stripping, especially in full cells, need further investigation.

Electrochemical stability. A wide electrochemical stability window of the inorganic SE is desirable. Beyond the stability window, SEs decompose at the interface, which could cause high interfacial resistance and cell failures.[7,71] Cyclic Voltammetry (CV) measurements have been shown to overestimate the stability window of SEs and thus their stability with Li metal or high-voltage PE compared to the electrochemical stability window calculated from DFT.[71–74] For instance, it was reported that sulfide-based SEs such as $Li_{10}GeP_2S_{12}$ (LGPS) have a wide stability window of $0-5$ V.[9] The apparent wide electrochemical stability window is caused by the very small decomposition current within the voltage window $0-5$ V in the CV measurement and limited kinetic reactions measured with a semi-blocking cell configuration (Li|LGPS|Au).[9,71] The measurement of the stability window using a

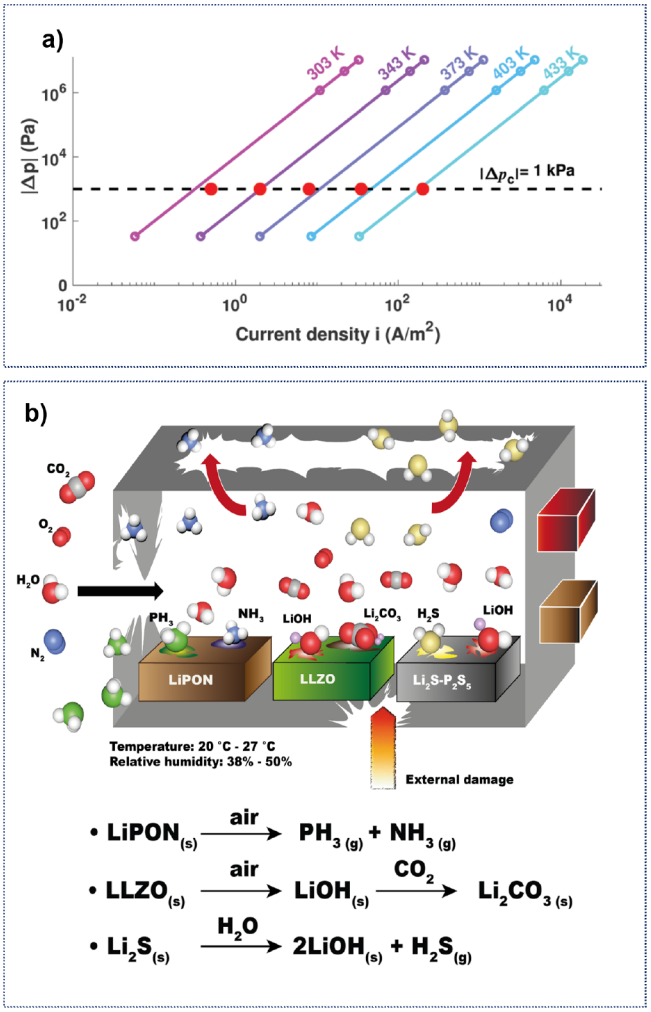


Figure 2.4 (a) The dependence of relative pressures on applied current densities and operating temperatures for Li|c-LLZO|Li: Whilst the current density was shown to increase with increasing operating temperatures from 303 K to 433 K, Li filaments nucleate whenever the current induces a critical pressure, which is far below the fracture stress for c-LLZO. Red dots indicate experimental critical currents. Reprinted with permission from Ref. 49, Copyright (2019), PCCP Owner Societies. (b) The chemical stability of LiPON, c-LLZO and LPS in air: LiPON generates toxic PH_3 and NH_3 gas,[67] whereas LPS forms LiOH solid and harmful H_2S gas.[68] Only c-LLZO was shown to form LiOH solid and Li_2CO_3 solid upon exposure to air.[69]

semi-blocking cell also does not reflect the solid-state composite electrode configuration, in which carbon black is often added as an additive to the SE and Active Materials (AM) to facilitate better electronic transport.[62,71,75] If the electrochemical stability window is measured with a Li|LGPS|LGPS-C|Pt cell configuration, LGPS was shown to have a limited stability window from $1.7-2.1$ V.[71] The decomposition products for LGPS include $Li_{15}Ge_4$, Li_3P, Li_2S, GeS_2, P_2S_5 and S.[71,72]

Although most oxide- and nitride-based SEs have a wider stability window than the sulfide-based electrolytes, it is worth noting that all oxide SEs form oxygen gas at high voltages (5 V).[72] Yu *et al.*[34] observed the formation of oxygen gas bubbles at the interface between LiPON and Pt

during an anodic voltage scan to 6 V, where the possible decomposition reaction was expressed as

$$2Li_3PO_4 \longrightarrow Li_4P_2O_7 + 1/2O_2 + 2Li^+ + 2e^-. \tag{2.2}$$

Chemical stability. The chemical stability in the atmosphere is also a significant feature. On exposure to ambient humid air (temperature: 20 °C, relative humidity: 50%), LiPON thin films were shown to react with air to form toxic PH_3 and NH_3 gas. As a consequence of this reaction, the surface RMS roughness increased from 28.8 nm to 612.8 nm and the ionic conductivity decreased from 2.8×10^{-6} S cm^{-1} to 9.9×10^{-10} S cm^{-1}.[67] Oxide-based SEs such as c-LLZO also react readily with humid air to form LiOH and Li_2CO_3, as shown by DFT calculation and X-ray Photoelectron Spectroscopy (XPS) analysis by Sharafi *et al.*[69] The formation of Li_2CO_3 on the surface of c-LLZO causes a significant increase in the Li|c-LLZO interfacial resistance.[29,76–79] Muramatsu *et al.*[68] investigated the stability of LPS SE after air exposure with Raman spectroscopy and an H_2S sensor. Sulfide-based SEs were shown to be hygroscopic and formed harmful H_2S gas on exposure to water molecules in the air (temperature: 26 °C – 27 °C, relative humidity: 38 – 39%).[68] The formation of these harmful gases due to the reactivity of the SEs with air has two significant implications. Firstly, all-solid-state batteries must be manufactured and assembled under a controlled environment such as a dry room. Secondly, mechanical damage of the batteries in real-world applications leading to exposure of the components to air could potentially cause health hazards to anyone nearby (see Figure 2.4b). It is worth noting that the amount of H_2S gas released was recorded for a pelletised cell in a controlled environment after exposure to air for a minimal period.[68] If solid-state batteries would be scaled up, in which each battery pack has hundreds of cells, and each unit cell has hundreds of layers, the impacts of harmful gas release due to mechanical damage such as battery crash cannot be neglected. This safety evaluation aspect is urgently needed before solid-state batteries can be employed for large-scale applications in electric vehicles or aircraft.

Relative permittivity. The relative permittivity is a physical property that characterises the strength of the electrostatic force acting between the electrodes and the SE in the space-charge layers. The relative permittivity of any given medium is inversely proportional to the electrostatic force, F_c as shown by Coulomb's law:

$$F_c = \frac{Q_1 Q_2}{4\pi\epsilon_0\epsilon_r d_{int}^2}, \tag{2.3}$$

where Q_1 and Q_2 are the charges of the bodies, ϵ_0 is the absolute permittivity of the vacuum, ϵ_r is the relative permittivity of the medium and d_{int} is the distance between the center of

the charges. The square root of the relative permittivity is directly proportional to the Debye length, λ, at the interface:[80,81]

$$\lambda = \sqrt{\frac{\epsilon_r \epsilon_0 R_{gas} T}{F^2 \sum_i z_i^2 c_{bulk}}}, \tag{2.4}$$

where R_{gas} is the universal gas constant ($R_{gas} = 8.314\,\mathrm{J\,mol^{-1}\,K^{-1}}$); T is the temperature; F is the Faraday's constant ($F = 96\,485\,\mathrm{C\,mol^{-1}}$); z_i is the number of proton charges carried by species i; c_{bulk} is the bulk concentration of the species. The Debye length denotes the characteristic length scale of the space-charge layer and usually has a thickness in the range of nm.[82–84] As shown by Table 2.1, the relative permittivity is different for LiPON and c-LLZO. It should be noted that the relative permittivity is also a function of frequency and temperature.[63,85] By using the zero-frequency limit of the relative permittivity, Braun *et al.* computed the thickness of the space-charge layers and showed that the fraction of cations at the interfaces depend strongly on the thickness of the space-charge layers.[82] A large relative permittivity indicates a thicker space-charge layer but a weaker electric field.[84] The implications of the space-charge layers on the cell performance will be further discussed in Section 2.3.1.3.

2.1.2 Thermal properties

Effects of operating temperatures. The operating and storage temperatures are critical parameters that affect the performance and lifespan of solid-state batteries. Temperature-dependent properties such as the ionic conductivity and the activation energy are usually described with the Arrhenius law.[23,24,60,61,63] High operating temperatures can facilitate better interfacial kinetics and ionic diffusion in the PE, but also accelerate the decomposition reactions. For example, Larfaillou *et al.*[63] showed that the LiPON SE had an electrolyte resistance up to 2000 Ω at −10 °C but dropped to 100 Ω at 30 °C. However, the lifespan of the cell also decreases significantly with increasing operating temperature. Wang *et al.*[86] showed that a cell cycled at 80 °C loses about 35% of the initial capacity while a cell cycled at 25 °C retains the same initial capacity. The loss of cell capacity at high operating temperatures was attributed to the decomposition reaction in the disordered $LiCoO_2$ (LCO) layer at the electrode-electrolyte interface.[86] Although a low operating temperature such as 0 °C could potentially reduce the rate of interfacial decomposition, studies in conventional Li-ion batteries show that other degradation mechanisms such as non-uniform Li plating could be significant under fast-charging at low temperature.[87] Moreover, the significant electrolyte resistance at low temperature indicates that sluggish ionic mobility in the SE would impede the overall cell performance.[63] Nonetheless, the lack of reports on low-temperature performance and degradation in solid-state batteries highlights a gap for future studies.

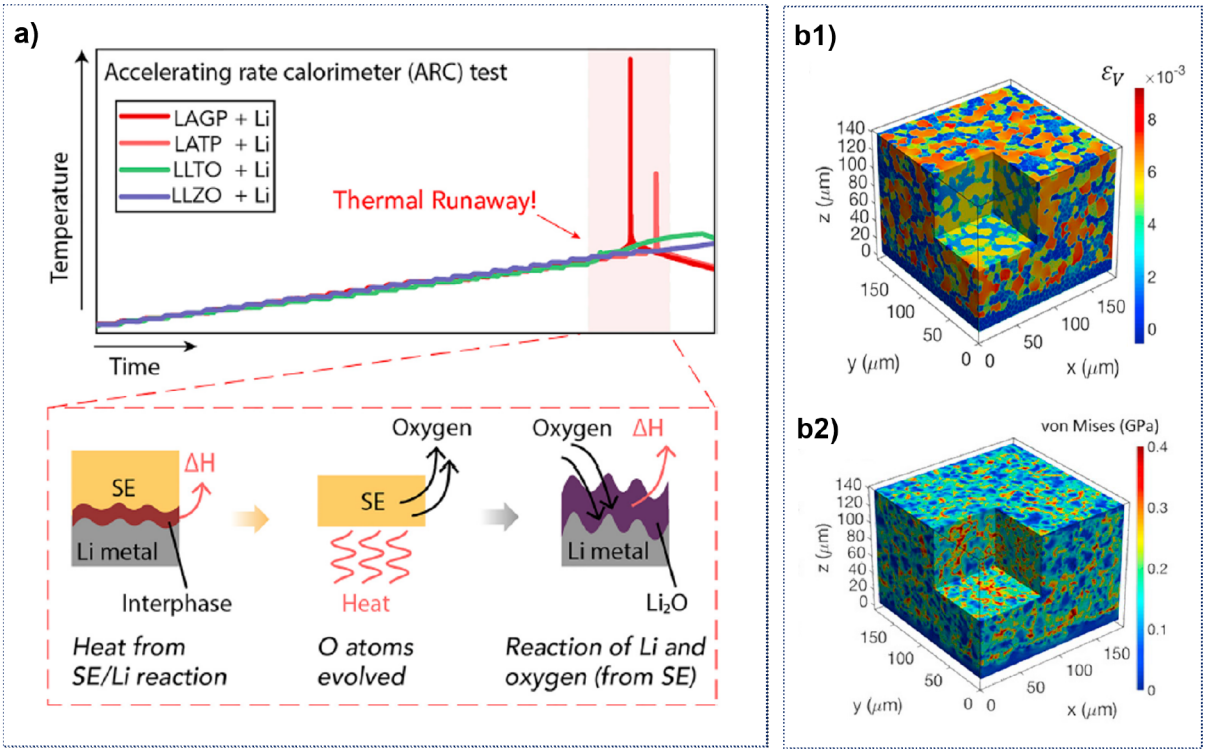


Figure 2.5 (a) Thermal stabilities of oxide-based SEs with Li metal: While thermal runaway behaviours could be observed with LAGP+Li, LATP+Li and LLTO+Li, c-LLZO SE exhibits no thermal runaway at elevated temperature. Reprinted with permission from Ref. 88, Copyright 2020, Elservier. (b) The impacts of a thermal contraction from 750 °C to 27 °C on the (b1) fractional volume change and (b2) von Mises stresses of the composite PE. The composite PE consists of NMC as AM, c-LLZO as SE and Ni as the electronic conductor. The fractional volume change indicates the volumetric contraction or expansion of the constituent particles relative to c-LLZO, whereas the von Mises stress quantifies the local combined thermal stress state of the composite particles. Reprinted with permission from Ref. 36, Copyright (2019), Elsevier.

Thermal stability. While safety is a concern for conventional Li-ion batteries due to flammable esters and ethers,[11] Chen *et al.*[88] demonstrated recently that the oxygen generation from oxide-based SEs at elevated temperature cause thermal runaway with highly reactive Li metal. By using Accelerating Rate Calorimeter (ARC) combined with first-principles calculations, they compared the thermal stability of Li metal with different SEs ($Li_{1+x}Al_xGe_{2-x}(PO_4)_3$ (LAGP), $Li_{1.2}Al_{0.2}Ti_{1.8}(PO_4)_3$ (LATP), $Li_{3x}La_{2/3-x}TiO_3$ (LLTO) and c-LLZO).[88] In SEs such as LAGP, LATP and LLTO, decomposition interphases formed after the Ti/Ge electrolytes contacted with the metallic Li. The release of oxygen from the SEs at elevated temperatures was shown to initiate a highly exothermic reaction with molten Li metal, leading to thermal runaway. However, c-LLZO was shown to have the highest onset temperature of O_2 release, indicating the thermal stability of c-LLZO with Li metal at elevated temperature (Figure 2.5a).[88]

On the other hand, the thermal stability of NMC-LPS composite PE was investigated by Tsukasaki *et al.*[89] By using a combination of experimental techniques such as Differential Scanning Calorimetry (DSC), *in-situ* X-ray Diffraction (XRD), *ex-situ* Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM), they showed a significant

morphological change occurring in the NMC-LPS composite PE after heating above 300 °C. NMC decomposed into transition metal sulfides and generated O_2 gas, further causing LPS to oxidise to Li_3PO_4.[89] When the LPS SE in the composite PE was replaced with Li_4SnS_4 (LSS) SE, the reactivity of LSS and NMC was shown to be much lower than that of LPS-NMC due to the stability of O_2 gas with LSS SE.[90]

Heat generations and transport. Because of the strong temperature-dependent cell behaviour, it is essential to analyse the heat generation mechanism inside the cell. The heat generation in a single-layer cell is insignificant because the surface-to-volume ratio is large.[35] However, for a cell stack with many units, the heat generation can be significant, especially for operating conditions at high current densities. In solid-state batteries, heat is generated due to irreversible heat sources such as ohmic transport across the SE, activation overpotential at both interfaces and species transport due to concentration gradients in the electrodes. Simultaneously, the reversible heat generation can also occur due to the structural change of the PE and NE. The generated heat is predominantly transferred to the surface through the heat conduction mechanism and is subsequently dissipated to the surroundings through convection and radiation.[35] Therefore, the heat generation and heat transfer mechanisms can be described by the energy balance as follows:[35,91]

$$\underbrace{\rho_{\text{eff}} C_{\text{p,eff}} \frac{\partial T}{\partial t}}_{\substack{\text{thermal} \\ \text{energy storage}}} = \underbrace{\frac{\partial}{\partial x}\left(k_{\text{x}} \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_{\text{y}} \frac{\partial T}{\partial y}\right)}_{\substack{\text{in-plane} \\ \text{heat conduction}}} + \underbrace{\frac{\partial}{\partial z}\left(k_{\text{z}} \frac{\partial T}{\partial z}\right)}_{\substack{\text{cross-plane} \\ \text{heat conduction}}} + \underbrace{Q_{\text{gen}}}_{\substack{\text{heat} \\ \text{generation}}} \underbrace{- Q_{\text{conv}} - Q_{\text{rad}}}_{\substack{\text{heat} \\ \text{dissipation}}}, \tag{2.5}$$

where ρ_{eff} is the effective density; $C_{\text{p,eff}}$ is the effective specific heat capacity; k_{x} and k_{y} are the in-plane thermal conductivity; k_{z} is the cross-plane thermal conductivity; Q_{gen} is the total heat generation; Q_{conv} and Q_{rad} are the heat dissipation by convection and radiation.

Specific heat capacity. A high effective specific heat capacity indicates a better storage of thermal energy and a smaller temperature increment for unit heat input. LiPON has a higher specific heat capacity (1400 $\text{J kg}^{-1}\text{ K}^{-1}$) than c-LLZO (553 $\text{J kg}^{-1}\text{ K}^{-1}$) (see Table 2.1).[92,93] In contrast, the current collector such as copper has a specific heat capacity of only 390 $\text{J kg}^{-1}\text{ K}^{-1}$. Such a low magnitude of specific heat capacity means that the temperature increase around the tabs and current collectors will be higher than the other cell components.

Thermal conductivity. In general, the thermal conductivity of a conventional Li-ion cell is highly anisotropic for cylindrical, pouch and prismatic configurations due to the layered arrangement of each component. Depending on the cell layer configuration, the effective thermal conductivity of a cell can be estimated from the thermal conductivity of each material by assuming parallel or series resistances for each cell layer (see Table A-1 in Appendix A).[94,95] While the difference between the cross-plane and in-plane specific heat capacity is negligible, the in-plane thermal conductivity of each cell component can be larger than the cross-plane thermal conductivity by a factor of $6-13$.[35,96] Xu *et al.* showed that LiPON has a cross-plane thermal conductivity of $1.4\ \mathrm{W\,m^{-1}\,K^{-1}}$.[92] Different cell manufacturing processes were also shown to affect the thermal conductivity. Bock and co-workers showed that a non-sintered c-LLZO has a cross-plane thermal conductivity of $0.22-0.23\ \mathrm{W\,m^{-1}\,K^{-1}}$, whereas a sintered c-LLZO has a thermal conductivity higher by a factor of two ($0.47\ \mathrm{W\,m^{-1}\,K^{-1}}$).[97] However, none of these reports have studied the effects of plane orientations on the measured thermal conductivity of the SE. For a layered PE such as LCO, Yang *et al.* showed from the first-principles calculation that the in-plane thermal conductivity is $53.6\ \mathrm{W\,m^{-1}\,K^{-1}}$, whereas the cross-plane thermal conductivity is only $8.4\ \mathrm{W\,m^{-1}\,K^{-1}}$.[98] This difference in the material thermal conductivity can be attributed to the higher mobility of the heat-carrying phonon modes in-plane compared to cross-plane.[96,98] Compared to the thermal conductivity of the SE or PE, Li metal has a higher thermal conductivity of $81.8\ \mathrm{W\,m^{-1}\,K^{-1}}$,[95] though it is not clear whether this value refers to the thermal conductivity of a single crystal Li or polycrystalline bulk Li. Although no studies have demonstrated the impacts of void formation on the interfacial thermal resistance of a solid-state cell, contact loss between the SE and the Li metal could potentially create additional thermal resistance to affect the effective heat transport. For a cell stack consisting of many unit cells, the smaller effective cross-plane thermal conductivity means a higher magnitude of heat accumulation across the stack thickness. Therefore, optimising the stack thickness and designing cells for effective thermal management are essential for large-format solid-state batteries.[35,99,100]

Thermal expansion coefficient. Recently, Yu *et al.*[36] evaluated the thermal stress in composite PEs due to cooling from the sintered temperature at 750 °C. The misfit strain resulting from the temperature change, ϵ_{T}, can be calculated by[36]

$$\epsilon_{\mathrm{T}} = (\alpha_{\mathrm{T1}} - \alpha_{\mathrm{T2}})\Delta T, \tag{2.6}$$

where α_{T1} and α_{T2} are the thermal expansion coefficients of bonded materials in the composite PE. c-LLZO has a thermal expansion coefficient of $1.5\times10^{-5}\ \mathrm{K^{-1}}$.[36,101] Figure 2.5b shows the simulated microstructures to assess the impacts of sintering and cooling on the thermal stresses in the composite PEs. By comparing the fractional volume change and dilatational stresses of the constituent particles in the composite, they found that NMC and Ni particles are under compression, whereas c-LLZO particles are under tension.[36] The von Mises stresses were shown

to concentrate on the boundaries between grains of two different materials in the composite. Therefore, intergranular cracks are more likely to occur than intragranular ones.[36]

Table 2.1 Multiphysical properties of three representative classes of inorganic SEs

Properties	LiPON	c-LLZO	LPS	Method	Ref.
Electrochemical/Chemical properties					
Ionic conductivity, σ_{elec}* [S cm^{-1}]	10^{-6}	10^{-4}	$10^{-4}-10^{-3}$	EIS	[23, 45, 63]
Electronic conductivity, σ_{e^-}* [S cm^{-1}]	10^{-14}	10^{-8}	10^{-9}	Hebb-Wagner DC polarisation	[31, 63, 102]
Electrochemical stability window vs. Li/Li$^+$ [V]	$0.68-2.63$	$0.05-{>}5$	$0-2.01$	DFT	[71, 72]
Relative permittivity, ϵ_r [–]	19.98 (thin-film)	40 (bulk) 152 (thin-film)	-	EIS	[24, 61, 63]
CCD, i_c** [mA cm^{-2}]	>10	$0.05-0.9$	$0.3-1.0$	Step-increased DC cycling	[23, 29–31, 47]
Exposure to moisture	Form toxic PH_3 and NH_3 gas	Form LiOH and Li_2CO_3	Form toxic H_2S	DFT, XPS, H_2S sensor	[67–69]
Thermal properties					
Specific heat capacity, $C_{p,SE}$ [J kg^{-1} K^{-1}]	1400	553	-	DSC, Neumann-Kopp calculation	[92, 93]
Thermal conductivity, k_{SE} [W m^{-1} K^{-1}]	1.4	0.47	-	MTRM	[92, 97]
Activation energy, $E_{A,SE}$ [eV]	0.51	0.42	$0.39-0.52$	Arrhenius	[23, 60, 103]
Density, ρ_{SE} [g cm^{-3}]	2.68	$5.08-5.34$	$1.45-1.91$	PUS, Mass and length	[18, 92, 104]
Mechanical properties					
Young's modulus, E [GPa]	77	147-150	8.8-25	Nanoindentation, impulse excitation, DFT, USV	[18, 19, 104]
Poisson's ratio, ν [-]	0.25	0.26	$0.27-0.33$	Assumption, RUS, USV	[19, 104, 105]
Shear modulus, G*** [GPa]	31	$58-60$	$3.4-9.5$	USV	[18, 19, 104]
K/G-ratio [-]	1.66****	$1.59-1.74$	$1.88-2.58$****	DFT	[18]
Fracture toughness, K_c [MPa m$^{1/2}$]	-	1.25	0.23	Vickers indentation	[106, 107]
Hardness, H_v [GPa]	3.9	6.3	1.9	Vickers indentation	[19, 105, 107]

† The definition of these metrics, acronyms and symbols can be found in the List of Acronyms and Symbols.

* Measurement at room temperature

** The CCD of fluoroethylene carbonate (FEC)-based electrolyte solution is 2 mA cm^{-2} (1100 cycles).[66]

*** The shear modulus of Li metal is 4.25 GPa.[18]

**** Calculated in this work

2.1.3 Mechanical Properties

Elastic moduli. In solid mechanics, the material's elastic, plastic, and fracture behaviour can be described by the material's stress-strain relationship. From the stress-strain measurements, mechanical properties such as the elastic moduli, yield strength, ultimate tensile strength and ductility, can be inferred.[108] An elastic solid will return to its original shape and size after the forces deforming the solids are removed. This elastic behaviour can be described by the linear relationship between the applied stresses and strains. Depending on the directions of the applied forces, the elastic moduli can be described with the Young's modulus (E), shear modulus (G) or the bulk modulus (K).

The Young's modulus can be measured with the nano-indentation, acoustic impulse excitation technique, load frame tensile or compression testing or Resonant Ultrasound Spectroscopy (RUS).[18,19,38,105,107,109] Masias *et al.* measured the Young's modulus of polycrystalline Li with the pulse-echo acoustic method and showed that the bulk polycrystalline Li has a Young's modulus of 7.8 GPa.[38] Unlike the polycrystalline Li, the elastic moduli of a single crystal Li were shown to vary significantly with the crystallographic orientations due to the high Zener anisotropy factor, A, of the body-centred cubic Li ($A = 8.52$).[38,110] It is worth noting that an isotropic material has an A-value of 1.[18,38] A high anisotropy factor of the single crystal Li implies that the local mechanical properties of Li grain may differ significantly from grain to grain, which causes different propensity for the propagation of Li filaments.[110] By conducting micro-pillar compression experiments in an *operando* SEM, Xu *et al.*[110] showed that Li exhibits an E value of approximately 5 GPa in the [100] orientation, whereas the E value is around 20 GPa in the [111] orientation.

Due to variances in the experimental setup (*i.e.*, a load frame tensile testing with and without the extensometer), the reported Young's modulus of the polycrystalline Li varies significantly between $1.9 - 7.8$ GPa.[38] Besides, a clear differentiation should be made between engineering and true strain measurements when measuring the stress-strain relationship. The stress and strain calculated with the original cross-section areas are known as the engineering stress and strain. In contrast, the stress and strain calculated with the cross-sectional area's instantaneous change are denoted as the true stress and strain. Both measurements of the same sample can yield very different results, as shown by Masias *et al.*[38] in Figure 2.7a. Nevertheless, it should be noted that for compression testing, the true stress should be smaller than the engineering stress due to the increase in the cross-sectional area with compression. LePage and co-workers showed that the instantaneous change of a cross-sectional area could be measured with the glove-box integrated digital-image correlation (DIC) (Figure 2.7b), in order to determine the true stress and strain of bulk Li metal.[111]

Compared to Li metal, SEs such as LiPON and c-LLZO have a high Young's modulus of 77 GPa and 150 GPa respectively.[18,19] In contrast, sulfide-based SEs have a low Young's modulus of only

8.8 – 25 GPa.[104,107] A lower Young's modulus also corresponds to a lower shear modulus and therefore a weaker ability to suppress the Li filaments, according to the Monroe and Newman's linear elasticity analysis.[17] Yu and co-workers calculated the anisotropy ratio of c-LLZO and showed that Al- and Ta-doped c-LLZO have an anisotropy ratio of 1.27 and 1.32, respectively. Compared to the anisotropy ratio of Li metal, the elastic properties of c-LLZO can be considered as isotropic.[18]

The pioneering work by Monroe and Newman[17] proposed the linear elasticity analysis and derived the interfacial stability parameter from a modified Butler-Volmer (BV) equation. Suppose the total interfacial stability parameter is positive. In that case, the roughness of the Li electrode tends to cause an unstable deposition due to a faster deposition on the peaks of the deformed electrode surfaces than on the undeformed electrode surfaces. Therefore, a negative stability parameter favours a stable deposition. When the shear modulus of the SE is lower than twice the shear modulus of the Li electrode, the total interfacial stability parameter becomes positive, indicating a faster deposition of Li on the local peaks. As a result, they suggested that a SE should have a shear modulus at least two times larger than the shear modulus of Li metal to prevent the Li filaments initiation (Figure 2.6).[17]

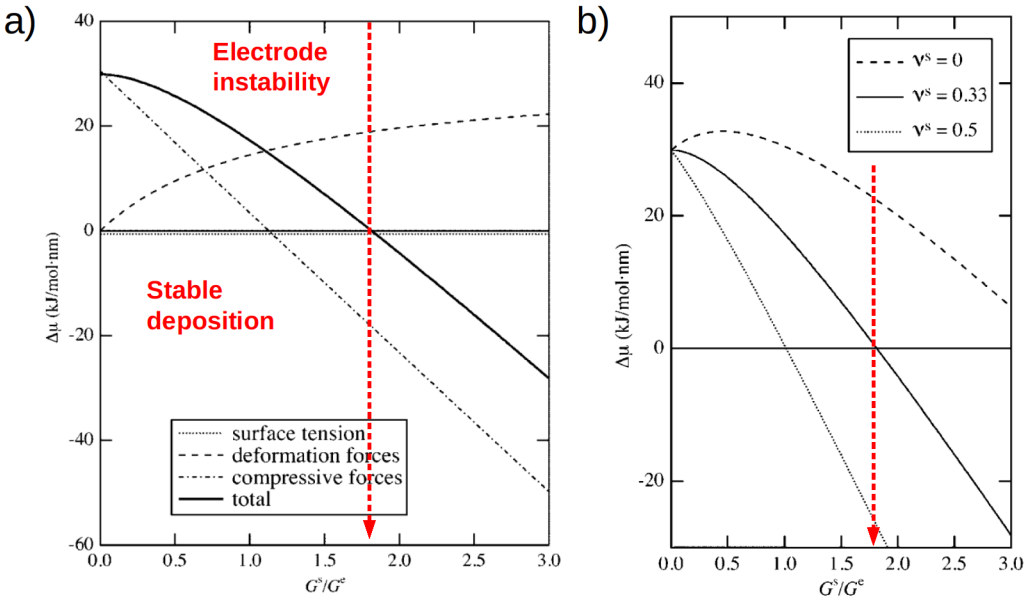


Figure 2.6 Interfacial stability criteria outlined in the Monroe-Newman model: a positive interfacial stability parameter indicates an unstable deposition, where the electrode roughness tends to amplify and the deposition rate on the peaks of deformed electrode surface would be greater than the undeformed surfaces. On the other hand, a negative interfacial stability parameter indicates a stable deposition, where the electrode roughness tends to decay and the deposition rate on the peaks of deformed electrode surface would be smaller than the undeformed surfaces. Reprinted with permission from Ref. 17, Copyright 2005, Elsevier.

The shear modulus of LiPON and c-LLZO are $7-14$ times larger than the shear modulus of Li respectively, whereas the LPS SE is just sufficiently compliant.[18,19,104] Yet, despite the high shear modulus of c-LLZO, the growth of Li filaments are still observable in c-LLZO.[15,112] Besides the shear modulus, the formation of Li filaments also depends on the critical plating and stripping current densities, grain morphologies of the SEs and the surface flaws.[23,26,31,65,113] Therefore, meeting Monroe's criterion should be a necessary criterion, but not an absolute sufficient condition to prevent an internal short-circuit.[17,18]

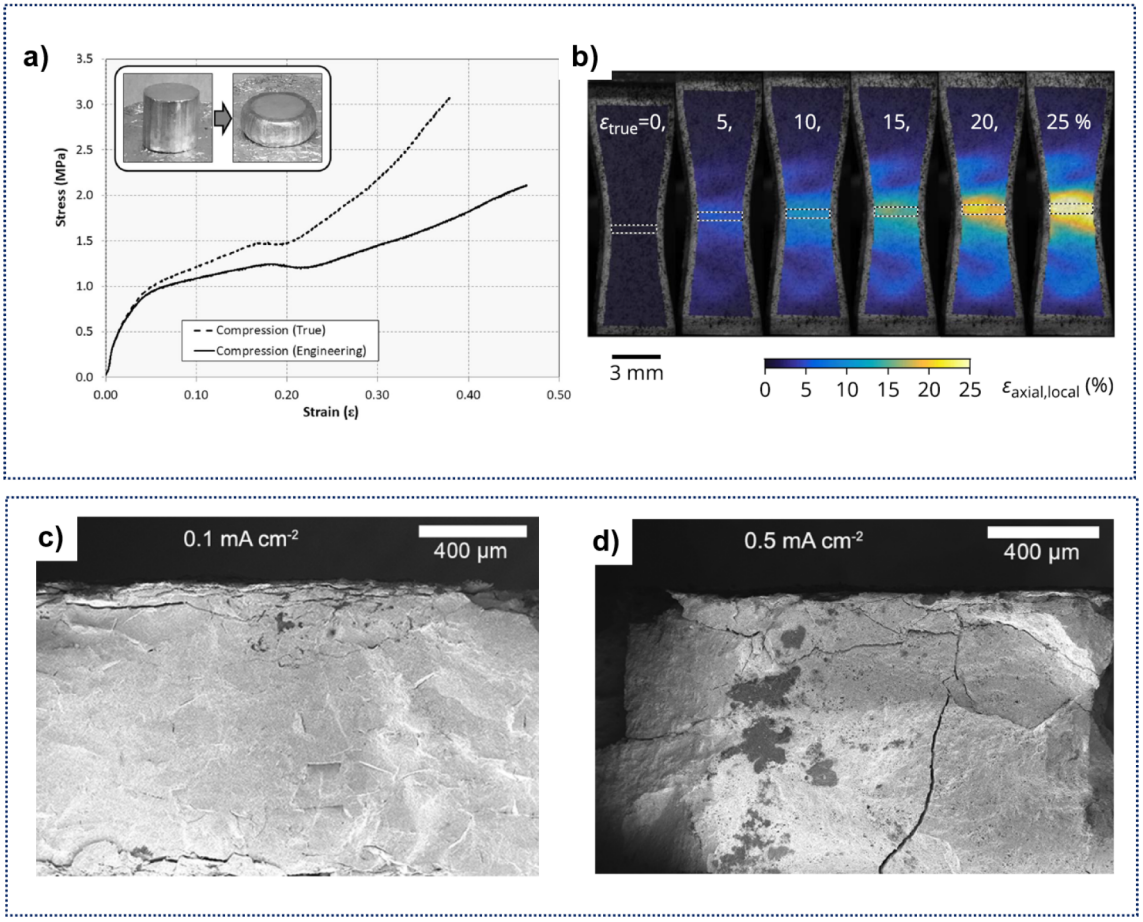


Figure 2.7 A contrast in the mechanical behaviour of a solid Li and a SE: A solid Li NE demonstrates a significant time-dependent deformation at room temperature under both (a) compressive (Reprinted with permission from Ref. 38, Copyright (2019), Springer) and (b) tensile testings (Reprinted with permission from Ref. 111, Copyright (2019), The Electrochemical Society). In Figure (b), the changes in the axial strain maps were obtained by using 3D digital image correlation.[111] Low-magnification cross-sectional Scanning Electron Microscopy (SEM) images of $Li_{1+x}Al_xGe_{2-x}(PO_4)_3$ (LAGP) cycled until failure at (c) $0.1\,mA\,cm^{-2}$ and (d) $0.5\,mA\,cm^{-2}$. Brittle cracks through the SE are observed at high current densities due to reaction processes at the LAGP|Li interface (Reprinted with permission from Ref. 33, Copyright 2019, American Chemical Society).

Plastic deformation. If the shear stress exceeds the critical shear stress in the slip plane and directions (*i.e.* a slip system with the largest Schmid factor), the lattice planes begin to slip, and an irreversible plastic deformation begins.

The Critical Resolved Shear Stress (CRSS) of metallic Li was shown to depend on the Li pillar diameters and temperatures.[110] Based on the micro-pillar compression measurements, Xu *et al.*[110] showed that the CRSS of Li decreases from about 30 MPa to about 6 MPa when the pillar diameters increase from 1 μm to 10 μm. These measurements imply that the deformation behaviour of Li filaments is highly dependent on the size of the filaments that form at the interface. They also showed that the CRSS decreases with increasing operating temperature. Li has a low melting point and a high homologous temperature (*i.e.* the ratio of absolute operating temperature to the absolute melting temperature). The homologous temperature of Li corresponds to 0.65 at 298.15 K and 0.8 at 363 K. Due to thermally activated processes such as cross-slip and dislocation climb, the dislocation movement is not limited to slip planes with the largest resolved shear stress when the homologous temperatures increase. Therefore, plastic deformation occurs more easily to induce more in-plane growth of Li, causing a smoother surface at the top of the deposit. As a result, they suggested that higher operating temperatures are more favourable in suppressing the Li filaments.[110] While a certain degree of plastic deformation is desirable to smoothen the local filament peaks, a high homologous temperature of Li also triggers Li creep (see Section 2.2.3).[38,111] An unrestrained creep could eventually cause an internal short-circuit against the PE.[38]

Compared to Li NE, a SE should exhibit minimal plastic deformation to withstand the propagation of Li filaments through the SE. The resistance of the SE to plastic deformation can be described by the parameter Vickers Hardness (H_v), and H_v was shown to decrease with increasing porosity.[105] For a volume fraction porosity of 0.03, c-LLZO has a H_v-value of $6.2-6.4$ GPa. As the volume fraction porosity increases to 0.06, the H_V-value decreases to $5.2-5.3$ GPa.[105] A SE with a higher porosity has more pores and less denser microstructures, which could cause more Li filaments to penetrate through the pores (see Figure 2.8). On the other hand, the LPS SE has a H_v-value of 1.9 GPa, which implies a lower resistance to plastic deformation compared to oxide-based SE.[107]

Fracture behaviour. The brittle nature of the ceramic-based SEs suggests that these SEs are more susceptible to cracks.[113,114] A crack will grow when the crack tip stresses exceed the critical stress threshold (fracture toughness, K_c).[114] In principle, K_c can vary depending on the crack mode (opening mode, sliding mode and tearing mode).[115] c-LLZO has a fracture toughness of 1.25 MPa $\mathrm{m}^{1/2}$, whereas LPS has a fracture toughness of 0.23 MPa $\mathrm{m}^{1/2}$.[106,107] A current collector made of aluminium has a fracture toughness of $25-35$ MPa $\mathrm{m}^{1/2}$.[18] A detailed discussion on the degradation mechanisms of electrode particles and SE cracking can be found in Section 2.2.1.

In contrast to the liquid electrolyte, which can penetrate through the pores and wet the solid electrodes, the problems of contact loss and voids are more apparent for a solid-solid interface.[26,116] Therefore, some degree of ductility is essential to maintain good interfacial contacts for a solid-state cell. The ratio of bulk modulus to the shear modulus (K/G)

indicates the ductile/brittle nature of a solid.[18,117] According to Pugh's criterion, the critical K/G ratio for a transition from brittle to ductile behaviour is 1.74.[18,117] This transition criterion was determined by grouping a wide range of brittle as well as ductile metals into groups according to their lattice structure and comparing their elongation percentage and Poisson's ratio at room temperature. A low K/G ratio corresponds to a brittle material, in which the stress concentration at the root of a crack will be high due to a negligible plastic flow.[117] c-LLZO has a K/G-ratio of $1.59-1.74$, which implies the brittle nature of the SE.[18] In contrast, the LPS SE has a K/G-ratio between $1.88-2.58$ (see Table 2.1), and the current collectors such as copper and aluminium have a K/G-ratio of 3 and 2.74 respectively.[117] Nevertheless, the mechanical properties of pure copper foils were also shown to depend on the thickness of the foils.[118] By investigating the effects of different thickness on mechanical properties of pure copper foil during cold rolling, Song *et al.*[118] showed that the ultimate strength of pure copper foil first increases from 310 MPa to 390 MPa when the foil thickness decreases from 300 μm to 100 μm. The further reduction of the foil thickness to 25 μm causes the ultimate strength to drop to 300 MPa due to the decrease in the dislocation density and micro-strain. Despite the high K/G ratios of copper, this experimental observation suggests that thinner copper foils are more brittle and susceptible to fracture and cracks.

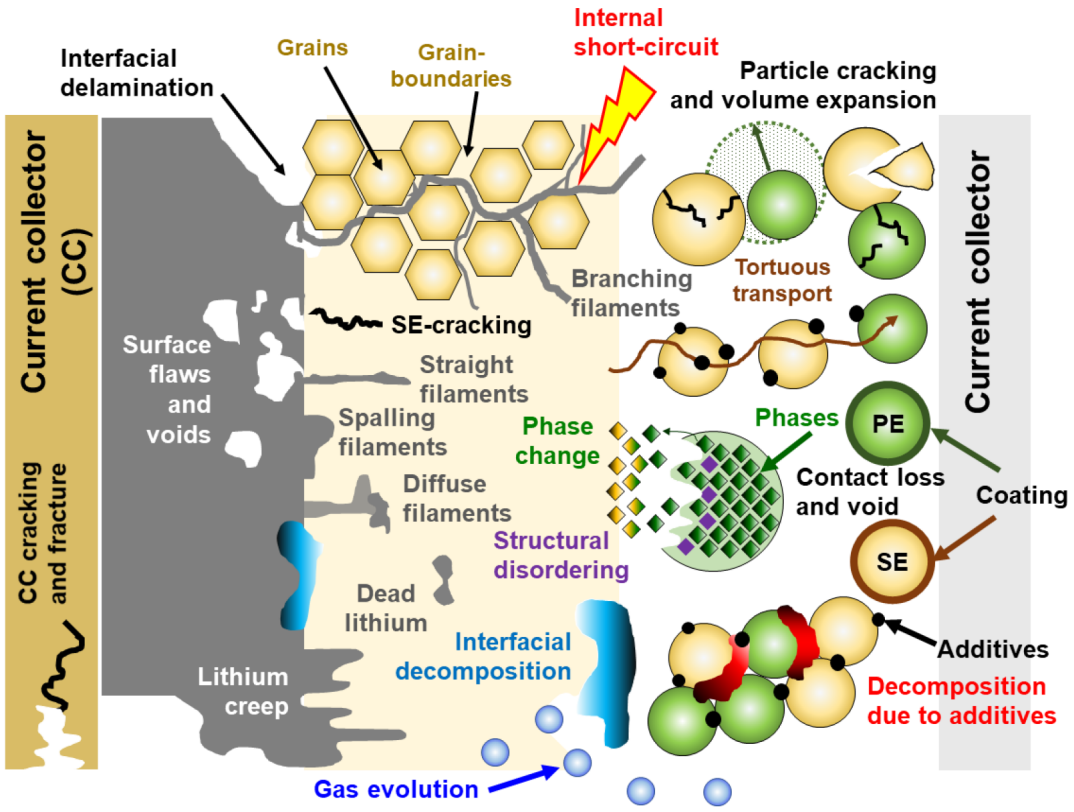


Figure 2.8 A summary of degradation mechanisms in a solid-state Li-metal cell, which include interfacial delamination, Li filaments propagation, surface voids and flaws, SE cracking, electrode particle cracking and volume expansion, tortuous transport, contact loss and void, interfacial decomposition, Li creep, decomposition due to additives, phase change, structural disordering, gas evolution, CC cracking and fracture.

2.2 Multiphysical degradation and failure modes

The complex interplay of different mechanisms in solid-state batteries induces various degradations and failure modes. For instance, although the addition of carbon black in the composite electrode improves electronic transport, it also causes an increase in the interfacial resistance and a faster capacity fade.[75,119,120] The irreversible capacity loss in solid-state batteries could also be caused by the formation of a passivating PE/electrolyte interface layer due to the decomposition of the electrolyte and the phase change/structural disordering of electrodes.[72,86,121] On the other hand, surface flaws and voids at the SE-NE interface can cause the nucleation of Li filaments and reduce the lifespan of solid-state batteries as a result of an internal short-circuit.[26,113,114] While the multiphysical properties of different cell components are discussed in Section 2.1, the degradation and failure mechanisms are analysed in this Section. The effects of different operating conditions on the solid-state battery degradation are also listed in Table 2.2. Many efforts have been made using experiments to understand the degradation of solid-state batteries. By coupling experimental observations with models, it is hoped that a clearer understanding of degradation can be achieved. The

development of *in-situ* techniques, such as *in-situ* XPS, Raman and Scanning Transmission Electron Microscopy (STEM), are being developed for characterisation of often-buried and air-sensitive interfaces. Table 2.3 summarises the experimental tools and techniques used for characterising degradation and referred to throughout this review.

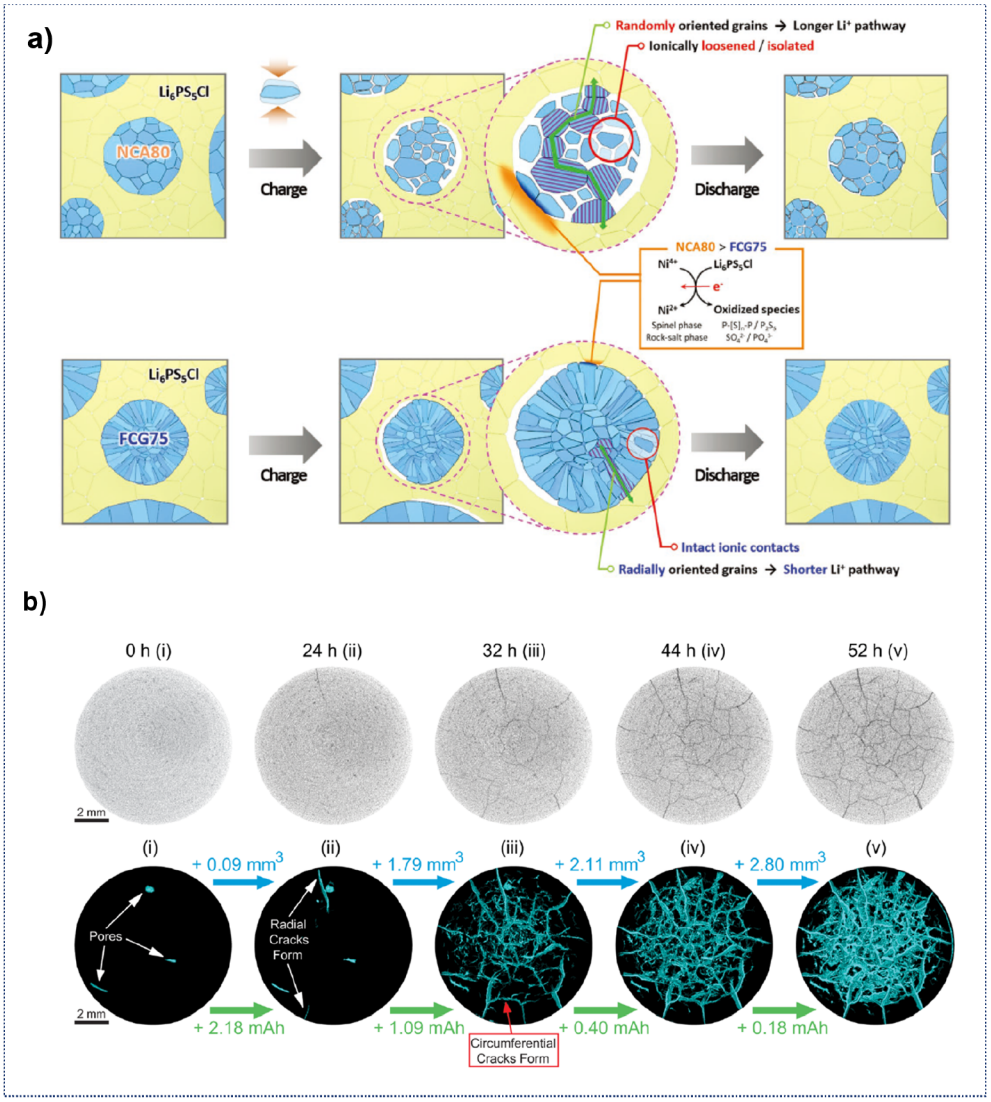


Figure 2.9 (a) Schematic depiction of the structural evolution in the NCA80 and FCG75 PE in all-solid-state cells. Reprinted with permission from Ref. 122, Copyright (2020), John Wiley and Sons. (b) *Operando* X-ray Tomography (XCT) observations of the crack formation within the LAGP SE. Reprinted with permission from Ref. 37, Copyright (2019), American Chemical Society.

2.2.1 Mechanical stresses

Due to the brittle nature of the inorganic SEs (see Table 2.1), as well as the rigid contact between the electrodes and the electrolyte, the accumulation of mechanical stresses in solid-state cells cause a more severe performance drop compared to liquid electrolytes. The propagation of stresses causes particle cracking, which eventually impedes ionic mobility and increases cell resistance.

2.2.1.1 Lithiation-induced stresses

The diffusion of Li-ions into and from the electrode host materials generates volume change.[123,124] This structural and morphological evolution can give rise to mechanical stress accumulation and significantly influence the cell performance.

Negative electrodes. The degradation mechanism of an intercalation electrode and a composite NE is different from that of a NE composed of pure metallic Li. A composite NE denotes an electrode composed of SE and NE (see Figure 2.14(c2)). The ionic diffusion in the electrode host, such as graphite, was shown to cause a structural change, as shown by Otoyama *et al.*[125] They employed *operando* confocal microscopy to observe the dynamic thickness evolution of graphite-based solid-state cells. During cycling, the graphite underwent irreversible volume change, and the thickness of the graphite layer increases due to the formation of voids and cracks, which cause the capacity to decay. Significant volume change was also reported in Si-based solid-state cells. Chen *et al.*[126] employed an *operando* NDP method to investigate the degradation of thin-film Si-Li_3PO_4-LCO cells. They demonstrated that the Si electrodes underwent a significant volume change during cycling that resulted in the penetration of the SE. Bucci *et al.*[127] proposed a coupled electrochemical-mechanical model based on the cohesive zone formulation to investigate the intercalation-induced stresses in the composite NE. By assuming Young's modulus of 15 GPa, the model predicted that the fracture could be prevented if the electrode particle's expansion is lower than 7.5% and the SE fracture energy is higher than $4\,J\,m^{-2}$.

Positive electrodes. The lithiation and (de)lithiation in the composite PE also causes a volume expansion and contraction, which introduces internal stresses. These stresses lead to the formation of cracks in both AMs and SEs to affect the cell integrity and lead to a severe increase in the interfacial resistance (Table 2.2). Liu *et al.*[128] revealed that the large volume change of LCO during cycling creates cracks in the electrodes of LCO/LLZ-Ta. As a result, the accumulated cracks disrupt the ionic diffusion path, causing an increase in the cell resistance leading to degradation.[128] The anisotropic plane orientations of the PE could also cause the formation of the concentrated stress within the particles. Jung *et al.*[122] investigated the volume change of $LiNi_{0.8}Co_{0.16}Al_{0.04}O_2$ (NCA-80) with randomly oriented grains in Li_6PS_5Cl based cells. They demonstrated that the anisotropic volume changes of primary particles in NCA-80 collectively cause the severe cracking of secondary particles (Figure 2.9a). However, in the $Li(Ni_{0.75}Co_{0.10}Mn_{0.15})O_2$ with radially oriented rod-shaped grains, the volume change and stress can be accommodated, resulting in mechanical integrity and cycle stability.[122]

In terms of physical modelling, Behrou and Maute[129] proposed an electrochemical-mechanical model, which describes diffusion-induced mechanical stresses in the PE. By modelling the

electrode diffusion as a function of the damage parameter, they showed that damage evolution in the PE causes the cell's capacity to fade during discharge.

2.2.1.2 Solid electrolyte cracking

Cracks can be formed in the SEs during cycling due to the interfacial decomposition or the growth of Li filaments.

NASICON-type Li conductors (general composition: $Li_{1+x-y}Al^{3+}_{x}M^{5+}_{y}M^{4+}_{2-x-y}(PO_4)_3$, where M^{4+} and M^{5+} are metal ions such as Ge^{4+} or Ti^{5+}) are unstable in contact with Li metal.[130] The electrolyte decomposes to form a new interface (a mixed ionic-electronic conducting interphase) between the electrolyte and the Li metal.[131] For example, Tippens *et al.*[37] investigated the evolution of mechanical damage within LAGP by *operando* X-ray Tomography (XCT) (see Figure 2.9b). The growth of a decompositon interphase with expanded volume introduce stresses on the electrolyte, resulting in the crack formation. The continuous reaction-driven degradation, rather than the interphase formation itself, was claimed to be the main cause for the observed increase in impedance.[53] Wu and co-workers[132] monitored the morphological dynamics in LPS by Synchrotron Radiation X-ray Tomographic Microscopy (SRXTM). They showed that horizontal cracks within the LPS electrolytes could be observed, which impede the Li-ion mobility, thus increasing the cell resistance.

The growth of Li filaments within the electrolytes also introduce severe localised stresses during cycling. Porz *et al.*[113] studied the Li deposition on four different SEs (LPS, β-Li_3PS_4, polycrystalline and single-crystalline LLZTO garnet) and showed that Li plating in pre-existing flaws would produce crack-tip stresses, which drive crack propagation in the SEs. Li *et al.*[133] directly observed the Li filament growth in LLZTO at the microscale by using *in-situ* NDP. The large volume changes due to Li plating and the mechanical stress would accelerate the crack propagation within LLZTO. However, they found that a well-designed 3D framework of the NE can accommodate the huge volume expansion during Li plating and regulate the Li deposition behaviour to inhibit Li filaments growth.[133] Klinsmann and colleagues[134] demonstrated *via* modelling that the insertion of Li filaments into pre-existing electrolyte cracks lead to increased pressure, which would lead to further cracking and finally, an internal short-circuit (Figure 2.10a).

2.2.2 Phase change and structural disorder

Many electrodes undergo phase changes during lithiation and de-lithiation, aggravated in solid-state cells due to the sluggish diffusion. Xia *et al.*[135] demonstrated that disordered LMO would form during cycling in LiPON-based thin-film cells. The formation of disordered LMO could reduce the accessible capacity and increase cell resistance. Subsequently, they developed

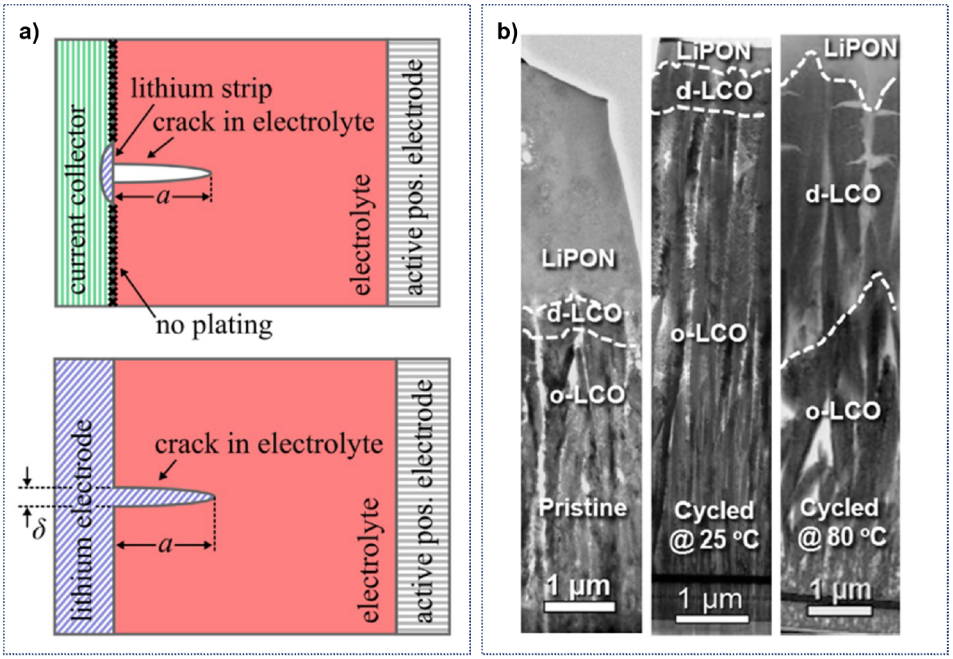


Figure 2.10 (a) A SE analytical model predicts the stress propagation due to the growth of Li filaments. Reprinted with permission from Ref. 134, Copyright (2019), Elsevier. (b) The formation of disordered phases between LCO and LiPON. Reprinted with permission from Ref. 86, Copyright (2016), Elsevier.

a 3-dimensional LMO electrode with a vertically aligned nano-wall array architecture, which increases the contact area at the interface and mitigates the formation of disordered LMO.[135] In another study, Jung *et al.*[122] monitored the phase evolution of $FeS_2/Li_7P_3S_{11}$ cells by using *operando* synchrotron X-ray nanotomography. They showed that the pristine FeS_2 phase transforms into the Fe phase, which subsequently penetrates the particle, resulting in a large volume expansion and cracking.[122]

High operating temperatures, overcharge and overdischarge could accelerate the phase changes in electrodes.[86,136,137] Wang *et al.*[86] used *in-situ* STEM coupled with Electron Energy Loss Spectroscopy (EELS) to elucidate the structural evolution in LCO/LiPON cells under different operating temperatures. As shown by Figure 2.10b, when cycled at 80 °C, LCO decomposed into disordered rocksalt phase comprising of cobalt oxide, Li_2O and Li_2O_2. The disordered LCO interphase consumed the AMs and increased the interfacial resistance, reducing the overall capacity and cycle life.[86] In addition, over-delithiation in overcharged batteries is reported to cause the phase transition and structural distortion of PEs in liquid electrolytes.[138–140] During deep overdischarge processes, overlithiation can also trigger phase changes and destroy the host structure.[141,142] It was also found that a severe phase change and structure disordering under high potential in Ni-rich NMC PE would accelerate the gas release (O_2) from the NMC lattice.[143,144]

2.2.3 Creep behaviour of Li metal

The unique mechanical properties (elastic, plastic and creep properties) of Li metal greatly influence its dynamic evolution during cycling under different operating conditions. The term creep describes the material behaviour to exhibit continuing deformation even though the stress is held constant.[115] The creep characteristics can be divided into three regions: primary creep, in which the material hardens and the creep-rate diminishes with time; secondary creep or steady-state creep, in which the hardening and softening mechanisms counteract to cause a constant creep rate; and tertiary creep, where the material softens until creep failure occurs.[115]

Although the permanent plastic deformation usually occurs above the yield strength, deformation can also occur below the yield strength for metallic Li.[38,111] Due to the high homologous temperature of Li, Li exhibits temperature, strain-rate, and pressure-dependent creep behaviour.[111] Therefore, the deformation of Li at stresses below the yield strength is caused by both elastic and creep strains.[111] Although the creep behaviour of Li metal is aggravated under high operating temperature, creep was also observed to be the dominant deformation mechanism over a wide range of temperature conditions (248 K - 398 K).[111] While a high external stack pressure such as 5 MPa is necessary to reduce voids and interfacial contact losses (see Section 2.2.5), Li creeps through the pores and grain boundaries of the SE to induce the propagation of Li filament if the stack pressure becomes too high. Doux *et al.*[145] showed that the cell shorted mechanically before cycling began when a high stack pressure of 75 MPa was applied. The problem of Li creep becomes more critical if the relative density of the SE is low and the porosity of the SE is high.[145] Under high external pressure, Li creeps and flows through the pores and grain boundaries of the SE, forming an electronic percolation between the NE and the PE to cause an eventual internal short-circuit.[145,146] Due to the low yield strength of polycrystalline bulk Li metal (0.6 MPa - 0.8 MPa),[38] a low stack pressure such as 5 MPa could already trigger the Li creep behaviour.[145] However, as discussed in Section 2.1.3, it should be noted that the local mechanical properties of Li metal such as the CRSS and yield strength can be very different from that of the bulk polycrystalline Li metal.[110] Although the external stack pressure is higher than the yield strength of the bulk polycrystalline Li metal, the difference between the local and bulk mechanical properties of Li metal may account for the stability of Li metal under the DC cycling with an external stack pressure of 5 MPa.

2.2.4 Electrode-electrolyte interfacial decomposition

In contrast to the widely-perceived idea of excellent stability of SEs,[51,147] most of the SEs studied have a limited intrinsic electrochemical stability and are predicted to form thermodynamically favourable decomposition interphases either at low or high potentials (see Figure 2.11f).[72,73] In this section, the interfacial decompositions at the NE-SE interface, SE-PE interface and the

decomposition due to carbon additives are briefly described. The reader is directed to other, more comprehensive reviews on the topic of interfaces in all-solid-state batteries.[51–53]

2.2.4.1 Negative electrode - solid electrolyte interface

Although the use of Li metal as the NE could improve the energy density in solid-state cells, its strong reduction potential can cause interfacial reactions at the electrode-electrolyte interface.[130] In principle, there are three different types of interfaces classified as (1) interphase layers of mixed ionic and electronic conductors (MCIs), (2) stable interfaces with negligible decomposition, and (3) ionically conductive but electronically insulating interphase layers.[73,130]

In contrast to the second and third types of interface, MCI is unstable (both thermodynamically and kinetically). In this type of interface, both Li and electronic conductivity lead to continuous decomposition reactions at the electrode-electrolyte interface.[130] For example, amongst the NASICON-type SEs, all members of this class are unstable in contact with Li metal. As shown by Figure 2.11b, the high valent state ions Ti^{4+} and Ge^{4+} can be reduced by Li metal to form a degradation interfacial layer, which decreases the Coulombic efficiency, increase the impedance and cause a capacity decay.[33,73,148,149] The decomposition interface layer comprises a mixture of Li_2O, Li_2O_2, Li_2CO_3 and the electronically conductive Ti^{3+} and Li-Ge alloy, which demonstrated mixed electronic and ionic conductivity.[73,149] LGPS can also form an MCI in contact with Li metal. The decomposition of LGPS leads to the formation of an interface composed of Li_2S, Li_3P and Li−Ge alloy, leading to a further continuous detrimental decomposition of the SE owing to the mixed electronic-ionic conductivity of the interphase formed.[150]

In the second type of interface (*e.g.*, stable interfaces with negligible decomposition), the SEs are thermodynamically and kinetically stable during cycling. However, due to the limited electrochemical window and the compatibility of the electrolyte/electrode interfaces, it is unrealistic to develop an intrinsically stable interface without decomposition over the entire cycling voltage range.[130] For example, c-LLZO is reported to have excellent stability against Li metal. Instead of triggering interfacial decomposition, the surface of cubic c-LLZO is slightly lithiated and undergoes a phase transition to its tetragonal phase (less than five cubic c-LLZO unit cells thick) when contacting the Li electrode (see Figure 2.11a).[151]

As for the third ionically conductive but electronically insulating interface, decomposition happens spontaneously but not continuously as in the MCI interface. Once formed, the electrochemically insulating interphase layer passivates the electrolyte interface and remains stable during further electrochemical cycling.[130] When LiPON is exposed to Li metal, a chemical reaction occurs and LiPON decomposes to form an interphase consisting of Li_3PO_4, Li_3P, Li_3N and Li_2O.[152] However, the reaction is intermittent, and the disrupted LiPON interface region is thin enough to allow the continuous migration of Li-ions, as well as being poorly electronically conducting. This characteristic demonstrates the high cycling stability of

solid-state cells using LiPON, caused by the formation of this kinetically-stabilising layer.[153–155]

Table 2.2 Solid-state cell degradation mechanisms: The effects of operating conditions, causes and consequences

Degradation mechanisms	High SOC	Low SOC	High temp	Low* temp	High C-rate	Low stack pressure	Causes	Consequences	Ref.
Electrodes and SE cracking							• Volume change of the AMs during charge/discharge; • Interfacial reactions and the resulting growth of decomposition layers; • Propagation of Li filaments through the SE.	• Disruption of the ionic diffusion path; • Contact loss between electrodes and the SE; • Increase in the interfacial resistance; • Decrease in the mechanical strength of the SE; • Faster and easier propagation of Li filaments.	[37, 128, 131, 132]
Phase change and structural disordering							• Sluggish ionic diffusion due to poor interfacial contacts; • Transition metal dissolution at the PE and SE interface.	• Capacity decay due to the loss of the AM; • Disordered/rock-salt phases between electrodes and the SE; • Increase in the interfacial resistance.	[86, 128, 156]
Li creep							• High homologous temperature of Li metal.	• Severe deformation and volume change of the NE; • Higher risk of internal short-circuit.	[38, 111, 157, 158]
Interfacial decomposition							• Limited chemical stability of the SE towards Li metal or high voltage transition metal oxide PE; • Carbon additives accelerate the decomposition of the SE.	• The growth of the decomposition layers increases the interfacial resistance; • Loss of the AMs decreases the capacity; • Produce localised pressure to trigger the formation of cracks in SE.	[33, 37, 86, 88, 148]
Surface voids and interfacial delaminations							• Voids or defects produced during materials processing; • Rigid contact between the electrodes and SE; • Volume change of the AMs during charge/discharge; • Li plating/stripping exceeding CCD.	• Poor contact causes insufficient ion diffusion and limits the rate performances; • Localised high current and pressure accelerate the growth of Li filaments.	[26, 116, 146, 159, 160]
Li filamentary growth							• Voids and flaws on the surface of SE trigger the heterogeneous diffusion of Li-ion; • Localized high current at the grain boundaries of SE; • Reduction of Li^+ within the SE due to high electronic conductivity of the SE.	• Internal short-circuit.	[23, 26, 30, 31, 145, 161]

*A low temperature in this table also includes the room temperature.

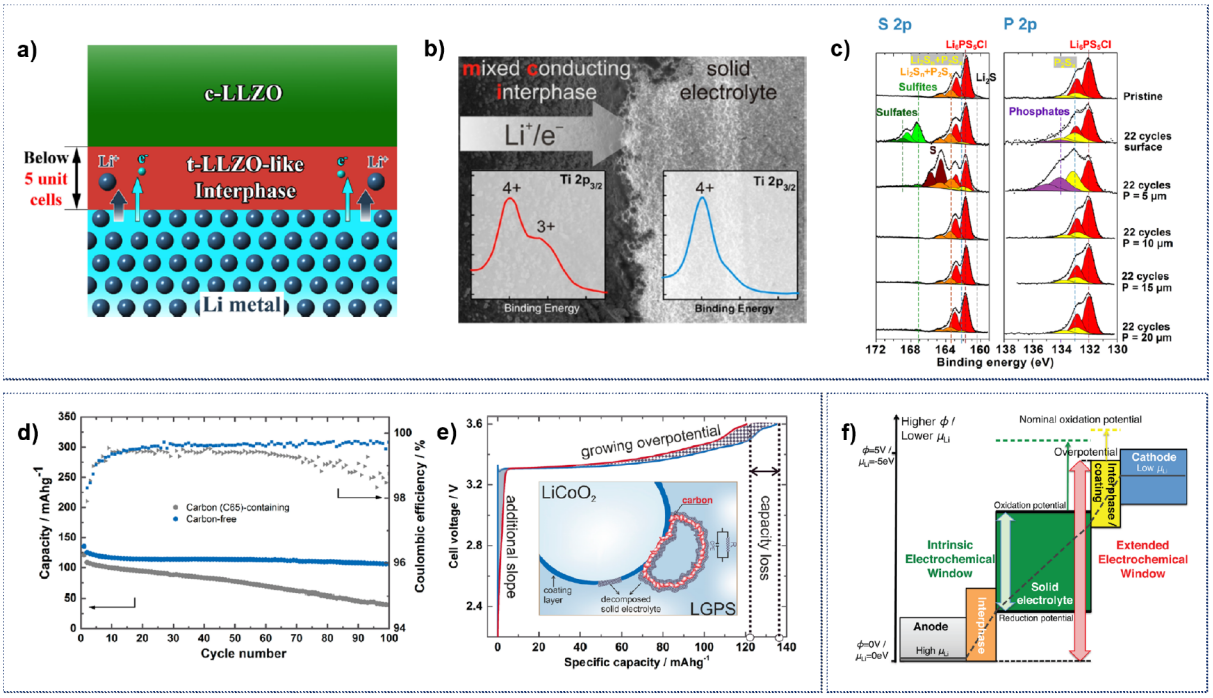


Figure 2.11 (a) The formation of the t-c-LLZO-like interface (Reprinted with permission from Ref. 151, Copyright (2016), American Chemical Society). (b) The reduction of Ti^{4+} to Ti^{3+} in the NASICON-type SEs and the resulting formation of the MCIs. Reprinted with permission from Ref. 149, Copyright (2013), American Chemical Society. (c) Interfacial stability of Li_6PS_5Cl toward NMC333. Reprinted with permission from Ref. 162, Copyright (2017), American Chemical Society. (d) Cycling performances with and without carbon additive in an all-solid-state cell consists of LGPS and LCO. (e) Illustration of the decomposition interaction between LCO and LGPS. Reprinted with permission from Ref. 119, Copyright (2017), American Chemical Society. (f) DFT calculation of the electrochemical and chemical stability of the SEs. Reprinted with permission from Ref. 72, Copyright (2015), American Chemical Society.†

Although the exact nature of the reaction products at the interface is difficult to predict, due to the interplay of thermodynamic and kinetic factors, computational methods have been useful in determining possible decomposition pathways, revealing trends in chemical reactivity, providing limits for electrochemical stability windows and guiding engineering of interfaces.[53] Three approaches have been adopted to evaluate the electrode-electrolyte interactions using first-principles methods: (1) electrochemical stability, (2) topotactic stability which provides the maximum voltage limits or widest electrochemical stability window in which there is maximum kinetic stabilisation and (3) chemical mixing reactivity.[53,72–74,74,163,164] The topotactic stability refers to a form of intercalation which is accompanied by a phase change, for example, Li insertion into the monoclinic binary MnP_4 phase to form a cubic ternary Li_7MnP_4 phase.[165] Explicit interface calculations assess energetics of interfacial species directly by using DFT on supercells. A structural-relaxation method optimises the atomic coordinates at the interface but cannot account for any activated processes, such as atomic diffusion or the nucleation of new solids.[53] This type of simulation has a high computational

† Link: https://pubs.acs.org/doi/10.1021/acsami.5b07517; Further permissions related to this material[72] excerpted should be directed to the ACS.

cost and typically only captures the dynamics of the system at elevated temperatures and limited time scales (< 1 ns).[25,29,53]

Engineering of Li/SE interfaces has been pursued in the community in order to mitigate the aforementioned interfacial effects.[166] For example, alloying of the Li NE has been explored, both to improve the Li diffusion coefficient (*e.g.* the Mg-Li alloy studied by Krauskopf *et al.*[167]), and to improve the chemical stability for the interface, such as Li-In used with thiophosphate-based electrolytes.[23,167,168] In the latter case, the Li-In alloy acts to raise the voltage of the NE material and reduce the volumetric strain on the metal.[168] Requirements for interlayer coatings include chemical and electrochemical stability with both the SE and electrode over the voltage range for the relevant electrode.[25,29,53,169] Introduction of artificial SEI through physical,[153,170] chemical[171] and electrochemical methods[172] is also an effective strategy to minimise the side reactions between Li metal and SE. Examples include the use of interlayers to act either as buffer layers preventing the reduction of SEs by alkali metals or used as mediators to improve wetting between two phases and subsequently lead to a reduction in Li filaments formation. For example, the use of binary layers such as LiF, Li_2O, Li_2S, Li_3N and Li_3P have been used as protective layers because of their intrinsic stability against Li metal.[25,29,173–175]

2.2.4.2 Solid electrolyte - positive electrode interface

Due to the strong oxidation of the transition metal species under high potential in the charged state, the interface between the PE and the SE is more complicated. The interactions between PEs and SEs include mutual diffusion of elements and the resulting phase change, the decomposition of electrolytes and growth of interphase. Sakuda *et al.*[176] studied the LCO/LPS interface using TEM and EDX. By using EDX mapping, they confirmed the mutual diffusion of Co, P, and S elements on the interface. High-resolution TEM results further revealed the growth of an interfacial layer between LCO and LPS after the initial charge process.[176] Park *et al.*[156] investigated the elemental diffusion on the LCO/c-LLZO surface by Time of Flight - Secondary Ion Mass Spectrometry (ToF-SIMS). Three-dimensional elemental distribution revealed that Co migrated into the c-LLZO while the La/Zr migrated to the LCO PE during high temperature processing. The resulting formation of the tetragonal c-LLZO phase at the SE/PE interface, therefore, deteriorated the electrochemical properties.[156]

In high performance batteries, layered PEs such as NMC and NCA have attracted great interest due to their high capacity. However, solid-state batteries using NMC or NCA PEs show a low Coulombic efficiency and a poor cycle stability.[162,177,178] In addition to the mechanical volume changes and resulting particle cracking and contact-loss (as discussed in Section 2.2.1.1), the interfacial side reactions and the growth of decomposition layer could also cause severe performance degradation. Koerver *et al.*[177] investigated the stability of thiophosphate-based

SEs (Li_3PS_4) against NMC-811. The results of *in-situ* XPS indicate the polymerisation and possible formation of $Li_2P_2S_6$, $Li_4P_2S_7$ and $Li_4P_2S_8$.

The argyrodite electrolyte, Li_6PS_5Cl, has been reported to possess a high ionic conductivity and an ease of processing. Auvergniot *et al.*[162] studied the interfacial stability of Li_6PS_5Cl against NMC-333, LMO and LCO by using Auger electron spectroscopy and XPS. Li_6PS_5Cl was oxidised to form elemental sulfur, Li polysulfides, phosphates, LiCl and P_2S_x ($x > 5$) (see Figure 2.11c). By using ToF-SIMS, Walther *et al.*[178] observed the interfacial decomposition of NMC-622/Li_6PS_5Cl. A Cathode Electrolyte Interphase (CEI) layer of at most 10 nm thickness was observed to have formed by the interfacial reaction between NMC-622 and Li_6PS_5Cl electrolyte. This CEI layer consisted of phosphate- and sulfate like species.[178] Surface coating of the PE materials with different protecting layers, such as $LiNbO_3$,[179,180] Al_2O_3,[181] Li_3PO_4,[182] and $Li_{3-x}B_{1-x}C_xO_3$, was shown to effectively reduce the side reactions.[183]

2.2.4.3 Instability of carbon additives

Composite electrodes of solid-state batteries typically consist of AMs, SEs, and carbon additives such as acetylene black. The electronically conductive carbon additives were shown to have both have positive and negative impacts on the rate performances and lifespan of solid-state batteries. Mizuno *et al.*[184] proposed that the addition of acetylene black was effective in decreasing the resistance of the LCO/LPS based solid-state cells. Many factors such as component proportion, morphology and specific surface of the carbon additives could affect the battery performances. Vapour-grown carbon fibre[185,186] and multiwalled-carbon-nanotubes[187] were found to enhance the capacity by constructing a continuous and long-range conducting path for electronic diffusion. Strauss *et al.*[188] investigated the specific surface of carbon additive and the relative battery performance. They showed that low BET surface material such as Super C65 carbon black could enhance the cyclability of NMC-622/thiophosphate-based bulk type solid-state cells compared to Ketjenblack and carbon nanofibers with a higher specific surface.[188]

While conductive carbon additives improve the kinetics and rate capacity, side reactions such as electrolyte decomposition also occur and cause cell degradation (Table 2.2). Oh *et al.*[189] investigated the interfacial phenomena between the $LiNi_{0.5}Mn_{1.5}O_4$ PEs and a sulfide electrolyte (LGPS). According to their research, electrochemical decompositions of LGPS continuously occur at the LGPS/acetylene black interface above 4.5 V (vs. Li/Li^+) that cause an irreversible capacity loss.[189] A similar interfacial issue was also found in LCO/LGPS based solid-state batteries, in which both acetylene black and Super P were shown to aggravate the oxidation of LGPS by forming inactive species on the electrode/electrolyte interface.[119] The inclusion of carbon additives was shown to produce faster electronic percolation paths in a composite PE. In the case of LGPS SE, carbon facilitates the oxidation from S^{2-} to S^0

(insulating polysulfides), which accumulate at the interface and isolates the Li^+ conduction pathway (see Figure 2.11d and Figure 2.11e).[119] A limited ionic transport in the composite PE ultimately causes an increasing interfacial resistance and a faster capacity fade.[119,190] Therefore, the development of more suitable carbon additives with an optimum balance between improving the rate performance and causing minimum degradation impacts are crucial to enhance the overall cell performances in different solid-state batteries.

2.2.5 Surface voids and interfacial delamination

The rigid nature of the SE and the low wettability at both interfaces have been identified as primary reasons causing the formation of voids during the fabrication of cells (Figure 2.12a).[25,191] Besides the pre-existing surface flaws, voids could form in *operando* under high current densities during the Li stripping process.[26] Figure 2.12 illustrates the mechanisms of voids formation at the SE-NE interface. If the applied current densities exceed CCD, the initial interfacial voids lead to the formation of occluded voids and the increase of contact loss after further stripping and plating (Figure 2.12b).[26]

Han *et al.*[25] studied the interfacial resistance of the $Li_7La_{2.75}Ca_{0.25}Zr_{1.75}Nb_{0.25}O_{12}$ (LLCZN)/Li metal electrode interface. The voids between the Li metal and the SEs were shown to reduce the surface contact and increase the resistance, creating a build-up of the overpotential and a drop in the cycle life.[25] In addition to the poor contact, the flaws and voids at the interface also act as active sites, where localised high current density and mechanical pressure initiate, triggering the growth of Li filaments and short-circuit problems. For bulk SEs, microstructural features such as pores and grain boundaries cause an inhomogeneous contact at the interfaces and within the SE (Figure 2.12e).[32] As a result, the rate of Li migration across the SE becomes non-uniform, which further promotes the nucleation of Li filaments.[22,23,32]

Based on the linear-elastic fracture mechanics

$$\sigma_{\mathrm{st}} \geqslant \frac{K_{\mathrm{Ic}}}{\gamma\sqrt{\pi a_{\mathrm{c}}}}, \tag{2.7}$$

where γ is the geometric factor of the surface crack shape and a_c is the flaw size, Porz *et al.*[113] developed an analytical model to study the effects of surface flaws on the Li electrodeposition in the SEs. Due to a lower surface overpotential, they showed that Li deposits preferentially in the pores and cracks of the SE. In the presence of pre-existing flaws, they showed that the critical overpotential threshold is low for cracks to propagate in the SE. However, Swamy *et al.*[114] showed later that Li filaments initiate favourably at the edges of the working electrodes, even when more significant surface defects are present near the edges. By correlating the optical microscopy observations with an electrochemical model, they showed that a stronger electric field causes the preferential initiation of Li filaments at the working electrode perimeters.

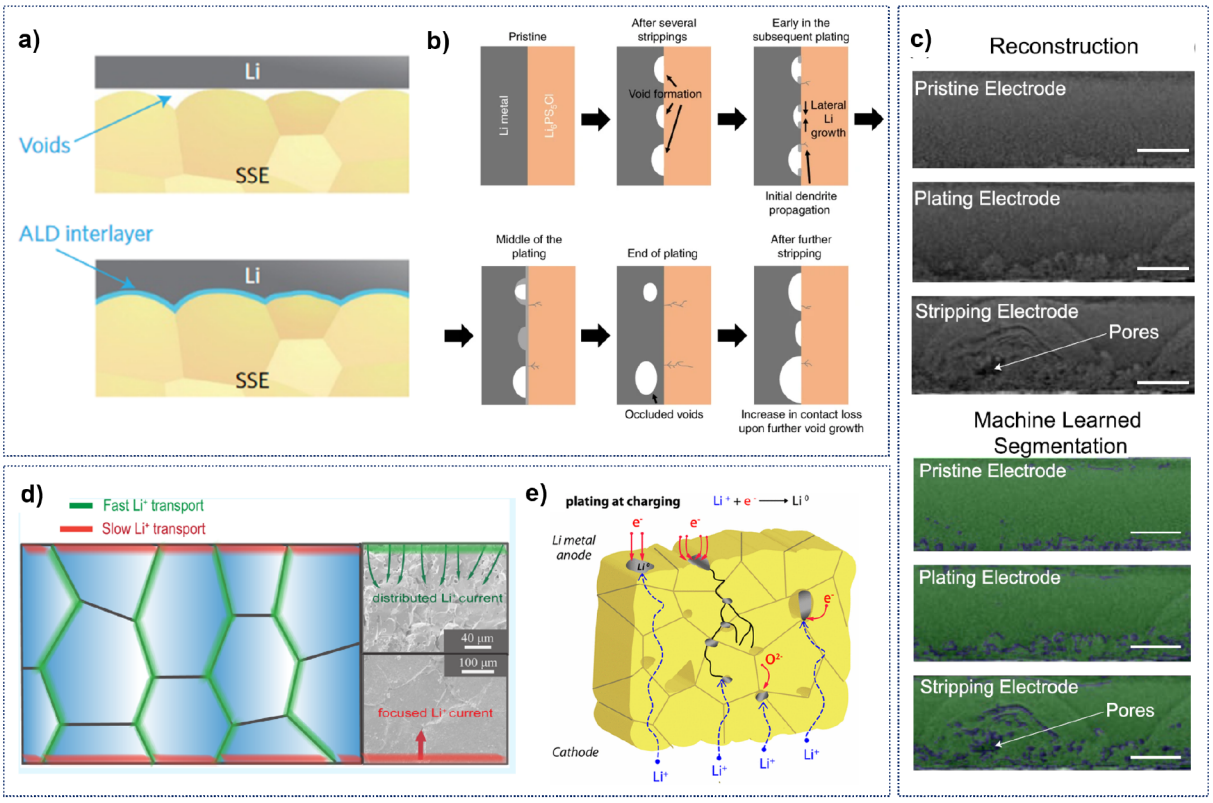


Figure 2.12 (a) Illustration of voids formation due to processing (Reprinted with permission from Ref. 25, Copyright (2017), Nature Materials) and (b) during electrochemical stripping and plating above CCD. Reprinted with permission from Ref. 26, Copyright (2019), Nature Materials. (c) A combined *In-situ* tomography imaging technique with machine learning computational method to track pores formation at the Li|SE interface. Deep convolution neural networks were trained on 800 images from one electrode and tested on additional 200 images from the same electrode to achieve a high confidence segmented image. Reprinted with permission from Ref. 192, Copyright (2020), American Chemical Society. (d) Grain orientations and grain boundary distribution within c-LLZO. (Reprinted with permission from Ref. 22, Copyright (2015), American Chemical Society) (e) The reduction of the Li^+ to Li_0 owing to the electronic conductivity of the SEs (Reprinted with permission from Ref. 32, Copyright (2017), American Chemical Society).

Tian and Qi[116] modelled the effects of imperfect contact areas in the film- and bulk-type solid-state cells. The exchange current density at the PE interface was modified to include a contact factor ($\gamma_c = A_{\text{imp}}/A_0$), where A_{imp} is the imperfect contact area and A_0 is the perfect contact area. They showed that the contact area loss causes local Li concentration accumulation at the interface and reduces the cell's accessible capacity. In another study, using the cohesive theory of fracture, Bucci *et al.*[39] formulated an analytical model to investigate the delamination of the electrode from the electrolyte. If the yield stress of the SE is lower than the interfacial cohesive strength, the plastic deformation of the SE occurs, which can prevent the delamination. Recently, Dixit *et al.*[192] used monochromatic, high-energy X-rays to capture low-density phases (voids and Li metal) in a Li|LLZO|Li model system. As quantification of the microstructural properties requires consistent segmentation procedures and the conventional thresholding methods could not segment the phases reliably in this case

(Figure 2.12b), deep convolution neural network was employed to obtain a high confidence segmented image (Figure 2.12c).[192] To mitigate surface voids and interfacial delamination, applied stack pressure and surface engineering strategies such as polishing the electrolyte surface with physicochemical methods, optimising the electrode structure with different size of electrolyte, coating protection, or wetting layers should be developed.[22,23,25,26,29,145,153]

High pressure such as 25 MPa (often accompanied by an elevated temperature) can be applied during cell fabrication to initially contact all components in a Li metal-containing cell.[52] The initial pressure used depends on the mechanical properties of the SE and the AMs, as well as the interfacial wetting properties with the Li NE.[52,145] If the stack pressure is increased from 3 MPa to 5 MPa during cycling, a sufficient contact during the lithiation and delithiation can be achieved to ensure a stable stripping and plating.[52,145,193] Doux *et al.*[145] investigated the effects of stack pressure on the degradation mechanism of Li metal/Li_6PS_5Cl solid-state cells. High-resolution XCT was employed to monitor the structural evolution of Li filaments during cycling. The interfacial resistance decreases under high stack pressure due to improved contact. However, as discussed in Section 2.2.3, they also showed an immediate cell failure due to Li creep if the applied stack pressure increases to 75 MPa.[145] Figure 2.13 summarises the complex relationship between the applied stack pressure, the interfacial contact behaviour and the cycling current densities.[52] Wang *et al.*[70] demonstrated that the stack pressure has dynamic effects on the overpotential required to cycle Li at constant current densities. They showed that a critical stack pressure was correlated to the overpotential, below which a significant voltage loss was observed.

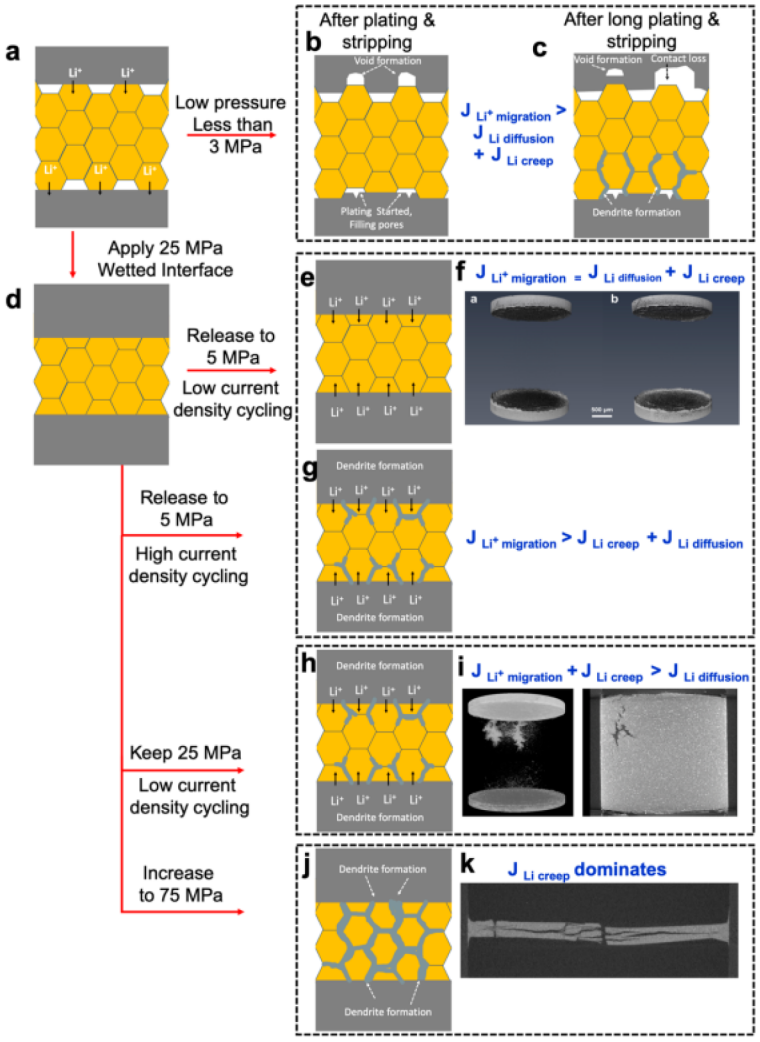


Figure 2.13 The impacts of stack pressure on the rate of Li^+ migration, Li^+ diffusion and Li creep across the SE. (a, b and c) A low stack pressure (< 3 MPa) would cause voids formation during stripping and Li filaments growth on the plating side after long plating and stripping. (d, e and f) When a high pressure of 25 MPa is applied initially to mechanically wet the interface and released to 5 MPa during low current cycling, a stable stripping and plating across the SE can be achieved. (g) However, if the current density is increased to more than 0.1 mA cm^{-2}, Li filament begins to occur and grow at both stripping and plating sides. (h) If the initial stack pressure is kept at 25 MPa, Li filaments were observed to occur even at low C-rate cycling. (j) If the stack pressure is increased to 75 MPa, an instantaneous short-circuit occurs without any applied current due to Li creep. Reproduced with permission from Ref. 52, Copyright (2020), American Chemical Society.

2.2.6 Li filamentary nucleation and growth

Li metal undergoes significant volume changes and is prone to interfacial instability, resulting in Li filament growth and interfacial reaction/delamination during electrochemical cycling. The accumulation or depletion of surface concentration at the interfaces can create an excess charge and induce instabilities (*e.g.*, Li filaments). By using *operando* video microscopy, Kazyak *et al.* [15]

identified four different types of Li-filaments in c-LLZO: branching, straight, spalling and diffuse filaments. Many experimental and theoretical efforts had been devoted to revealing the causes leading to the Li-filaments formation, which include:

(1) **Discontinuous interfacial contact and inhomogeneous ionic flux.** As discussed in Section 2.2.5, both the processing as well as the cycling conditions would introduce voids (see Figure 2.12a and Figure 2.12b),[15,25,26] increase the porosity,[194] or cause surface defects.[195] In addition, the Li metal shows poor compatibility with some SEs. These physical properties introduced heterogeneous ionic flux and distribution within these limited spaces, which increase the local electric driving force and become the "hotspot" for preferential Li filamentary growth.[195] To further achieve a sufficient interfacial contact, different strategies such as cleaning the surface of Li metal and the SE,[29,196] applying appropriate stack pressure[70] and introducing soft interlayers[25,169] have been proposed.

(2) **Grain boundaries.** Grain boundaries were also reported as the preferential sites for the penetration of Li-filaments (Figure 2.12d).[22,197,198] The grain boundaries situation is far from simple and depends on numerous factors, including mechanical and transport properties.

The mechanical properties of the grain boundaries differ from the grain interior, which can lead to filament propagation if they have a lower yield strength than the grain interior. It is possible that stress can be alleviated in certain SEs as Li is deposited along grain boundaries, preventing cracking of the SE. Furthermore, as the grain boundaries have high surface energy, they can have a lower stiffness than the grain interior. They have been found to have a 50% lower shear modulus,[199] which can mean they fall under the criteria for Li filaments formation according to the Monroe-Newman model.[17] Regarding the ionic conductivity of grain boundaries, in materials with a higher grain boundary conductivity, Li might be expected to accumulate more quickly in the grain boundaries than the grains, resulting in a limit for the CCD. However, it is mostly unclear whether the grain boundary conductivity exceeds that in the grains in many systems, in part due to difficulties in characterising the grain boundaries experimentally and potentially substantial differences in the conductivity depending on the synthesis and processing parameters. For example, in the case of c-LLZO, Ga-doped c-LLZO was shown to tolerate higher current densities than Al-doped c-LLZO, where Al-doped c-LLZO was shown by ToF-SIMS to contain both Al and Li, while Ga-doped c-LLZO contained only Li,[200] even though the grain boundary conductivity was reported to be higher in Ga-doped c-LLZO. This report also demonstrated a preferential growth of Li filaments along grain boundaries even when the grain boundary conductivity is lower than in the bulk material.

On a related note, the grain boundary reactivity may also play a role – the preferential reaction of grain boundaries in *e.g.*, c-LLZO to form LiOH and Li_2CO_3[78] may further exacerbate an inhomogeneous contact of the surface of the SE with Li metal, altering the inherent mobility/flux of Li across this interface. There are contrary reports regarding the effect of grain size – Sharafi *et al.*[201] reported that the CCD increased with increasing grain size in c-LLZO – this was

attributed to the increased effective contact area between Li metal and the grain instead of the grain boundaries. However, Cheng *et al.*[202] showed that the CCD increased as the grain size is reduced, which was attributed to the larger area fraction of grain boundaries. It is possible that differences in the grain boundary structure, orientation and composition as a result of different synthesis protocols even with the same nominal SE could be responsible for these different observations. In fact, it has been suggested that the difference in interfacial energies of grain boundaries and the SE/Li interface will dictate the propensity for filaments to form preferentially along grain boundaries.[49]

(3) **Electronic conductivities.** High electronic conductivities introduced Li filaments formation within the SEs. c-LLZO and Li_3PS_4 have high electronic conductivities, thus electrons and negative charges could be trapped within the bulk SE, causing the reduction of Li^+ to Li^0 and initiating the formation of Li filaments within the SE (Figure 2.12e).[31,32] An empirical criterion was further demonstrated, which shows that the electronic conductivities of SEs should be lower than 10^{-10} S cm^{-1} and 10^{-12} S cm^{-1} for a filaments-free Li plating at 1 and 10 mA cm^{-2}, respectively.[31]

Barai *et al.*[203] studied the impacts of external pressure and electrolyte transport properties on the Li filamentary growth *via* an electrochemical-mechanical coupled model. By modifying the Butler-Volmer's expressions derived by Monroe and Newman,[17] they showed that the minimum pressure required to suppress Li filaments' growth depends strongly on the current densities and elastic moduli of the SEs. They also found that increasing the electrolyte conductivity and transference number can reduce Li filamentary growth.[203] In a subsequent electrochemical-mechanical coupled model,[197] they modelled the growth of Li filaments through the SE microstructure. Due to the lower Young's modulus of the grain boundaries versus the grain interiors by two orders of magnitude, they predicted higher effective stress-induced current density at the grain boundaries. The stress-induced current densities were shown to further cause an accumulation of strain energy that induces crack formation in the SE.[197] These studies show that filament growth can preferentially occur at the grain boundaries even when they have a lower ionic conductivity than the grain interior. Both microstructural and chemical inhomogeneities play a role in the electrochemical-mechanical formation of such Li filamentary growth (Table 2.2).[200]

While many efforts have been devoted to developing SEs with high ionic conductivity, the electronic conductivity should also be considered another critical criterion for high-performing solid-state batteries. Surface engineering strategies such as doping and thin coatings have been developed to decrease the electronic conductivity.[204,205] The creation of compressive stress at the surface of the SE has been suggested to reduce stress-induced Li filament penetration by Qi *et al.*[206] with ion implantation.

Fundamental analysis of various materials behaviours and the multiphysical interactions between different cell components is essential to overcome the degradation challenges in

solid-state batteries. The investigation of solid-state batteries involving multiscale and multiphysical material characterisations include: (1) intrinsic properties such as crystal structures, electronic conductivity, ionic conductivity and electrochemical windows; (2) morphological and structural evolution (*e.g.*, grain boundaries evolution, volume change, particles cracking); (3) reaction between different cell components and the resulting chemical analysis of the elemental distribution; (4) gas formation; (5) thermal stability and runaway; (6) pores tracking and Li filaments formation. Different multiscale advanced characterisations techniques have been employed to gain insights into the complex multiphysical mechanism. Table 2.3 summarises diverse advanced characterisation methods, both *in-situ* and *ex-situ*, in solid-state battery research. As there have been several reviews discussing these working principles,[52,207] only the applications of these methods in solid-state batteries and their limitations are outlined.

Table 2.3 A summary of characterisation techniques to identify different degradation mechanisms in solid-state batteries

Techniques	Degradation mechanisms	Challenges and limitations	Ref.
CV	• Electrochemical stability windows; • Redox reaction analysis.	• The absence of voltammetric currents may be caused by passivation layers rather than indicative of lack of a thermodynamically favourable reaction for electrolyte decomposition; • Too high scan rates are often employed; • The stability of SE should be measured with a non-blocking cell configuration.	[71, 135, 208] [189, 209]
DEMS	• Measuring the gas release during the decomposition of SE and PE.	• Special cells are needed to monitor the gas release with the mass spectrometry. • Isotope labelling are needed to distinguish the allotrope.	[144]
DSC and ARC	• Thermal stability and thermal runaway.	• Only heat generation is recorded.	[88, 210]
EIS	• SEI formation; • Time-dependent charge-transfer or diffusion-controlled mechanisms.	• Convolution of electrochemical processes with similar resistance or capacitance; • Separation of electrode and electrolyte behaviour requires a reference electrode.	[7, 211, 212]
NDP	• Tracking movement of Li-ions through measuring the Li content in SE.	• NDP is sensitive only to the ^{6}Li isotopes; • Neutron generation and handling on the laboratory scale is difficult; • NDP analysis is time-consuming due to the small neutron fluxes; • Samples with magnetic properties cannot be tested; • Special cells are needed during *in-situ* tests.	[31, 126, 213]
NMR-MRI	• 3-dimensional spatial tracking of Li filament growth during cycling, microstructural growth.	• Imaging dimensions limited to 300 μm.	[214]
Optical microscope	• Morphological evolution: Volume change, crack and voids formation; • Li-filaments growth; • Colour change during cycling.	• Limited resolution ($\approx$ 200 nm), only macro-structural changes can be observed.	[15, 125, 195] [113, 215]
Raman	• Reaction products at the surface of SE, probing compatibility of electrode and electrolyte and their decomposition products; • SEI formation during Li deposition; • Phase change and the SOC distribution.	• Sensitive to particle size and preferential crystallite orientations; • Need to tune the laser specific power to achieve reliable signal-to-noise ratios, whilst avoiding laser-induced sample transformations; • Samples must have Raman-active vibrational modes; • Proper selection of laser source wavelength, power and exposure time to optimize the resolution.	[216–218] [202, 219, 220]
SEM and EDX	• Interfacial and sub-surface decomposition, particle cracking, Li filament formation in the bulk SE.	• Samples must be representative for different measurements; • Strict operating conditions such as high vacuum and conductive samples; • High electron energy may damage the sample.	[122, 189, 221] [32, 113, 128]

† The acronyms in this table can be found in the List of Acronyms.

Techniques	Degradation mechanisms	Challenges and limitations	Ref.
SIMS	• Interlayer formation, possible to follow isotopically labelled species.	• Destructive technique, matrix effects limits the interfacial quantification; • Only thin layers near-surface of the sample are accessible; • High energy ion beam may damage the sample and trigger side reactions; • The quantification of SIMS needs standard samples.	[78, 222, 223] [178, 224]
Solid-state NMR	• Composition analysis of (amorphous) decomposition products at the interface and their impact on Li^+ transport; • Li microstructural growth and Li^+ dynamics.	• The *ex-situ* approach does not capture short-lived metastable or reactive phases, which may react further before the NMR spectrum is acquired; • ^7Li is used as the probe nucleus, which may be difficult to distinguish from the similar Li content in electrodes and electrolytes; • Challenging to separate the resonances from the different components and to determine what signal corresponds to which part of the cell.	[32, 225, 226] [214, 227]
TEM and EELS	• Phase change and the formation of disordered interface; • Atomic scale structural and chemical analysis; • Observation of interfacial chemical and structural changes, Li filaments formation during cycling.	• Samples must be electrically conductive; • The sample preparation is complicated due to FIB processing; • *In-situ* TEM experiments need special sample holders and fabrication of nano-cells, with an air-sensitive sample transfer. • High energy electrons can destroy the sample.	[33, 151, 217] [86, 228, 229] [226]
XPS	• *Ex-situ* composition analysis of reaction/decomposition products at the interface; • *In-situ* observation of SEI formation, onset voltages for redox products, SE chemical decomposition pathways (chemical information with time).	• Surface sensitive with shallow detection depth; • High energy ion flux during etching process may affect the chemical component and bring side reactions; • Li is supplied to the SE surface through physical means instead of electrochemical cycling during *in-situ* tests.	[119, 152, 217] [150, 228, 230]
XCT	• Correlate pores, voids, defects with CCD for Li filament formation; • Interfacial growth and cracking of SE.	• Need a synchrotron source; • Differentiating between voids (air) and Li metal is challenging; • Lack of chemical specificity towards Li and only indirect observation of filament growth is possible.	[145, 194, 231] [37, 132, 160]
XRD	• *Ex-situ* rudimentary studies of chemical stability/compatibility, decomposition products of mixing reactions; • *In-situ* monitoring of local structural changes as a function of current and potential.	• Sensitive to bulk only, Li has a low electron scattering factor. • During *in-situ* XRD testing, X-rays may be consumed by non-targeted materials (such as current collector) resulting in a decreased intensity and data quality.	[209, 232, 233] [234]

†The acronyms in this table can be found in the List of Acronyms.

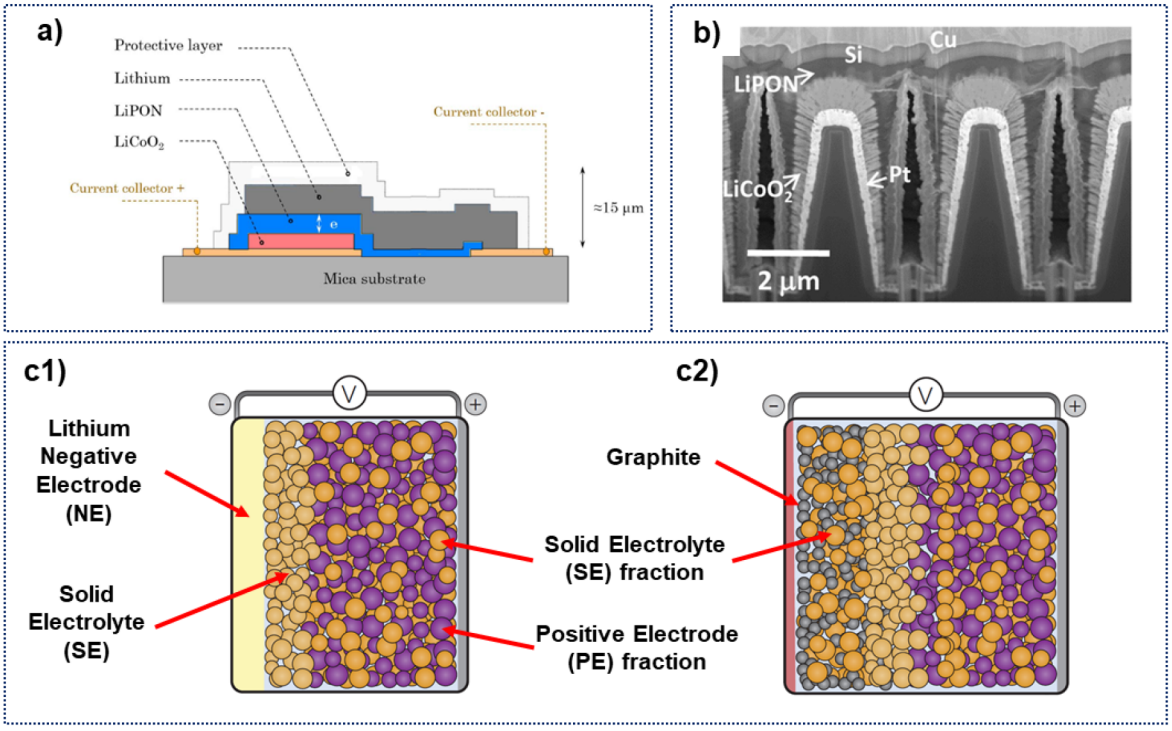


Figure 2.14 (a) Schematic of the planar thin-film solid-state cell. Reprinted with permission from Ref. 235, Copyright (2015), The Electrochemical Society. (b) Cross-sectional SEM image of the interdigitated three-dimensional solid-state cell. Reprinted with permission from Ref. 236, Copyright (2016), American Chemical Society. (c1) The composite solid-state cell with metallic Li film (light yellow) as the NE. (c2) The solid-state cell using composite electrodes as both the PE and NE: Grey circles in the NE represent graphite; dark orange circles denote the SE fractions in both composite electrodes and violet circles in the PE represent a layered transition metal oxide. Lighter orange circles in the electrolyte denotes a different SE than the SE used in the electrodes. Reprinted and adapted with permission from Ref. 8, Copyright (2016), Nature Energy.

2.3 Solid-state physics and cell architecture engineering

There are three different types of solid-state cells in terms of cell architecture: planar thin-film, three-dimensional interdigitated and composite solid-state cells. Figure 2.14a shows the schematic of the planar thin-film cell, in which the electrodes are fabricated into a thin, non-porous layer.[63,235] The electrochemical reactions take place at the planar surface between the SE and electrodes. However, the energy per unit area of planar thin-film cells is insufficient to meet the power demands of micromachined sensors and actuators.[237] Figure 2.14b shows the SEM micrographs of the interdigitated three-dimensional solid-state cells, where the cell components are fabricated in an array of three-dimensional columns.[236] Due to a shorter mass transfer transport distance and a larger electrode surface area per footprint area, the interdigitated electrodes in the fully conformal three-dimensional configuration show promise to meet the required energy per unit area.[237,238] In contrast, a composite electrode is typically made of

three components, which include AMs, SEs and electronic conductive agents such as carbon black.[41,62,75] The AMs and carbon black act as the electronic conducting phase, whereas the SE in the composite cell is the ionic conducting phase.[62] The composite solid-state cell can use either metallic Li or composite electrodes as the NEs, as shown in Figure 2.14(c1) and Figure 2.14(c2), respectively.[8]

2.3.1 Thin-film solid-state cell

In this section, the solid-state physics of different cell components such as the Li NE, SE, non-porous PE and the space-charge formation at both interfaces on the overall thin-film cell behaviour are reviewed.

2.3.1.1 Low melting temperature of Li metal

Thin-film solid-state cells have a low capacity in the range of μAh and mAh.[63,239] Potential low power density applications for these cells include micromachined sensors and actuators, implantable medical devices and smart cards.[237] Some of the electronic circuit boards are manufactured with the solder reflow assembly, in which the integrated circuits are heated to 250 °C for a short time, and all the components are soldered simultaneously.[239,240] Under this solder reflow manufacturing condition, thin-film solid-state cells using pure metallic Li as the NEs fail due to the low melting temperature of metallic Li (180 °C).[239,240] The molten Li metal could penetrate through the grain boundaries of the SE and cause an internal short-circuit. As a result, compounds that alloy with Li have been proposed to replace the pure metallic film as the NE.[236,241,242] However, the delithiation of these compounds could cause a significant volume change up to 4.07 times of the initial volume and a significant irreversible capacity loss during the first cycle.[241]

Another feasible solution to address the high solder reflow temperature is the fabrication of a NE-free thin-film cell (Cu|SE|LCO).[239,240] In this configuration, a copper current collector is deposited over the electrolyte in place of the NE.[239] As a result, the NE-free cell can be soldered onto the Si wafers and integrated directly into the electronic circuit boards before the electrochemical cycling.[240] Li from the LCO is then plated between the copper current collector and SE on the initial charge.[239] One drawback of this cell configuration is that its cycle stability requires a gastight seal provided by an overlayer, such as parylene to reduce the partial pressure of oxygen and moisture. Without an overlayer, half of the reversible capacity was reported lost during the initial cycle due to the formation of Li_2O and LiOH.[240]

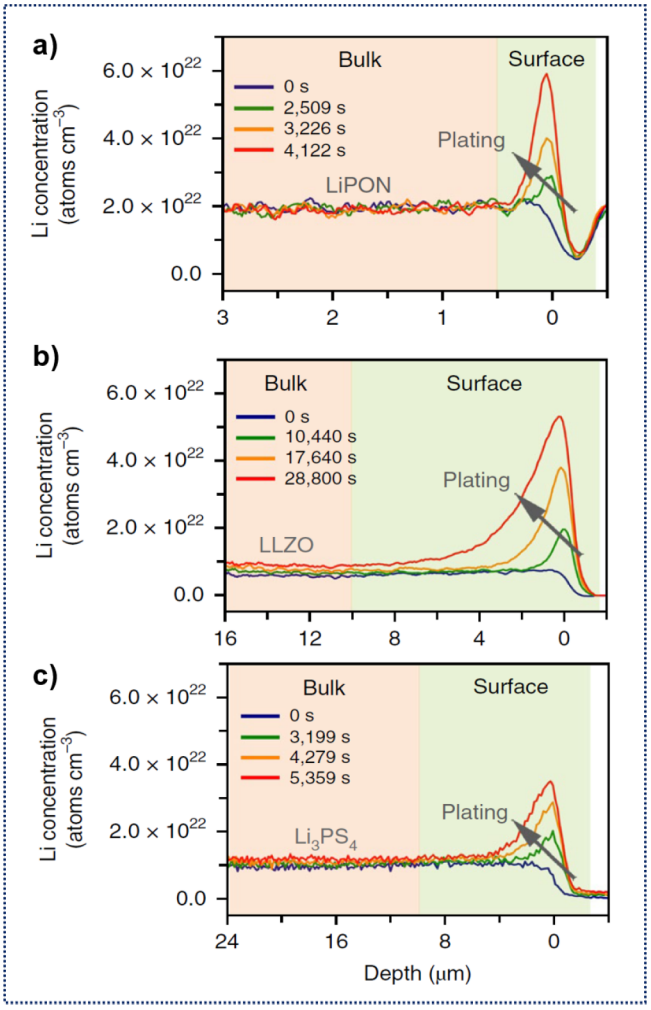


Figure 2.15 A comparison in the distribution of the Li concentration across the bulk SE and at the electrode-electrolyte interfaces. The absence of concentration gradients across (a) LiPON, (b) c-LLZO and (c) Li_3PS_4 SE implies a near-unity transference number in the bulk SE. However, the variation of Li concentrations at the interface indicates that the local space-charge layers are non-electroneutral. Reprinted with permission from Ref. 31, Copyright (2019), Nature Energy.

2.3.1.2 Conduction mechanism in the bulk solid electrolyte

For all types of cell architecture shown in Figure 2.14, a thin-layer of bulk SE is used as the separator and ionic conductor between the NE and the PE. An inorganic SE can be considered as a single-cation ionic conductor when the mobility of the anion is negligible.[243] In the case of LiPON SE, Yu *et al.*[34] postulated that the oxygen, nitrogen and phosphorus atoms are rigidly bound in the framework structure of LiPON. The single-cation ionic conductance feature can be verified by the measurement of cationic transference number (T^+) on a non-blocking symmetrical cell (Li|SE|Li) as follows:[244]

$$T^+ = \frac{I^s(\Delta V - I^0 R_1^0)}{I^0(\Delta V - I^s R_1^s)}, \tag{2.8}$$

where I^{s} is the steady-state current, ΔV is the potential difference, I^{0} is the initial current, R_1^0 is the initial resistance and R_1^s is the steady-state resistance.

The transference number for the inorganic SE is often considered as near-unity.[60,245] Conventional liquid electrolytes such as those based on $LiPF_6$ salts have a transference number between $0.3 - 0.5$.[246,247] A low transference number implies that mobility of anions in the electrolyte and their accumulation at the electrode surface cause the concentration gradients of Li-ions in the SE, which creates a concentration overpotential that subsequently limits the cell performance.[7,248] While a near-unity transference number in the inorganic SE can reduce the amount of heat generated in the SE, all other processes described in Section 2.1.2 still generate a considerable amount of heat. Han *et al.*[31] measured the concentration of Li-ions in the bulk SE for LiPON, c-LLZO and amorphous Li_3PS_4 using the time-resolved *operando* NDP method. According to their measurements, all three different SEs exhibit constant concentration profiles in the bulk electrolyte at different times during Li plating (Figure 2.15).[31] A near-zero concentration gradient shows that the migration of Li-ions due to the hopping of Li-ions from one site to the neighbouring site is the primary conduction mechanism in the bulk SE.[7]

2.3.1.3 Space-charge formation at the interface

At the interface between the electrode and the electrolyte, a space-charge region with two oppositely charged layers is formed due to the difference in the chemical potentials of the electrodes and the SE.[83] As illustrated by Figure 2.15 and 2.16a, the accumulation or depletion of the charged species at the interface causes the surface concentration of the species to deviate from the bulk concentration and the formation of a local electric field at the interface.[84] Due to variations of surface concentration and local electric potential at the interfaces, the space-charge layers are non-electroneutral.[84,249–251] The characteristic length scale of the space-charge layers can be estimated from the Debye lengths. Wan and Ciucci showed that the Debye length of the NE at the NE-SE interface is 9.66 nm, whereas the Debye length of the SE at the same interface is 0.63 nm. At the SE-PE interface, the Debye lengths of the electrolyte side and PE side are 0.71 nm and 0.49 nm respectively.[84] Different Debye lengths indicate different electric potential gradients at each side of the same interface. For instance, at the NE-SE interface, the maximum electric potential gradient is 5.68×10^5 V m^{-1} in the NE side and 3.42×10^7 V m^{-1} in the SE side.[84] The thickness of the Debye length does not only depend on the relative permittivity of the materials (see Section 2.1.1),[82] but also on the surface concentration and the potential difference of the electrode and the electrolyte during operation.[83] Figure 2.16(c1) and 2.16(c2) illustrate the electric potentials across the cell for the electroneutral model and the non-electroneutral model. In the electroneutral model, an instantaneous change of the concentration and electric potential are assumed at the interfaces, whereas the electric potential is continuous in the non-electroneutral model following Maxwell's first law.[84] The space-charge layers act as a shock absorber, which allows the electric potential to change gradually at the interfaces.[252]

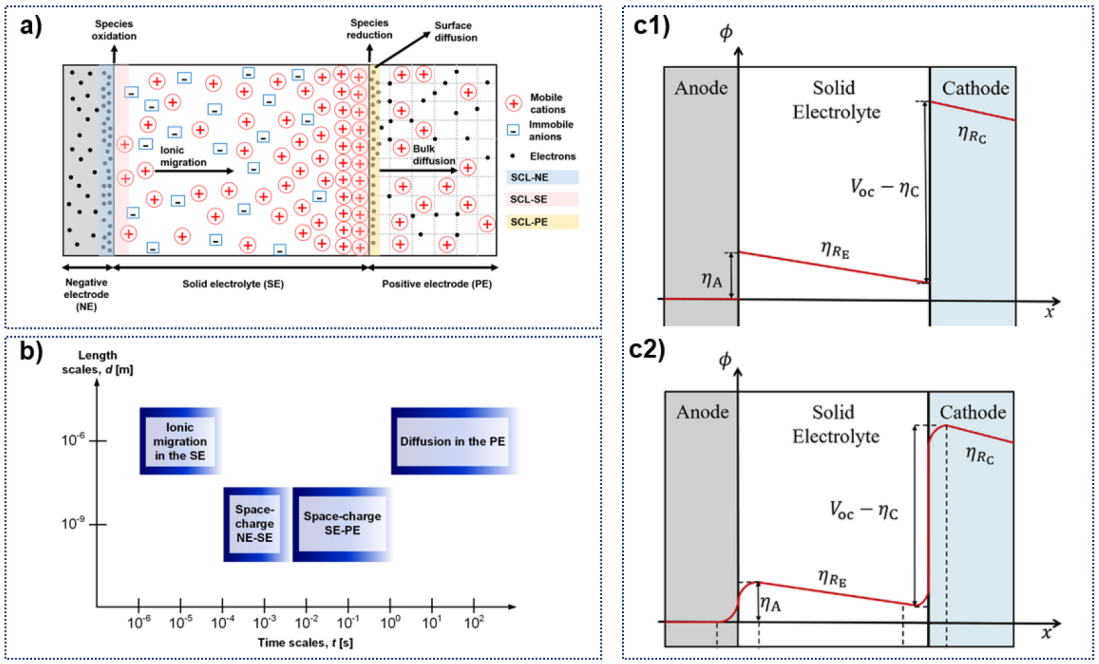


Figure 2.16 (a) An illustration of different possible mechanisms occurring during discharge in the domains of space-charge layers, bulk SE and across the PE. (b) A mapping of the mechanisms in an ideal thin-film solid-state cell according to the time and length scales. The time scales were estimated from the EIS measurement,[7,40,62] whereas the length scales of the space-charge layers were taken from the non-electroneutral model computed by Wan and Ciucci.[84] The length scales of the bulk electrolyte and the non-porous PE were given by their thickness.[63] The electric potential variation across the cell represented by the electroneutral model (c1) and the non-electroneutral model (c2). Reprinted with permission from Ref. 84, Copyright (2020), Elsevier.

One should note that the formation of a space-charge layer is different from the formation of the passivating layers, though both mechanisms occur at the interface.[83,84] A passivating layer is formed as a result of the decomposition reactions whereas a space-charge layer is formed due to the non-homogeneous charge distribution at the interfaces.[72,83,84] Most solid-state relevant space-charge models proposed in the literature do not account for the effects of interfacial decomposition reactions.[40,82–84,249,253] The charge-transfer at both interfaces (NE-SE and SE-PE) can be represented by the Kröger-Vink notation as[84]

$$\mathrm{Li(NE)} + \mathrm{V}'_{\mathrm{Li}}\mathrm{(SE)} \rightleftharpoons \mathrm{Li}^{\mathrm{X}}_{\mathrm{Li}}\mathrm{(SE)} + e^{-}\mathrm{(NE)}, \tag{2.9}$$

$$\mathrm{Li}^{\mathrm{X}}_{\mathrm{Li}}\mathrm{(SE)} + e^{-}\mathrm{(PE)} \rightleftharpoons \mathrm{Li}^{\mathrm{X}}_{\mathrm{Li}}\mathrm{(PE)} + \mathrm{V}'_{\mathrm{Li}}\mathrm{(SE)}, \tag{2.10}$$

where SE, PE and NE denote the solid electrolyte, positive electrode and negative electrode, respectively.

In general, the charge distributions at the interfaces can be described with the Helmholtz model, Gouy-Chapman's model or Stern's model.[254–258] Different variations of these models have been proposed to account for the surface concentrations and potential drops at the interfaces.[259] Depending on the electrical forces between the electrodes and the charged species, specific adsorption of the charged species can also happen.[250,260] In the context of solid-state batteries, the BV kinetic relation has been used to model the charge-transfer at the interfaces:[7,60,261]

$$i = i_{0,\text{neg}}\left[\exp\left(\frac{\alpha_{\text{ox}} F \eta^{\text{ct}}_{\text{neg}}}{R_{\text{gas}} T}\right) - \exp\left(\frac{-\alpha_{\text{red}} F \eta^{\text{ct}}_{\text{neg}}}{R_{\text{gas}} T}\right)\right], \tag{2.11}$$

$$i = i_{0,\text{pos}}\left[\exp\left(\frac{\alpha_{\text{ox}} F \eta^{\text{ct}}_{\text{pos}}}{R_{\text{gas}} T}\right) - \exp\left(\frac{-\alpha_{\text{red}} F \eta^{\text{ct}}_{\text{pos}}}{R_{\text{gas}} T}\right)\right], \tag{2.12}$$

where α_{ox} and α_{red} are the oxidation and reduction charge transfer coefficient, respectively; and $i_{0,\text{neg}}$ and $i_{0,\text{pos}}$ are the exchange current densities at the NE-SE and PE-SE interface. The BV model assumes a single-step reaction across the interfaces between the bulk electrode and the bulk SE without accounting for the space-charge effects. As a result, this kinetic model cannot reproduce the high-frequency semi-circles as observed by the impedance measurement. Only the low-frequency impedance model governed by the diffusion mechanisms can be described by the standard BV model.[250,251]

To account for double-layers' effects, the exponential term in Butler-Volmer's kinetic model can be corrected to describe the potential difference across a Stern layer between the electrode and the electrolyte. This kinetic relation is known as the Frumkin-Butler-Volmer (FBV) model and was implemented by Landstorfer *et al.* and Rossi *et al.* to model an electrolyte membrane comprised of fixed anions and mobile cations.[249,251,253] The FBV model at the NE and electrolyte interface can be represented by[249]

$$j = k_{\text{ox}} \exp\left(\frac{\alpha_{\text{ox}} F n}{R_{\text{gas}} T} \Delta\phi_{\text{NE-SE}}\right) - k_{\text{red}} \frac{c_+}{c_{+,0}} \exp\left(\frac{-\alpha_{\text{red}} F n}{R_{\text{gas}} T} \Delta\phi_{\text{NE-SE}}\right), \tag{2.13}$$

whereas the FBV at the electrolyte and PE interface is given by[249]

$$j = k_{\text{ox}} \exp\left(\frac{\alpha_{\text{ox}} F n}{R_{\text{gas}} T} \Delta\phi_{\text{SE-PE}}\right) - k_{\text{red}} \frac{c_+}{c_{+,0}} \exp\left(\frac{-\alpha_{\text{red}} F n}{R_{\text{gas}} T} \Delta\phi_{\text{SE-PE}}\right), \tag{2.14}$$

where k_{ox} and k_{red} denote the oxidation and reduction rate-constant; and c_+ represents the concentration of mobile cations. $\Delta\phi_{\text{NE-SE}}$ and $\Delta\phi_{\text{SE-PE}}$ are the correction terms that describe the linear potential drop between the electrodes and the reaction planes at each interface. The reaction plane was defined as the intersection between the Stern layer and the diffusive layer, where the Faradaic charge-transfers occur.[249]

The capacitive contribution to the electrode reactions can also be modelled by modifying the interfacial current to include the faradaic current due to charge-transfers at the interfaces (i_{ct}) as well as the non-faradaic current due to charge/discharge of the double layers (i_{DL}).[40,252] Therefore, the sum of interfacial current, i_{int} becomes[40,251,252]

$$i_{\mathrm{int}} = i_{\mathrm{ct}} + \underbrace{C_{\mathrm{int}} \frac{\partial(\phi_{\mathrm{s}} - \phi_{\mathrm{e}})}{\partial t}}_{i_{\mathrm{DL}}}, \tag{2.15}$$

where C_{int} is the interfacial capacitance. The academic discussions on the effects of the space-charge layers have been debatable. Klerk and Wagemaker[83] calculated the space-charge capacitance and resistance for the c-LLZO and the LATP SEs at both interfaces. The space-charge resistance and capacitance were shown to depend on the applied voltage. By accounting for the Coulomb interactions between charged defects, they concluded that the space-charge effects are negligible at the device level due to the small space-charge resistance and capacitance. On the other hand, Wan and Ciucci[84] suggested that the accumulation or depletion of the charged species at the interface limits the charge-transfer reaction, which reduces the exchange current densities and increases the charge-transfer resistance. Although the maximum electric potential gradients at both interfaces reach a magnitude between $10^5 - 10^{10}\ \mathrm{V\,m^{-1}}$, the charge-transfer overpotential calculated from the non-electroneutral model is negligible at the NE-SE interface and varies between $\approx 0.02 - 0.12\ \mathrm{V}$ at the SE-PE interface.[84] However, these electric potential gradients can induce Maxwell stresses at the interfaces.[84,262]

By comparing the electroneutral and non-electroneutral model, Wan and Ciucci showed that the space-charge layers affect the exchange current density term of the kinetic model.[84] The exchange current density can be defined as the current density at equilibrium, where both the forward and reverse reactions have the same rate.[81] It is also a model parameter that can be estimated from the EIS measurement, in which the space-charge effects are considered in the model implicitly.[60] Nevertheless, the EIS measurement of the exchange current density has one limitation due to the assumption of the linear current-voltage relationship. For a small perturbation amplitude ($\leq$ 20 mV), the current response to an applied potential can be approximated as linear.[263] As shown by the CV measurement of thin-film solid-state cells, the relationship between the current and voltage is highly non-linear.[264] This non-linearity can be attributed to interfacial reactions, current-strength dependent solid-state diffusion losses and strong concentration gradients in the electrode under load.[62] For an operating condition near equilibrium, the kinetic parameters estimated from the linear EIS is sufficient to describe the cell behaviour. If the operating conditions deviate significantly from the equilibrium, such as under high current densities ($\geqslant 7\,\mathrm{C}$), the assumption of a linear current-voltage relationship is no longer valid, and the non-linear losses must be taken into account.[62] In contrast to the linear EIS, the report of using the Non-Linear Electrochemical Impedance Spectroscopy

(NLEIS) method is scarce due to the requirement of multiple instruments such as function generator and high-speed digitisers in addition to the different control, data acquisition and signal processing programs.[263,265] However, kinetic parameters estimated from the NLEIS measurements could provide valuable insights in choosing the most appropriate electrochemical kinetic model. The response at fundamental frequencies to large amplitude excitations can reveal additional mechanisms indistinguishable with the use of linear EIS.[263,266]

In reality, the effects of space-charge at the interfaces are coupled with the charge-transfer and the surface diffusion.[40,250,252] The underlying physics governing the space-charge behaviour is the time scales, during which the space-charge effects are most dominant.[7,40,62,252] However, the time scales due to space-charge effects obtained by EIS frequency measurements are different from the time evolution in NDP measurements. While space-charge effects are usually shown to occur in short time scales corresponding to high-frequency and mid-frequency regions (1 MHz - 1 Hz) from EIS measurements,[7,40,62] Han *et al.*[31] demonstrated that the surface concentration continues to change above thousands of seconds in NDP measurements. Further works are required to study these differences in the future. Figure 2.16(b) illustrates the mapping of the space-charge effects, the ionic conduction in the bulk SE and the Li diffusion in the PE according to their time and length scales. For an ideal solid-state cell without considering the interfacial decomposition reactions or the nucleation of Li filaments, the space-charge effects are most visible within the time scales between μs and ms, and the length scales are on the orders of 10 nm.[7,84] The ionic conduction in the bulk SE occurs on a short time scale (μs) but over a longer length scale (μm). On the other hand, the mass transport in the non-porous PE happens in a longer time scale ($\geqslant 1$ s) and also a more extended length scale (μm).[7,63] Comparing the length and time scales of the space-charge effects to the bulk ionic conduction or diffusion in the electrode does not imply the insignificance of the space-charge models. In contrast, the space-charge models are especially relevant when analysing the impacts of doping on the interfacial properties or the effects of charge accumulation/depletion on the degradation behaviour.[84,251] Compared to a thin-film cell configuration, which only has one interface between the SE and the electrodes, a composite solid-state cell Li cell has multiple interfaces. Therefore, the effects of space-charge may be more dominant in such cell architecture. Further studies are required to evaluate the impacts of space-charge and its interplay with surface diffusion on cell performance under different operating conditions.

2.3.1.4 Diffusion limitations in non-porous positive electrodes

One major feature differentiating the thin-film and the composite solid-state cell configuration is the PE. The PE in the thin-film configuration is non-porous. Therefore, the electrochemical oxidation and reduction occur only at the external surface between the bulk SE and the PE.[7,60] The crystalline LCO and nano-crystalline $LiMn_2O_4$ (LMO) are the commonly studied PEs for

the thin-film cell configuration.[239] Due to more phases and wider stoichiometry in the LMO PE, the hysteresis observed in the LMO film is more significant compared to that in the LCO films.[239]

Bates and co-worker[267] measured the principal diffraction lines of LCO-films and found that the grain orientations are strongly dependent on the film thickness. Three types of grain orientations can be observed from the XRD analysis in the LCO films: (003)-oriented grains, (101)-oriented grains and (104)-oriented grains. The film with more percentages of (101) and (104)-orientations are more favourable to the Li diffusion compared to the (003)-grains due to the in-plane diffusion. For a film with (003)-orientation, Li must diffuse in the perpendicular direction through the close-packed oxygen layers. It should also be noted that the deposition temperature also affects the grain distribution significantly. The film deposition at higher temperatures causes the formation of larger grains and more void fraction, which subsequently increases the film resistance.[267]

Other than the grain orientations, the phase transformation in the LCO film is another critical variable affecting the diffusion coefficient of Li^+. The diffusion coefficient in the LCO film is not constant as commonly assumed but varies with the Li concentration upon lithiation and delithiation.[7,60] The diffusion coefficient can be measured with either the Galvanostatic Intermittent Titration Technique (GITT) or the PEIS method.[7,60,268] Matsuda *et al.*[216] measured the structural change of the LCO electrode with the *in-situ* Raman spectra and observed the formation of five phases in the film. Phase changes have two significant implications. Firstly, a thicker bulk PE was shown to demonstrate a higher percentage of capacity drop compared to a thinner PE at high current densities.[27] Secondly, the phase transformation in the PE causes large voltage change and contributes to the reversible heat generation. For a cell with the LCO electrode, the rate of reversible heat generation due to the structural change can be as large as 700% of the irreversible heat generation in the operating regime of C/8 and 5-40% SOC.[264]

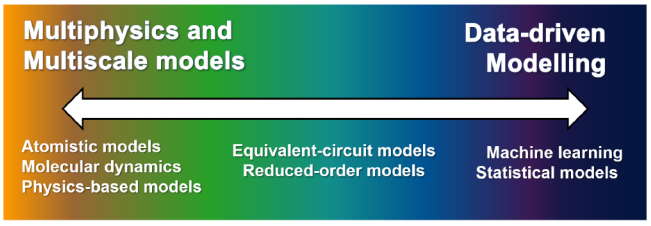


Figure 2.17 An illustration of battery modelling spectrum: On the left end, multiscale and multiphysics models are typically constructed based on first-principles and fundamental physics of a battery. On the right end of the spectrum, data-driven models such as statistical and machine learning approaches are mechanisms-agnostic models that do not require prior knowledge of the battery chemistries. In the middle of the spectrum, equivalent-circuit models and reduced-order models are semi-empirical models developed based on experimental data.

2.3.1.5 Overpotential analysis

In the absence of current flow, the cell potential is known as the equilibrium or Open-Circuit Potential (OCP), which denotes the maximum work achievable in batteries. During discharge, the current enters through the negative current collector and travels through the solid NE to the NE-SE interface, where oxidation occurs. Then, the current travels through the SE to the SE-PE interface, where the reduction occurs, and the current is transferred into the non-porous PE. Finally, the current travels through the PE until it reaches the positive current collector.[269] The passage of current through the cell causes different resistance and voltage losses. Therefore, the cell voltage, V, can be expressed by[40]

$$V = U_{\mathrm{PE}}(c_{\mathrm{s}}) + \eta^{\mathrm{diff}}_{\mathrm{PE}} + \eta^{\mathrm{mt}}_{\mathrm{PE}} + \eta^{\mathrm{ct}}_{\mathrm{PE\text{-}SE}} - \eta^{\mathrm{mt}}_{\mathrm{SE}} - \eta^{\mathrm{ct}}_{\mathrm{SE\text{-}NE}} - U_{\mathrm{NE}}, \tag{2.16}$$

where $\eta^{\mathrm{diff}}_{\mathrm{PE}}$ is the diffusion overpotential in the PE; $\eta^{\mathrm{mt}}_{\mathrm{PE}}$ is the mass-transfer overpotential due to the electronic transport in the PE; η^{ct} is the charge-transfer overpotential at the respective interface; $\eta^{\mathrm{mt}}_{\mathrm{SE}}$ denote the ohmic losses in the SE and U_{NE} is the OCP of the NE. In a solid-state cell, in which a metallic Li is used as the NE, the term U_{NE} is zero.

The analysis of overpotentials is often used in physics-based models to estimate the performance of solid-state batteries. For instance, Raijmakers *et al.*[40] and Wan and Ciucci[84] showed that the ohmic loss in the SE is the dominant overpotential during the low and high C-rate of constant-current discharge. Under pulse operating conditions, the diffusion overpotential in the PE was found to be dominant for long and short pulse durations.[7,40] During the interruption of external currents, the development of the local concentration gradients in the solid electrode causes the redistribution of material and the diffusion overpotential.[270] The voltage losses can be reduced by improving the ionic conductivity of the SE, reducing the thickness of the SE, decreasing the thickness of the PE or modifying the cell architecture altogether from a thin-film configuration to a three-dimensional or composite configuration.[7,62,238,271,272]

While physics-based models are useful in understanding the internal dynamics of a battery, this modelling approach requires the estimation of many parameters. The measurement of real-world parameters in battery research is challenging due to manufacturing defects, cell-to-cell variability, measurement uncertainties as well as the evolution of grain boundaries and interfaces over time.[273–276] Recently, Wu *et al.*[277] proposed the fusion of multiphysical and multiscale modelling approaches with machine-learning methods as a possible solution to address the problems of inherent cell-to-cell variability.[277] Figure 2.17 shows a spectrum of battery modelling approaches, consisting of multiscale and multiphysics models on the left end and data-driven models such as machine learning models on the right end. Due to the extensive and even destructive characterisation experiments required for physics-based model parametrisation, it becomes impractical to measure all the parameters for every single cell.[277]

By learning the battery behaviour and improving the performance from training data, machine learning approaches such as artificial neural networks and Gaussian/Bayesian regression have shown promise to adapt to the inherent variability in batteries.[277] However, this method requires a large amount of training data to produce an accurate predictive model. Therefore, high-fidelity multiphysical and multiscale models could be used to train machine-learning models, creating new opportunities for fusing the advantages of both modelling approaches.[277] By using these hybrid models to estimate the state-of-charge, state-of-available-power and state-of-health, dynamic limits that account for real-world operating conditions can be used as a basis for intelligent solid-state battery management and diagnostics.[277]

2.3.2 Three-dimensional solid-state cells

For a thin-film cell configuration, increasing the electrode thickness is not proportional to the improvement in the cell's rate capability due to a longer diffusion distance of Li-ions into the PE.[7,60,278] One alternative to improving the energy and power density is the fabrication of a fully conformal three-dimensional solid-state cell.[236,238,279,280] Figure 2.18a shows the schematic of a planar thin-film cell and a three-dimensional solid-state cell.

Talin *et al.*[236] fabricated a 3D solid-state cell (Si|LiPON|LCO) by using the Physical Vapour Deposition (PVD) and compared the performance of the 3D cells to planar thin-film cells. While the planar thin-film cells could deliver a specific capacity of approximately 20 μAh cm^{-2} up to 3.3 C, the specific capacity achieved with the 3D solid-state cells was less than 5 μAh cm^{-2} at 1.2 C. The lower specific capacity of the 3D solid-state cells was attributed to the non-uniform electrolyte thickness. As a result, the 3D solid-state cell had an inhomogeneous internal current distribution and a significant potential drop towards the bottom of the microcolumns. Pearse *et al.*[238] showed that the problem of non-uniform electrolyte thickness could be overcome by fabricating a fully conformal 3D solid-state cell using the Atomic Layer Deposition (ALD). They introduced a metric known as the Area Enhancement Factor (AEF) to quantify the performance of the 3D cell:[238]

$$AEF = \frac{A_{\text{int}}}{A_{\text{f}}}, \tag{2.17}$$

where A_{int} is the true internal surface area and A_{f} is the footprint area of the cell on the substrate. The AEF can be enlarged by increasing the depth of microcolumns. They demonstrated that the 3D conformal cell with AEF10 has a higher discharge capacity compared to AEF4 and AEF1 (planar cell) for all current densities ($\leqslant 10000\ \mu$A cm^{-2}) up to 100 cycles.[238] This performance improvement was attributed to a shorter diffusion distance in the non-porous PE and a larger uniform interfacial area, which result in lower overpotentials.[238]

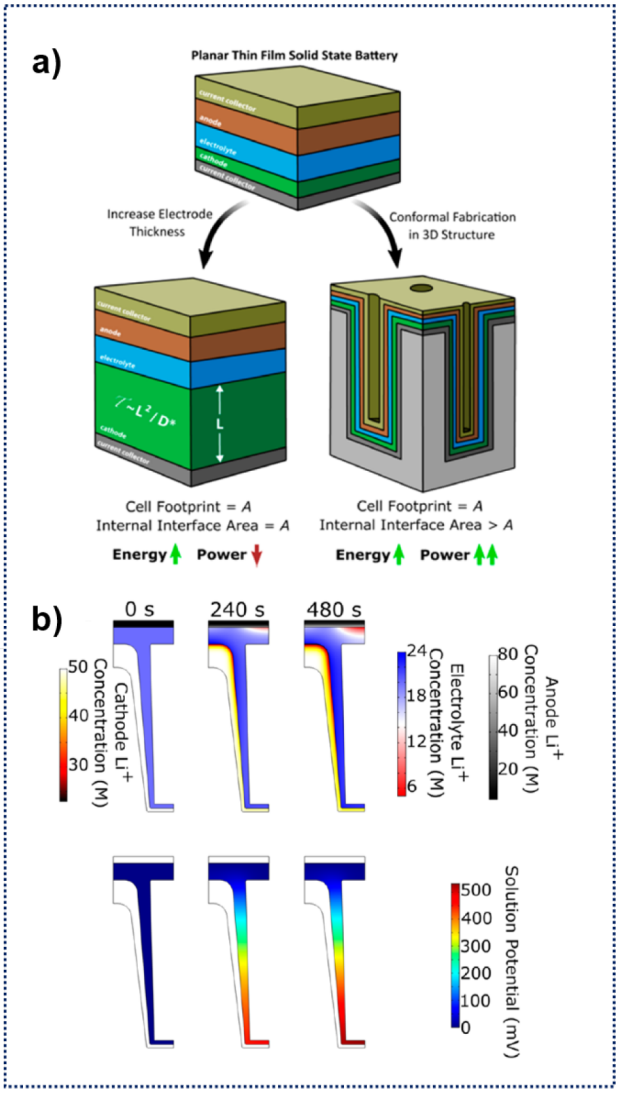


Figure 2.18 (a) A comparison of a thick planar thin-film cell with the 3D conformal solid-state cell. For the planar thin-film cell, an increase in the electrode thickness causes a drop in the power density due to the diffusion limitation across a thick electrode. By enlarging the internal surface area, a 3D structure improves the energy density without sacrificing the power density. Reprinted with permission from Ref. 238, Copyright (2018), American Chemical Society. (b) Physics-based model of a 3D solid-state cell: the inner column represents the concentration distribution of Li^+ in the PE, whereas the outer column depicts the concentration of Li^+ and potential gradients in the SE. The significant potential gradient towards the bottom of the microcolumns was attributed to the non-uniform electrode and electrolyte structures. Reprinted with permission from Ref. 236, Copyright (2016), American Chemical Society.

2.3.3 Composite solid-state cells

Unlike the thin-film cell architecture, the electrochemical oxidations and reductions occur at the various interfaces between the SE and AMs in a porous composite electrode.[62] Randomised orientations will also occur between crystal particles in the SE and electrode, which may have a mixture of 2-dimensional and 3-dimensional Li^+ diffusion pathways, leading to a mixture of favourable and unfavourable interfaces between the particles for fast Li^+

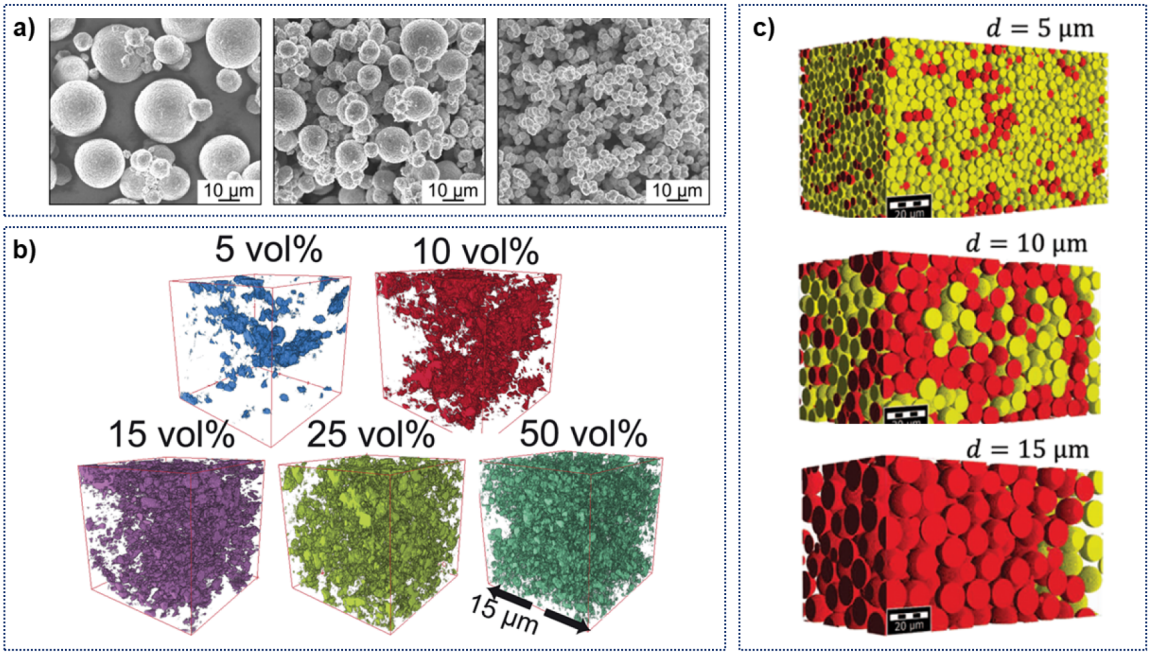


Figure 2.19 (a) Scanning Electron Microscopy (SEM) visualisation of the non-coated $LiNi_{1-x-y}Mn_xCo_yO_2$ (NMC)-622 composite PE: NMC-Large, NMC-Medium and NMC-Small. Reprinted with permission from Ref. 120, Copyright (2018), American Chemical Society. (b) 3D reconstructed hybrid SE with different volume fraction of Al-LLZO (5-vol%, 10-vol%, 15-vol%, 25-vol%, 50-vol%) using the synchrotron nano-tomography. Reprinted with permission from Ref. 281, Copyright (2019), Royal Society of Chemistry. (c) Numerical generation of synthetic composite electrodes with different particle sizes ($5\,\mu m$, $10\,\mu m$, $15\,\mu m$): the yellow particles denote percolated particles in the electronic conduction clusters whereas the red particles represent unconnected particles. Reprinted with permission from Ref. 41, Copyright (2019), American Chemical Society.

transport across all possible combinations of particle surface orientations. Therefore, an in-depth understanding of the microstructural morphology such as particle sizes, size distribution, porosity and tortuosity are essential in optimising the electrode composite design.[41,75,282–284] In general, there are three different approaches to study the microstructures of a composite electrode. The first approach involves reconstructing the microstructures from real electrodes and measurement of the microstructural parameters using SEM,[120,282,284,285] Focussed-Ion-Beam Scanning Electron Microscopy (FIB-SEM)[272,283] or XCT.[281,284] The second approach is the numerical generation of synthetic electrode microstructures by ordered or disordered packing of spherical particles in a three-dimensional simulation box.[41,75] In the third approach, the microstructural behaviour can be described based on an assumed average particle coordination number and the percolation theory.[281,286]

2.3.3.1 Performance limiting mechanisms

Particle sizes of the composite electrode. The effects of the NMC particle sizes and LPS SE on the electrode performance were first investigated by Sakuda *et al.*[282] The NMC particles

had an average size of 9 μm and 5 μm, whereas the SE has an average size of 4 μm and 16 μm respectively.[282] They showed that the reversible capacity obtained with the SE-4 μm and NMC-5 μm is larger than those using SE-16 μm and NMC-9 μm.[282] Based on the complementary SEM results, the higher reversible capacity achieved with the smaller particles was attributed to the homogeneous distribution of SE particles and smaller void volume in the composite electrode.[282] This conclusion can be corroborated with the results obtained by Ito and co-workers,[285] who fabricated all-solid-state composite cells (In|LPS|LCO) by cold-pressing LPS coated LCO particles without the sintering process. Smaller particle sizes and narrower size distribution are often correlated to better rate performance due to shorter diffusion pathways of Li^+ and larger surface-to-volume ratio to enhance the interfacial kinetics.[287–290]

Effects of electronic conductivity. Strauss *et al.*[120] further studied the effects of non-coated NMC particles sizes on the capacity of the cells and categorised the particle sizes into three groups: NMC-Large ($d_{50} = 15.6\,\mu$m, $d_{90} = 26.1\,\mu$m), NMC-Medium ($d_{50} = 8.3\,\mu$m, $d_{90} = 13.0\,\mu$m) and NMC-Small ($d_{50} = 4.0\,\mu$m, $d_{90} = 4.8\,\mu$m). The loss in the specific capacities for NMC-M and NMC-L was correlated to the fraction of inactive materials. Based on the results obtained from the *ex-situ* XRD analysis, they showed that the fraction of inactive material increases from 2% for NMC-S to 27% for NMC-M and 31% for NMC-L. By measuring the mean ionic and electronic partial conductivity using ion or electron-blocking electrodes, the loss of inactive NMC is shown to be dominated by the electronic conductivity of NMC particles. The electronic conductivity of NMC particles decreases from 10^{-3} S cm^{-1} for NMC-S to 10^{-6} S cm^{-1} for NMC-L.[120]

The conclusions obtained by Ref. 120 are different from the experimental results shown in Ref. 75. Shi *et al.*[75] studied the effects of particle size on the specific capacity of the all-solid-state cell using NMC ($d_s = 5\,\mu$m, $d_L = 12\,\mu$m) as the AMs and LPS (1.5 μm – 8 μm) as the SE. They showed that the cell with larger NMC particle size has a higher specific capacity than the cell with smaller particle size. It should be noted that the NMC particles were coated with Li_2O-ZrO_2 in Ref. 75 but no coating was applied to the AMs in Ref. 120. The contradiction was attributed to the carbon additives in the composite material.[75] While carbon nanofibers were included in the composite PE in Ref. 75, no carbon additives were used in the experimental cells of Ref. 120 due to the severe degradation effects of the additives.[119] The use of carbon additives mitigates the electronic percolation limitation in the composite PE and therefore larger NMC particles were shown to deliver higher capacity compared to smaller NMC particles.

Effects of composite electrode composition. Zhang *et al.*[284] showed that composition electrode composition affects the electrode utilisation as either a high-energy or a high-power cell. The composite PE comprised of $LiNb_{0.5}Ta_{0.5}O_3$-coated LCO mixed with LGPS and were made in different mass ratios (LCO:LGPS in 40:60, 50:50, 60:40, 70:30 and 80:20). The accessible capacities of the composite cell increase with a higher mass ratio of LCO for low operating current densities (< 2C). For a high discharge C-rate (10C), they showed that the composite cell with 70% and 80% of LCO has no specific capacity compared to the composite cell with

50% and 60% of LCO loading. This result implies that a sufficient electrolyte fraction in the composite cell is necessary to facilitate fast transport of Li^+. The capacity retention of the composite cells was also analysed after 100 cycles. The cell with 70% of LCO was shown to retain 80% of the initial capacity.[284] This conclusion agrees very well with the experimental and modelling analysis by Shi and co-workers,[75] where they showed that an optimum electrode utilisation and high specific capacities could be achieved with 60-70 wt-% of NMC particles. The performance of a solid-state composite cell depends on optimising the electronic and ionic paths within the composite electrode: Too much of SE fractions prevent sufficient electronic pathways in the AMs, whereas too high of AM mass ratios limit the ionic transport within the network of electrode particles.[284]

2.3.3.2 Microstructural modelling of the composite electrode.

Reconstruction of the microstructural electrodes. From the reconstructed composite electrode based on FIB-SEM, Hlushkou *et al.*[283] proposed in their studies that the void phase could occupy up to 13.2% in the composite PE. Due to the void phase, the ionic transport in a composite electrode is reduced compared to that in an ideal composite electrode, where the ions migrate along the straight and uniform pathway. The reduction in ionic transport can be described with the parameter known as tortuosity. The simulated tortuosity in the reconstructed composite electrode is 1.74, which is close to the tortuosity estimated from the EIS measurement (1.6 ± 0.1). By replacing the void space with the SE in the model, they showed that the SE volume fraction could increase from 53.7% to 66.9%, and the tortuosity of the SE phase could be reduced from 1.74 to 1.27.[283] Finsterbush *et al.*[272] have also fabricated a fully inorganic, garnet-based all-solid-state cell and performed a 3D microstructure resolved continuum simulations of the composite cell (Li|LLZ:Ta|LLZ:Ta-LCO). The model predictions show a reasonable agreement with the experimental measurement at 100 °C but a significant deviation of 98% can be observed at room temperature.[272] While the choice of the representative reconstructed microstructures could be one possible reason causing this deviation, further works are necessary to identify whether the significant deviation is caused by physical phenomena not captured in the model or estimation of the model parameters at room temperature.

Table 2.4 A summary of modelling techniques with their applications and limitations in solid-state battery research

Modelling avenues	Applications/Advantages	Challenges and limitations	Ref.
DFT models	• Investigate atomistic structure, interfacial stability, synthesisability and conductivity of SEs; • Databases of DFT calculated energies of bulk structures, such as the Materials Project and the Open Quantum Materials Database, allow for the rapid calculation of grand potential phase diagrams and the assessment of interfacial stability of SE materials against both the NE and PE.	• Expensive so only small systems can be used (< 1000 atoms); • Enumerating all possible interface orientations between two materials is computationally challenging. Many studies thus use a limited number of interfaces, chosen based on experimentally observed orientations of the materials or by joining two low energy surfaces of the two materials.	[72–74] [53, 291, 292] [293–295]
Analytical models	• Low computational costs in modelling specific mechanisms;	• Interdependence and full coupling between solid-state electrochemistry and other mechanisms are often not represented by analytical models;	[39, 97, 113, 134]
Physics-based models	• Analyse the internal dynamics of a cell (*e.g.* overpotentials and concentration gradients); • Predict the battery behaviour under different operating conditions; • Design prototype for next-generation solid-state batteries.	• Requires extensive and even destructive experiments to estimate the model parameters; • Uncertainty and variability of the parameters could affect the model predictions; • High computational costs in solving coupled physics-based models.	[40, 60, 261] [7, 84]
Microstructural models	• Models the effects due to particle sizes, composite electrode distributions, volume fractions and voids on the cell performance; • Reconstructed microstructures using tomography resembles realistic electrode/SE compositions; • Random packing of spherical particles in synthetic microstructural models;	• The choice of representative reconstructured microstructures could affect the model predictions; • High computational costs to resolve the mesh and to solve coupled mechanisms; • High computational costs to account for the effects of carbon additives.	[41, 272, 283] [75, 285]
Transmission line models	• Estimate the internal resistance due to different components in a composite cell. • Predict the cell discharge behaviour under different operating conditions.	• The model assumes an ideal RC impedance behaviour. • The cell impedance must be converted into a time-dependent overpotential using a series of RC circuits.	[62]
Machine learning models	• High throughput discovery and screening of potential materials for solid-state batteries; • Can be combined with DFT models to predict structure-property relationships. • Deep convolution neural network can be used to track pores formation at the Li|SE interface.	• Requires a large amount of training and test datasets to achieve a high confidence in model predictions.	[55, 64, 192] [296, 297]

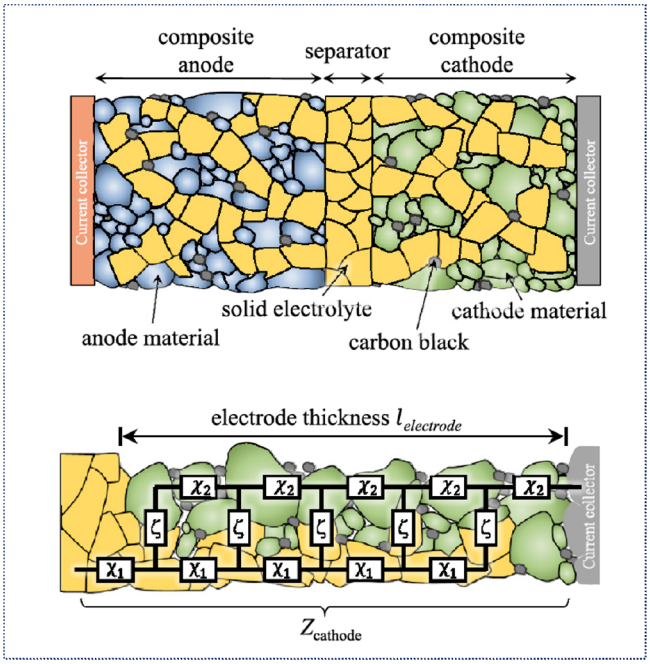


Figure 2.20 The 1D transmission line model represents the microstructure of a composite positive electrode ($Li_{10}GeP_2S_{12}$-$Li_4Ti_5O_{12}$). The yellow particles depict the SE fractions and are modelled by χ_1. The green particles denote the PE fractions and are modelled by χ_2 in the transmission line model. ζ describes the charge transfer at the interface and the solid-state diffusion in the AM. Reprinted with permission from Ref. 62, Copyright (2018), Elsevier.

Numerical generation of synthetic microstructure. Ito *et al.*[285] modelled the microstructural behaviour by placing the spherical particles randomly in a simulation box. The phase-field method was further used to obtain a smooth interface and to construct the 3D electrode microstructure.[285] Bielefeld *et al.*[41] generated synthetic 3D microstructures with particle sizes ranging from 3 μm to 15 μm to study the effects of particle size, volume fractions of AMs, composition, porosity and electrode thickness on the utilisation level and specific surface area of the composite electrode. The model accounts for the ionic conducting phase due to the SE and the electronic conducting phase due to the AMs. Smaller particles were shown to have higher electronic percolation and lower percolation threshold. The model prediction also demonstrated that the specific active interfacial area increases with smaller porosities, indicating that a denser composite electrode could form better conduction clusters.[41] However, the conclusions shown in Ref. 41 differ from the recent modelling works reported in Ref. 75. In Ref. 75, it was shown that a large ratio of d_{AM}/d_{SE} yields a high utilisation of the composite PE, whereas Ref. 41 showed that the electronic percolation decreases for larger electrode particles. Due to the computational limitation (10^{10} number of particles),[75] both models did not account for the carbon additives explicitly. Therefore, more modelling works that include carbon additives are required in the future to examine the overall effects of particle sizes and electronic conductivity on the performance of composite PE.

Transmission line model. Braun *et al.*[62] developed a one-dimensional homogenised transmission line model to estimate the internal resistance due to the ionic conducting phase of the SE

and the electronic conducting phase of the AMs in the composite cell (Figure 2.20). While the model predicts the cell discharge behaviour of LCO-LGPS|LGPS|$Li_4Ti_5O_{12}$-LGPS at near equilibrium and for low C-rate (< 7C) relatively well (with a maximum deviation of 13%), the model prediction deviates from the experimental measurement by 150% for high C-rates (> 45C).[62] The difference between experimental measurements and model predictions can be attributed to two possible reasons. Firstly, the 1D transmission line model assumes an ideal RC behaviour, whereas the experimental impedance measurements often exhibit a non-ideal RQ behaviour.[23,40,47,62] Secondly, the large deviation under high-current load could be caused by non-linear losses (see the description of NLEIS in Section 2.3.1.3). It is also worth noting that the cell impedance estimated from the transmission line model must be first converted into a time-dependent overpotential using a series of RC circuits. Therefore, transient cell behaviours cannot be predicted directly with the proposed model.[62]

2.4 Conclusions and perspectives

2.4.1 Review conclusions

The conclusions obtained through this literature review are compared against the research questions outlined in Section 1.3 as follows:

What are the impacts of electrochemical, chemical, thermal and mechanical properties of different inorganic SEs on the performance of solid-state Li-metal and Li-ion batteries?

A holistic approach is taken to describe the multiphysical behaviour of solid-state cells, encompassing their electrochemical, chemical, thermal and mechanical properties. Although LPS SE has a higher ionic conductivity and critical current densities than c-LLZO SE, LPS has a shear modulus much lower than c-LLZO. According to the linear elasticity analysis from Monroe and Newman,[17] the mechanical strength of LPS SE is just sufficiently compliant to suppress the Li filaments propagation. Nevertheless, the compounded effects between the shear modulus and critical current densities should be a subject of further investigation to understand the susceptibility of SEs to Li filamentary nucleation and penetration. On the other hand, oxide-based SEs were predicted *via* first-principles modelling to generate oxygen gas at higher voltages, which could react with the Li NE to cause adverse decompositions. Most importantly, all SEs should be manufactured and assembled under an inert environment: on exposure to air, LiPON generates PH_3 and NH_3 gas, whereas c-LLZO reacts to form LiOH and Li_2CO_3; LPS is hygroscopic and forms H_2S gas. Whether the release of these gases also poses a safety hazard if batteries are mechanically damaged during operation is yet to be established.

Which degradation mechanisms are dominant in solid-state batteries? What are the impacts of different operating conditions on the failure modes of solid-state batteries?

This review also summarises the impacts of multi-physics mechanisms on various degradation modes under different operating conditions. Besides the intercalation-induced stresses and SEs cracking, other degradation mechanisms include phase change and structural disordering, temperature and pressure-dependent Li creep, electrode-electrolyte interfacial decompositions, instability of carbon additives, surface voids, interfacial delamination, Li filamentary nucleation and current collector fracture. As summarised by Table 2.2, it is essential to note the effects of operating conditions on triggering different degradation mechanisms. While high operating temperatures reduce the electrolyte resistance and increase the critical current densities, operating at high temperatures also accelerates the interfacial decomposition and Li creep. Compared to low C-rates, although operating at high current densities could achieve higher power densities, but high C-rates also cause more electrolyte and electrode particle cracking, the formation of surface voids and Li filaments.

2.4.2 Perspectives

By reviewing the recent progress on experimental investigation and computational modelling, pathways for further investigation could be summarised as follows:

Performance limiting mechanisms. Although there are different avenues to improve the rate-performance of solid-state batteries, this chapter shows that a systematic design principle focussing on the critical mechanisms limiting the performance is lacking. While many studies have used experimental approaches to identify different bottlenecks, such methods are costly and time-consuming, especially when the performance-limiting mechanisms change under different operating conditions for various materials. Physics-based models could reveal the performance limiting mechanisms due to different cell components and materials for diverse application-relevant operating conditions. This research gap will be studied in Chapter 3 of this thesis, and guidelines for next-generation solid-state cell designs will be proposed.

Upscaling of solid-state batteries. Despite the advantages of inorganic SEs in terms of their non-flammability, solid-state Li-metal batteries have not reached the technical maturity to meet the energy and power densities demand of electric vehicles and aircraft. Most studies in the literature focus on researching the performance of a single-layer cell, whose capacity is insufficient to achieve the total energy and power output required for large-scale applications. By using dimensionless governing equations, the performance of different large-format solid-state Li-metal batteries can be studied and compared. A model-based upscaling approach will be further discussed in Chapter 4.

Thermal behaviour of large-format solid-state Li-metal batteries. Even if the transference number of the inorganic SEs is near-unity, solid-state batteries still generate a considerable amount of heat due to other processes such as activation overpotentials at the interface, solid diffusion overpotential in the electrode and joule heating from the current collectors and tabs. Significant heat generations could lead to temperature gradients in large-format solid-state Li-metal batteries, which will be analysed in Chapter 4 of this thesis.

Mechanical behaviour of inorganic solid electrolytes. Many existing literature reports have studied the mechanical behaviour and electrochemical ionic transport in an inorganic SE individually. In reality, the inorganic SE mechanical properties are correlated to the electrochemical transport properties such as diffusion coefficients and ionic conductivities. Chapter 5 reveals how fundamental mechanical properties such as brittleness and viscoelasticity affect the ionic transport in an inorganic SE.

Acknowledgements and author contributions

M.-C. Pang and X. Liu initiated and defined the framework of this review project. M.-C. Pang reviewed and wrote Section 2.1 and Section 2.3. Section 2.2 was reviewed and written by M.-C. Pang, K. Yang and R. Brugge. The perspectives were reviewed and written by M.-C. Pang, K. Yang, R. Brugge and T. Zhang. G. J. Offer, H. Wang, M. Marinescu, B. Wu, A. Aguadero, F. Pan and S. Yang supervised and reviewed the written manuscript.

Chapter 3

Experimental and numerical analysis of solid-state lithium-metal battery cells: understanding the performance limiting mechanisms and effects of cell design under pulse operating conditions

While there is an array of different possibilities to improve the rate performance of solid-state Li-metal batteries, there is a lack of systematic design principles to focus on the critical aspects of the cell design. The performance limiting mechanism in solid-state batteries under realistic operating conditions has received little attention.

In the literature, Danilov *et al.*[261] used the Nernst-Planck governing equation to model the ionic flux due to diffusion and migration in the SE and Fick's equation to model the transport mechanisms in the PE. The charge transfer kinetics at both interfaces were modelled using the Butler-Volmer's equations. Figure 3.1 illustrates the relationship of different equation elements used in the governing equations of Danilov *et al.*[261] The first drawback of this model is the description of the transport mechanisms in the SE, where both ohmic and concentration overpotentials are considered in the model. Because of considering the concentration gradients of mobile Li^+-ions across the SE, the transference number calculated with Danilov's parameters is 0.15.[261] This value is smaller than the transference number in standard liquid electrolytes $(0.3-0.5)$[243,247,298] and deviates significantly from the material description of the ceramic-based SE. Secondly, the model also considers an ionisation reaction in the SE to

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conserve the electroneutrality with Li^+ and n^-. As a result, the reaction rate in the electrolyte includes three additional parameters: (1) Li^+-ions recombination reaction rate, (2) dissociation rate constant in the SE and (3) fraction of free Li^+ ions in equilibrium.[261] As discussed in Chapter 2, due to the complexity of decoupling the various phenomena occuring in the SE, the feasibility of measuring these parameters in reality is low. Figure 3.2 summarises the list of parameters used in Danilov's model. Their model has 12 fitted, 3 designed, 3 fixed, 2 calculated and 1 measured parameters.[261] For a SE with a unity transference number, the transport mechanisms across the SE can be simplified to modelling with Ohm's law (see Section 3.1.2). This simplification allows the reduction of non-measurable parameters in the SE to one single parameter, which is the ionic conductivity that can be determined from EIS measurements. Although the present research has reduced the number of fitted parameters significantly compared to the literature, the rate-constant at the PE-SE interface is used as a free-standing fitting parameter in this work. Section 4.2.4 in Chapter 4 discusses the fitted rate-constant as a function of temperatures and the impact of using this parameter on the model prediction in terms of its sensitivity.

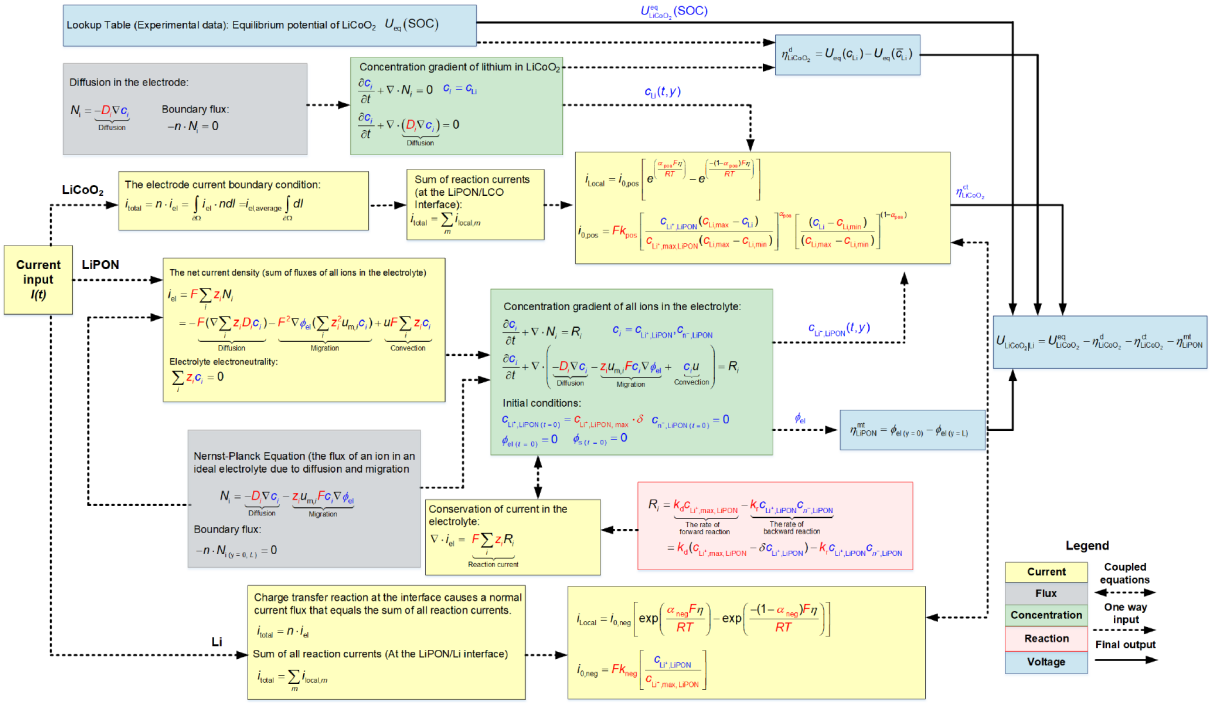


Figure 3.1 A flowchart constructed using the governing equations described by Danilov *et al.*[261] to link the governing equations and mechanisms represented in the SE and the PE.

Thirdlly, Danilov *et al.*[261] have also assumed the diffusion coefficient across the non-porous PE to be constant and has a value of $1.76 \times 10^{-15}\ m^2\ s^{-1}$. As shown by Fabre *et al.*[60] and the measurement in this thesis, the diffusion across the non-porous PE exhibits a non-linear behaviour, where the diffusion coefficient at low Li stoichiometry in the PE has an approximate range at $10^{-13}\ m^2\ s^{-1}$ and decreases with higher Li content in the PE towards $10^{-14} - 10^{-15}\ m^2\ s^{-1}$.

Model parameters				
Variable	**Parameter**	**Unit**	**Description**	**Source**
Geometry				
L	1500	nm	Thickness of electrolyte	Design parameter
M	320	nm	Thickness of electrode	Design parameter
A	1	cm^2	Geometrical surface area	Design parameter
Concentration				
$c_{Li+,\,max,\,LiPON}$	6.01E+04	mol/m^3	Total concentration of Li ions in Li_3PO_4 matrix	Measured
$c_{Li,\,max}$	2.33E+04	mol/m^3	Selected maximal activity of Li, positive electrode	Calculated
$c_{Li,\,min}$	$c_{Li,\,max}/2$	mol/m^3	Minimum Li concentration, positive electrode	Calculated
$c_{Li+,\,LiPON\,(t=0)}$	$c_{Li+,\,max,\,LiPON}$*delta	mol/m^3	Initial Li ion electrolyte concentration	Optimised
$c_{Li,\,(t=0)}$	$c_{Li,\,max}/2$*1.01	mol/m^3	Initial Li concentration, positive electrode	Optimised
Diffusion coefficients				
$D_{Li\text{-}ion}$	9.00E-16	m^2/s	Diffusion coefficient for Li ions in electrolyte	Optimised
$D_{n\text{-}}$	5.10E-15	m^2/s	Diffusion coefficient for n in electrolyte	Optimised
D_{Li}	1.76E-15	m^2/s	Diffusion coefficient for Li, positive electrode	Optimised
Charge transfer coefficients				
α_{pos}	0.6	-	Charge transfer coefficient, positive electrode	Optimised
α_{neg}	0.5	-	Charge transfer coefficient, negative electrode	Optimised
k_{pos}	5.10E-04	$mol/(m^2\ s)$	Rate constant charge transfer reaction, positive electrode	Optimised
k_{neg}	1.00E-02	$mol/(m^2\ s)$	Rate constant charge transfer reaction, negative electrode	Optimised
Reaction rate in the electrolyte				
delta	0.18	-	Fraction of free Li ions in equilibrium	Optimised
k_r	9.00E-09	$m^3/(mol\ s)$	Li ion recombination reaction rate	Optimised
k_d	k_r*$c_{Li+,\,max,\,LiPON}$*delta ^2/(1-*delta*)	1/s	Dissociation rate constant in electrolyte	Optimised
Global parameters				
C_rate	1	-	C rate parameter in parametric sweep	Fixed
i_1C	1.00E-05	A/cm^2	1C current	Fixed
T	298.15	K	Temperature	Fixed

Figure 3.2 A summary of the parameters used by Danilov and co-workers:[261] their model has 12 fitted, 3 designed, 3 fixed, 2 calculated and 1 measured parameters.

The discrepancy in modelling the ionic transport across the SE was addressed by Fabre *et al.*[60], where they proposed a one-dimensional charge/discharge mathematical model, in which Ohm's law was used to relate the electric potential to the current density in the PE and the SE. Although the modelling results were validated with experimental measurements, the performance limiting mechanisms due to different cell components have not been quantified and compared. Moreover, batteries are not always subjected to constant current charge and discharge, and the current profiles are often dynamic with varying pulse amplitudes. Therefore, an understanding of the cell's response to pulse current operations can contribute to the optimal cell design for next-generation solid-state Li-metal batteries. This research question is addressed in this work by first analysing the cell response under pulse discharge and charge experimentally and then constructing a physical model to help reveal the performance-limiting factors. Mathematical models can provide valuable insights into the mechanism limiting cell behaviour and thus form an essential tool in cell design and upscaling for applications. By using the physics-based model, a maximum thickness of the non-porous PE is identified to avoid unnecessary voltage loss and increased internal resistance under pulse operating conditions. A maximum ionic conductivity is also proposed, beyond which no further performance gains are obtained. Section 3.1 illustrates the governing model equations.

Section 3.2 describes the electrochemical test rig and the experimental procedures. Section 3.3 presents the experimental results and the data analysis for model parametrisation. Finally, in Section 3.4, the rate-limiting mechanisms under different application-relevant operating conditions are identified, and the model-based cell design optimisation is performed.

3.1 Model formulation

3.1.1 Computational domain

In general, three transient phenomena occur when the external current is interrupted: relaxation of the double-layer capacitance, local equalisation of the state-of-charge and reduction of concentration gradients in the solid electrode.[270] This work focuses on the continuum modelling of pulse behaviour and relaxation phenomena in solid-state Li-metal cells. Figure 3.3 illustrates the domain modelled in this work. Assuming isotropic material properties in the x- and y-direction, the three-dimensional model (xyz) was reduced to a one-dimension model (in the z-direction). As the NE is a pure Li metallic thin film, no ohmic losses were assumed across the thin film such that the model considers the SE and the PE only. Therefore, the origin of the z-axis was defined at the interface between the Li-metal and the SE.

During discharge, Li is oxidised to form Li^+-ions. The Li^+-ions migrate through the SE due to potential gradients. Reduction takes place at the interface between LiPON and LCO, and Li atoms diffuse into the PE. The reverse processes occur during charging.

3.1.2 Governing equations in the Solid Electrolyte (SE)

In the literature, the Poisson-Nernst-Planck (PNP) equation has been used at the microscopic[299] and the macroscopic level[253,300] to depict the transport mechanism in the SE. However, the mass transfer mechanism in the SE can also be represented with a simple Ohm's law.[60,245] The relationship between the comprehensive PNP model and Ohm's law is not well understood and has not been clearly described in the literature. This relationship will be illustrated in this section with the derivations based on the dilute solution theory.[81]

LiPON is a glassy inorganic SE developed by Bates *et al.*[301] at Oak Ridge National Laboratory. The acronym LiPON denotes an inorganic compound with the generic composition $Li_xPO_yN_z$, in which the stoichiometric coefficients are related to each other via the charge neutrality condition: $x = 2y + 3z - 5$.[302] Unlike conventional liquid electrolytes, where both cations and anions are mobile, only the Li^+ ions are mobile in the SE. Deng *et al.*[303] presented a detailed analysis of Li-ions conduction mechanism in the SE with the MD simulation method. Their simulation results

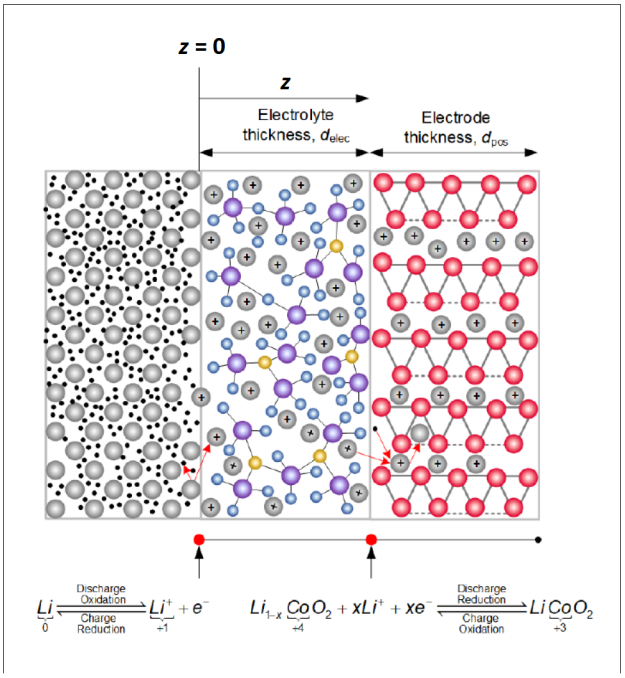


Figure 3.3 The model domain, where the origin of the z-axis is defined at the interface between the negative Li electrode and the LiPON SE. In this thesis, z-axis denotes the through-plane coordinate.

propose a cooperative knock-on like mechanism: the migrating interstitial Li^+ displaces another Li^+ towards a neighbouring site, which subsequently leads to a further Li^+ migration. Hence, the inorganic SE used in Li-metal batteries is often known as a single cation ionic conductor. The transference number for Li^+, T^+ can be defined as the amount of Li per Faraday of charge carried by migration across the SE.[244] The transference number for SE is established by Patterson to be greater than 0.99.[304] When $T^+ \approx 1$, only the flux of Li^+ constitutes the electric current. At the continuum level, it can be assumed that the rate of migration is equal to the rate of oxidation or reduction. This assumption has two implications. Firstly, there will be no concentration gradients of Li^+ and therefore no concentration polarisation in the SE. This assumption has been shown valid through the *operando* NDP measurement of Li concentration profiles in the SE, where a constant concentration has been observed in the bulk SE (LiPON) at different times (see Figure 2.15).[31] Secondly, this assumption implies that the impacts due to degradations such as voids formation and Li creep are not considered in current works, where the rate of migration will not be the same as the rate of oxidation or reduction at the NE-SE interface.[26] The effects of degradation on cell performance will be a subject of further investigations in future works.

Based on the single-cation conduction mechanism and the unity transference number of the inorganic SE, the Nernst-Planck equation (Equation 3.1), which represents the flux of species in the SE, can be simplified by removing the diffusion term. Because the SE does not move at any point of time, the convection term can also be eliminated. Generally, the Nernst-Planck equation is strictly applicable to describe the mass transfer mechanism in a dilute solution only, *i.e.* when the ionic species do not interact with each other in the electrolyte.[81] This assumption is deemed valid because only Li-ions are the only mobile ions in the inorganic SE and no reactions occur

between these mobile cations and the neighbouring atoms. Therefore, the flux density of the only mobile species in the electrolyte, Li^+, is given by:

$$\underbrace{N_{Li^+}}_{\text{flux density of species } Li^+} = \underbrace{-D_{Li^+}\frac{\partial c_{Li^+}}{\partial z}}_{\text{diffusion}} \underbrace{- z_{Li^+} u_{Li^+} F c_{Li^+} \frac{\partial \phi_{elec}}{\partial z}}_{\text{migration}} + \underbrace{c_{Li^+} v}_{\text{convection}}, \tag{3.1}$$

where D_{Li^+} is the diffusion coefficient of Li-ions in the SE, c_{Li^+} is the concentration of Li-ions in the SE, $\partial c_{Li^+}/\partial z$ is the concentration gradient due to diffusion in the electrolyte, z_{Li^+} is the number of proton charges carried by an ion, u_{Li^+} is the mobility of Li-ions in the electrolyte, $\partial \phi_{elec}/\partial z$ is the potential gradients, F is the Faraday's constant ($F = 96,485\,\mathrm{C\,mol^{-1}}$) and v is the bulk velocity of the SE.

The flux of charged particles constitutes the current, i in the electrolyte. This mechanism can be represented as:

$$i = F \sum_i z_{Li^+} N_{Li^+}. \tag{3.2}$$

Combining Equation 3.1 and 3.2, the current in the electrolyte becomes

$$i = -\underbrace{F^2 \sum_i z_{Li^+}^2 u_{Li^+} c_{Li^+}}_{\text{Electrolyte conductivity}} \frac{\partial \phi_{elec}}{\partial z}. \tag{3.3}$$

By defining the ionic conductivity as the sum in front of the differential $\partial \phi_{elec}/\partial z$, Equation 3.3 becomes

$$i = -\sigma_{elec} \frac{\partial \phi_{elec}}{\partial z}. \tag{3.4}$$

Equation 3.4 is equivalent to Ohm's law, in which the current density is proportional to the potential gradient. This expression was used for solid-state Li-metal cell modelling by Fabre *et al.*[60] to simulate a constant current charge and discharge profile in the solid-state battery, and by Thomas-Alyea[245] to describe an electrochemical model for a porous solid anolyte, in which Li could deposit on the surface of the electrolyte to reduce the risk of cracks due to dendrites. The current work focuses instead on the effects of pulse current profiles on cell behaviour and identifying the rate-limiting mechanism for different pulse operating conditions.

Usually, the Poisson equation in the PNP expression is used to describe the non-constant electric field at the electrode-electrolyte interface ($\leq 10\,\mathrm{nm}$) due to unequal distribution of cations and

anions.[253,300] Instead, this model conserves charge through a one Li^+ in and a one Li^+ out in the Butler-Volmer's boundary conditions. Uniform current is imposed throughout the electrolyte:

$$\frac{\partial i}{\partial z} = 0. \tag{3.5}$$

3.1.3 Governing equation in the Positive Electrode (PE)

The governing equation describing the Li transport in the positive LCO electrode is the Fick's second law of diffusion (Equation 3.6). As the experimental characterisation results show that the diffusion impedance changes with the SOC, the diffusion coefficient in the PE is modified to be dependent on the amount of (de-)intercalated Li:

$$\frac{\partial c_{\mathrm{Li}}}{\partial t} = \frac{\partial}{\partial z}\left(D_{\mathrm{Li}}(x_{\mathrm{Li}})\frac{\partial c_{\mathrm{Li}}}{\partial z}\right), \tag{3.6}$$

where c_{Li} is the Li concentration, D_{Li} is the solid diffusion and x_{Li} is the Li stoichiometry in the PE. The concentration-dependent solid diffusion mechanism will be further elucidated in Section 3.3.3. Depending on the SOC, LCO has an electronic conductivity of $14-31\ \mathrm{S\,cm^{-1}}$ at 25 °C.[305] As this electronic conductivity is 10^7 orders of magnitude higher than the ionic conductivity in the SE, the potential drop due to the mobility of electrons in the non-porous PE is negligible. Therefore, for a non-porous PE, the cell voltage in the model can be determined by solving the surface electrode potential across the SE.

3.1.4 Boundary conditions

The two boundary conditions required for solving the governing equations in the SE domain are described as follows:

$$\phi_{\mathrm{elec}}\Big|_{z=0} = 0, \tag{3.7}$$

$$\sigma_{\mathrm{elec}}\frac{\partial \phi_{\mathrm{elec}}}{\partial z}\Big|_{z=d_{\mathrm{elec}}} = i_{\mathrm{pulse}}, \tag{3.8}$$

where i_{pulse} is the externally applied pulse current density. The initial conditions for each pulse were taken from the initial voltage given by experimental measurements.

The Butler-Volmer equations were used to describe the rate of Li flux between the domains. By using the Butler-Volmer equation, it is assumed only one reaction is occurring at the interface, and that the current is proportional to the net rate of the reaction given by the difference

between the rate of anodic reaction (*i.e.* the first term in Equation 3.9 and 3.10) and the rate of cathodic reaction (*i.e.* the second term):[81]

$$i = i_{0,\mathrm{neg}}\Bigg[\underbrace{\exp\left(\frac{\alpha_{\mathrm{neg}} F \eta_{\mathrm{neg}}}{R_{\mathrm{gas}} T}\right)}_{1} - \underbrace{\exp\left(\frac{-(1-\alpha_{\mathrm{neg}}) F \eta_{\mathrm{neg}}}{R_{\mathrm{gas}} T}\right)}_{2}\Bigg], \tag{3.9}$$

$$i = i_{0,\mathrm{pos}}\Bigg[\underbrace{\exp\left(\frac{\alpha_{\mathrm{pos}} F \eta_{\mathrm{pos}}}{R_{\mathrm{gas}} T}\right)}_{1} - \underbrace{\exp\left(\frac{-(1-\alpha_{\mathrm{pos}}) F \eta_{\mathrm{pos}}}{R_{\mathrm{gas}} T}\right)}_{2}\Bigg], \tag{3.10}$$

where α_{neg} and α_{pos} are the charge transfer coefficients, which denote the fraction of applied potential that favours the respective reactions;[81] R_{gas} is the universal gas constant ($R_{\mathrm{gas}} = 8.314\,\mathrm{J\,mol^{-1}\,K^{-1}}$), T is the cell temperature, $i_{0,\mathrm{neg}}$ and $i_{0,\mathrm{pos}}$ are the exchange current densities at the respective interface. While $i_{0,\mathrm{neg}}$ is determined from the experimental measurement, $i_{0,\mathrm{pos}}$ is dependent on the Li concentration at the interface between the SE and the PE:[60]

$$i_{0,\mathrm{pos}} = F k_{\mathrm{pos}} (c_{\mathrm{LCO,max}} - c_{\mathrm{Li}})^{\alpha_{\mathrm{pos}}} (c_{\mathrm{Li}})^{1-\alpha_{\mathrm{pos}}}, \tag{3.11}$$

where k_{pos} is a free-standing fitting parameter in this model and $c_{\mathrm{LCO,max}}$ is the theoretical maximum molar density of Li in the PE.

$\eta_{\mathrm{pos/neg}}$ is the overpotential defined as the potential difference between the respective electrode potential, ϕ_{s} and that of the SE, ϕ_{elec}, minus the open-circuit potential of the electrodes, U:[81]

$$\eta_{\mathrm{pos/neg}} = \phi_{\mathrm{s}} - \phi_{\mathrm{elec}} - U. \tag{3.12}$$

Solving the governing equation in the PE required two additional boundary conditions. The first boundary conditions (at the LiPON-LCO interface) describes the Li flux density into the PE and can be represented by Fick's first law as follows:

$$D_{\mathrm{Li}}(x_{\mathrm{Li}}) \frac{\partial c_{\mathrm{Li}}}{\partial z}\bigg|_{z = d_{\mathrm{elec}}} = -\frac{i}{F}. \tag{3.13}$$

The second boundary condition in the PE domain stipulates a zero-flux condition at the electrode and current collector interface, as Li cannot diffuse into the current collector:

$$D_{\mathrm{Li}}(x_{\mathrm{Li}})\frac{\partial c_{\mathrm{Li}}}{\partial z}\bigg|_{z\,=\,d_{\mathrm{elec}}+d_{\mathrm{pos}}} = 0. \tag{3.14}$$

The system of DAEs in this continuum model was solved using the finite element method in COMSOL Multiphysics® V5.4.

3.2 Experimental procedures for parametrisation and model validation

Pulse current experiments were carried out to characterise the cell behaviour at different SOCs and 25 °C ambient temperature followed by the impedance experiments to measure the model parameters. As this model focuses on understanding the cell response to the pulse operations, the experimental pulse discharge and charging measurements were also used as model validations in this work. This section describes the experimental setup (Section 3.2.1), followed by experimental procedures to characterise the relaxation behaviour and measure the model parameters (Section 3.2.2).

3.2.1 Experimental setup

Experiments were conducted on solid-state microcells from ST Microelectronics (Enfilm™ EFL700A39, nominal capacity $0.7-1.0$ mAh and nominal voltage window $3.0-4.2$ V) with Li NE, LiPON SE and LCO PE.

Larfaillou *et al.*[63] showed that the non-porous PE has a thickness of $5-8\,\mu$m, whereas the SE has a thickness of $2-4\,\mu$m. The cell encapsulation has a surface area of $4\,\mathrm{cm}^2$. However, the graphical representations of the internal structures published by STMicroelectronics reveal a different size of the interfacial area between the two electrodes and the electrolyte within the encapsulation (see Figure 3.4).[63,235] These two schematics imply that the internal cell architectures were not drawn to scale. In fact, in a modelling study affiliated with STMicroelectronics, Fabre *et al.*[60] mentioned explicitly that the exact surface area is unknown. Therefore, the surface area in this work was approximated with a length and width of 1.4 ± 0.2 cm. The parameters calculated with this approximation (Table 3.2) were compared with literature values[60] and show a reasonable agreement.

The cells were placed inside a transparent housing on top of a Peltier element thermoelectric cooler (European Thermodynamics APH-127-10-25-S: 17 W, 1.9 A, $\Delta T = 68$ K), which was used to control the cell's temperature throughout the experiments. The thermocouples type K were fixed on the surface of the cell. The Peltier element inside the transparent housing was attached to an aluminium cooling block, which was used as a heat sink with a through-hole for water flowing. The water flow through the aluminium blocks was maintained via

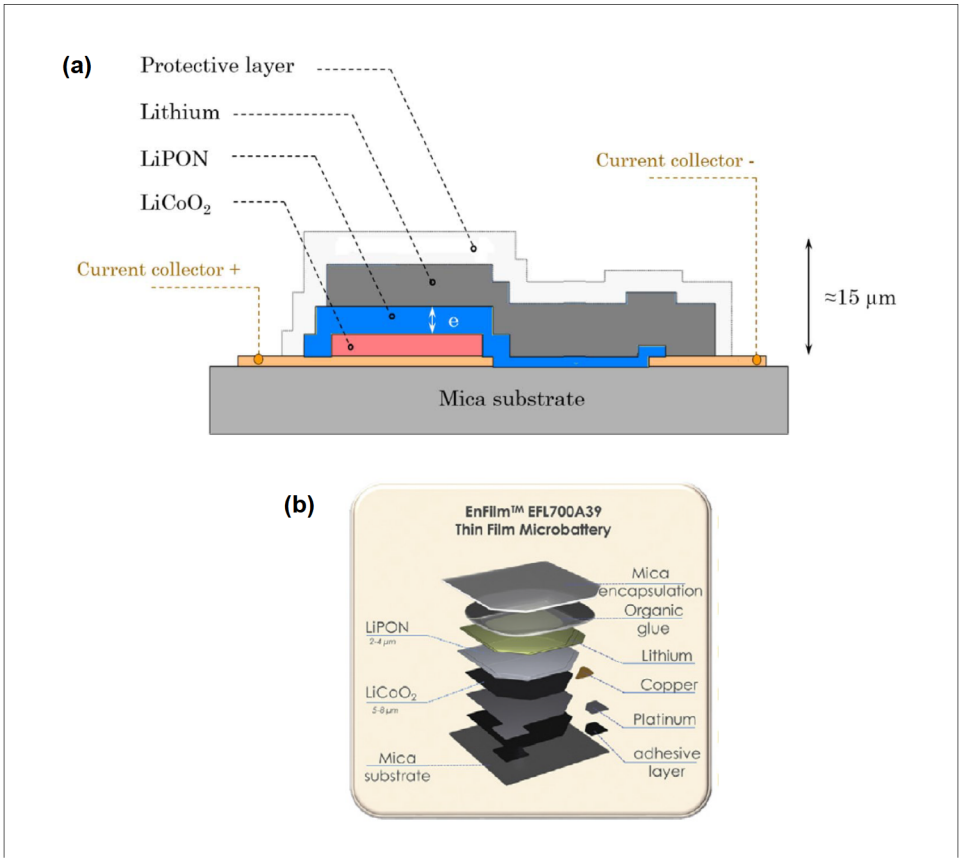


Figure 3.4 The internal architecture of solid-state Li-metal cell: both graphical representations published by STMicroelectronics reveal different cell architectures, implying that the exact electrochemical active surface area cannot be estimated precisely. Figure (a) is reprinted with permission from Ref. 235, Copyright (2015), The Electrochemical Society. Figure (b) is reprinted with permission from Ref. 63, Copyright (2016), Elsevier.

a water pump. A radiator was also used to dissipate the heat into the environment. Six identical rigs were constructed to run parallel experiments under different operating conditions. The electrochemical experiments were conducted with Gamry Interface 1000 (frequency range: 10 μHz − 1 MHz; current range: 10 nA − 1 A).

3.2.2 Experimental procedures

A combination of Galvanostatic Intermittent Titration Technique (GITT) and Potentiostatic Electrochemical Impedance Spectroscopy (PEIS) techniques was deployed to characterise cell behaviour and measure the model parameters. The experimental procedures from Birkl *et al.*[306] were adapted to include PEIS measurements at the open-circuit voltage of each pulse. The cell was first equilibrated at 25 °C by using the temperature control with the Peltier element before being charged with a CC-CV procedure to 4.2 V and relaxed for three hours. Complex impedance as a function of frequency from 1 mHz to 1 MHz with an AC signal of 5 mV was then performed to measure the impedance of the cell. After the first PEIS characterisation, the cell was discharged with a current of 0.1C to remove 10% of the nominal cell capacity. After the

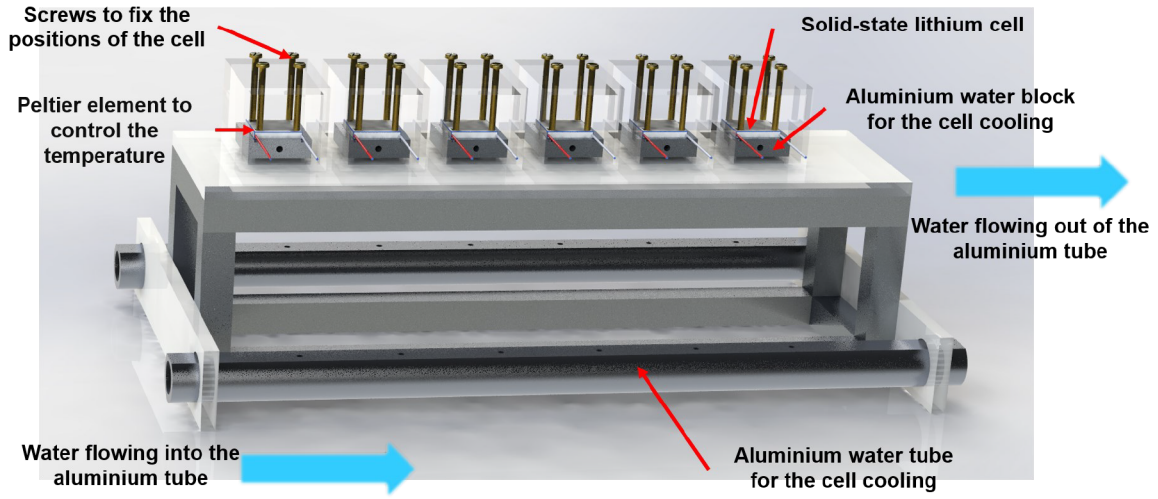


Figure 3.5 Schematic drawing of the electrochemical test bench: The test bench consists of six rigs to run parallel experiments under different operating conditions. The cells were placed on top of Peltier Element thermoelectric coolers, which were attached to aluminium blocks.

current was interrupted, the cell was relaxed for 3 h before the next PEIS measurement. The cell was subsequently discharged at 0.1C followed by the voltage relaxation and PEIS measurement until the cell voltage reached the lower limit of 3 V.

PEIS was implemented at the open-circuit voltage of each pulse in order to characterise the impedance of the cell as a function of SOC. From the impedance spectra, the ionic conductivity of the SE, exchange current densities and the concentration-dependent diffusion coefficient of Li in the PE were extracted. OCV as a function of Li content was also measured.

3.3 Experimental characterisation results and parameters analysis

This section first describes the experimentally measured pulse behaviour (Section 3.3.1) and the PEIS impedance spectra obtained as a function of SOC (Section 3.3.2). As the impedance spectra are subsequently used to estimate the values of model parameters, the linear Kramers-Kronig validity test was used to quantify the experimental reliability in the measurements. Distribution of relaxation times analysis is used to help identify the electrochemical processes in the solid-state Li-metal cell. Finally, Section 3.3.3 discusses how the model parameters were obtained from the experimental data measurements.

3.3.1 Pulse behaviour

Figure 3.6(a) shows the voltage measurement during the pulse discharge at 0.1C. Figure 3.6(b) shows how information is extracted from the experimental pulse measurements. Transient

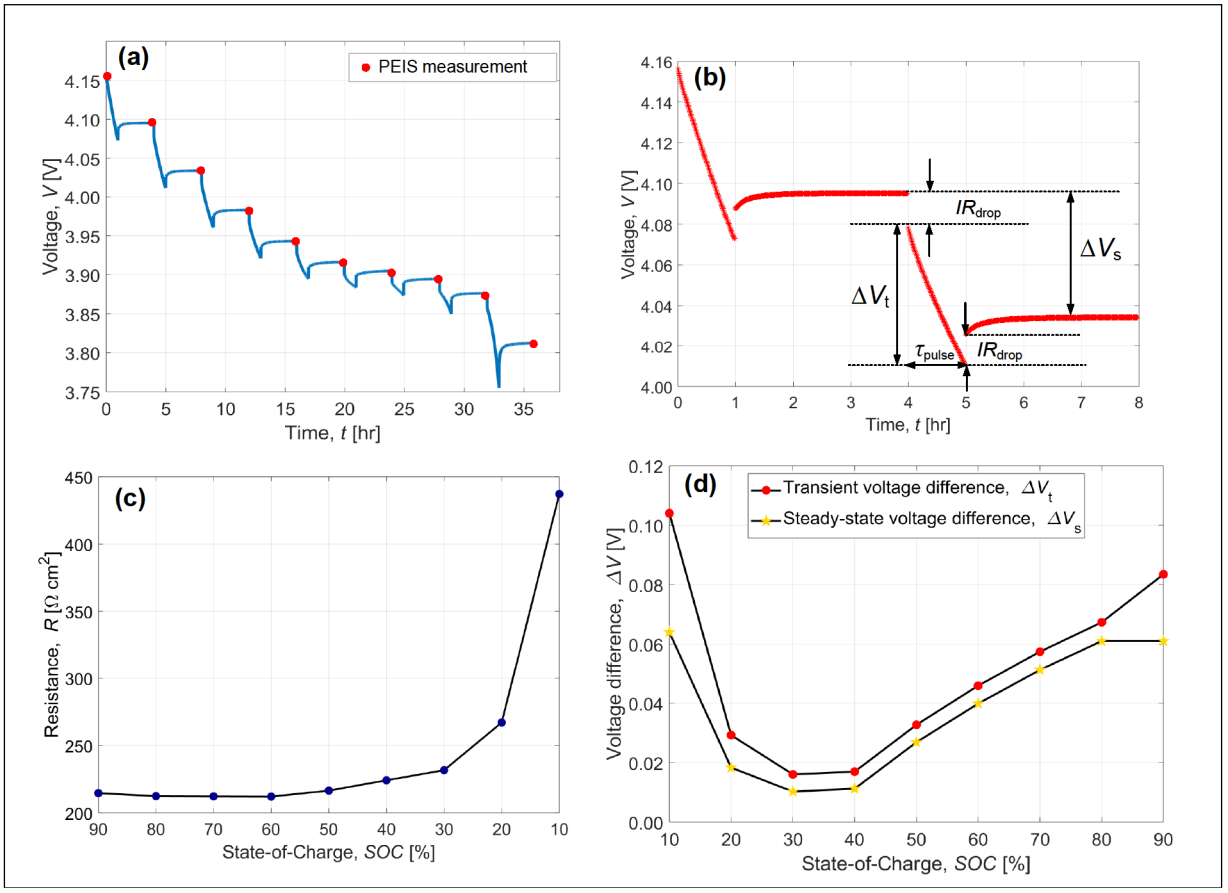


Figure 3.6 (a) Experimentally measured pulse discharge and OCV with the GITT method. The red dot indicates the point in time, at which the PEIS measurement was taken. (b) An illustration on how ΔV_t, ΔV_s, τ_pulse and IR_drop are extracted from the experimental data. (c) The calculated resistance for all pulses: The resistance have similar values from 90% SOC to 30% SOC, but a significant increase can be observed for SOC less than 30%. (d) The increase in ΔV_t and ΔV_s at the end of SOC can be correlated to the increase in the cell internal resistance.

voltage difference, ΔV_t can be calculated by determining the voltage difference of each pulse discharge, and steady-state voltage difference, ΔV_s can be calculated from the voltage difference between two consecutive relaxation points. The pulse time constant, τ_pulse is the period of each pulse discharge, whereas the voltage drop, IR_drop is the instantaneous voltage drop at the beginning of each pulse or the end of each pulse. Figure 3.6(c) illustrates the calculated cell internal resistance for all pulses. The internal resistance of the solid-state Li-metal cells obtained from GITT is several orders of magnitude higher than Li-ion cells, which is usually in the $m\Omega$ range.[56,307] The internal resistance increases marginally at the beginning of SOC but rises drastically to $\approx 450\,\Omega\,\mathrm{cm}^2$ at the end of discharge. The calculated ΔV_t and ΔV_s for each pulse is displayed in Figure 3.6(d). Both ΔV_t and ΔV_s first decrease from the first pulse discharge towards the sixth pulse discharge but increase drastically at the end of SOC due to the rise in the cell internal resistance.

3.3.2 Impedance and distribution relaxation times analysis

Figure 3.7(a) shows the impedance spectra at the 90% and 10% SOC. The possible assignment of the semi-circles to the corresponding physical mechanism will be discussed along with the DRT analysis. The tail of the impedance spectra is attributed to diffusion and varies most between the two SOCs. The diffusion impedance at 90% SOC has a nearly 90° slope, whereas the diffusion impedance at 10% SOC has a nearly 45° slope. As SOCs decreases, the gradient of the diffusion slopes decreases and the magnitude of the impedance increases. The near 90° angle diffusion as observed at 90% SOC can be associated to a large ratio of $D_{\mathrm{Li}}/d_{\mathrm{pos}}^2$ (*i.e.* a thin electrode or a large diffusion coefficient) whereas the near 45° angle diffusion at 10% SOC can be correlated to a small ratio of $D_{\mathrm{Li}}/d_{\mathrm{pos}}^2$ (*i.e.* a thick electrode or a small diffusion coefficient).[308] In this work, as the impedance spectroscopy was carried out under the same frequency sweep on the same cell and assuming a negligible change of thickness during the impedance measurement, the most probable explanation for the difference in the experimental measurement of the impedance spectra is the decrease in the effective diffusion coefficient as the depth-of-discharge increases. The linear Kramers-Kronig validity test[309] was used to quantify the experimental reliability in the impedance measurements. Figure 3.7(b) shows the residual plots of the impedance spectra at 90% SOC and 10% SOC. The Kramers-Kronig relation tests the stability, causality and linearity of the impedance measurement.[310–312] A high residual denotes the failure of the experimental measurements.[312] In this work, the impedance measurement residual plots indicate an acceptable deviation of approximately $\pm\,0.5\%$. Detailed discussions on the linear Kramers-Kronig validity test can be found in Appendix F.3.

In this study, an equivalent circuit model fitted to experimentally measured impedance data was constructed to extract electrochemical parameters required by the continuum model. Equivalent circuit model fits can be ambiguous since the different arrangement of the circuit elements can be fitted to obtain similar impedance curves.[313] As the cell polarisation processes often appear convoluted in the Nyquist or Bode plots,[314] the Distribution Function of Relaxation Times (DRT) analysis[315] is used to distinguish the electrochemical processes in the solid-state Li-metal cell *via*[313,315,316]

$$\begin{aligned} Z(\omega) &= R_{\mathrm{ohmic}} + Z_{\mathrm{pol}}(\omega), \\ &= R_{\mathrm{ohmic}} + \sum_{k=1}^{N} \frac{R_{\mathrm{pol,k}}}{1 + j\omega\tau_{\mathrm{k}}}, \end{aligned} \tag{3.15}$$

where R_{ohmic} is the frequency-independent ohmic resistance, and $Z_{\mathrm{pol}}(\omega)$ denotes the polarisation part of the impedance.[313,315,316]

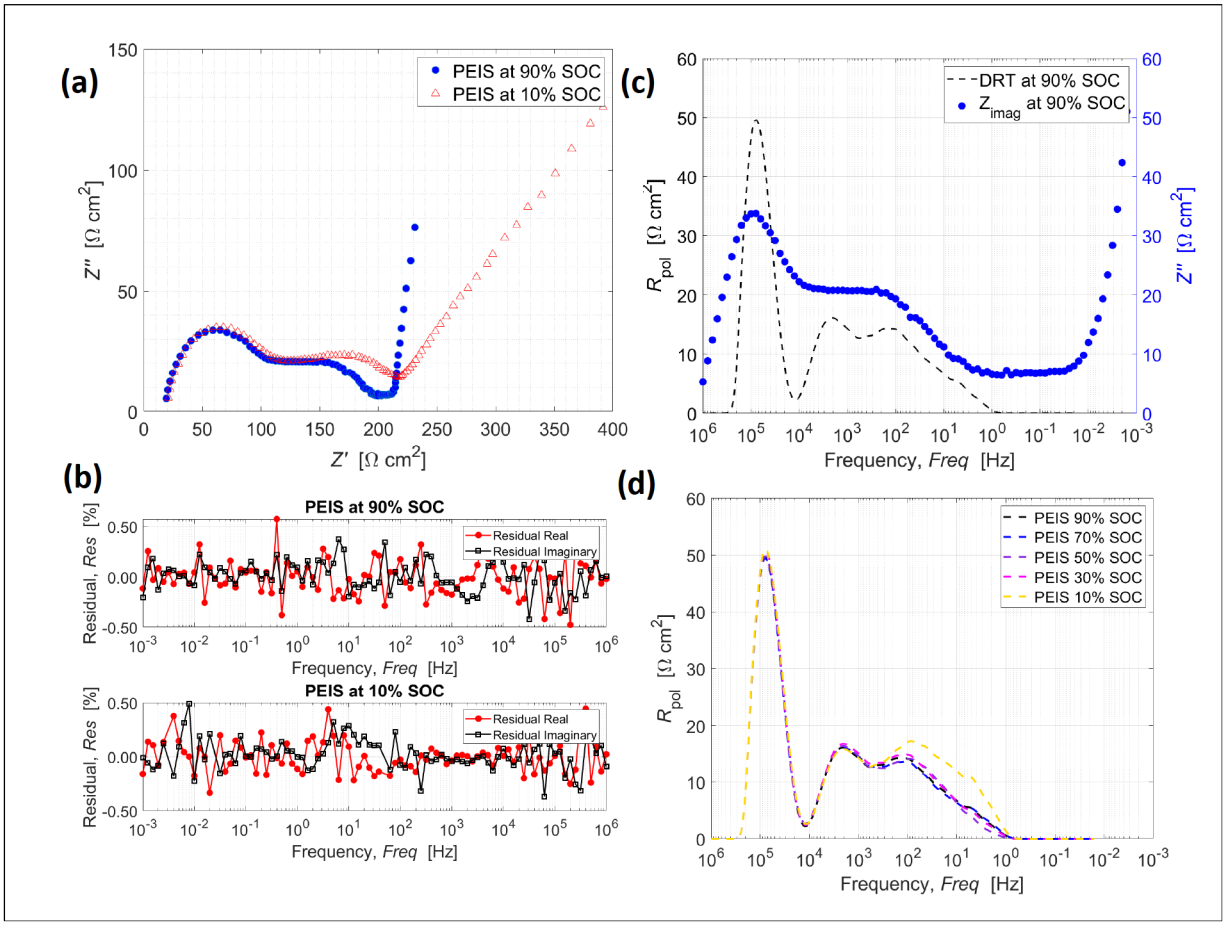


Figure 3.7 (a) Experimentally measured PEIS at 90% SOC (blue marker) and 10% (red marker) SOC. (b) Relative errors of the real and imaginary experimental data: The experimental data have residuals of $\approx \pm 0.5\%$ and a maximum residual of 0.57%, which means the measurements are compliant with the KK-relations. (c) Imaginary part of the PEIS compared to the DRT spectrum: the DRT analysis reveals a third semi-circle within the convoluted semi-circles from the PEIS measurement. The impedance spectrum due to the diffusion in the PE was truncated for the DRT analysis (black dashed line). (d) Overlay of the DRT spectrum as a function of SOC: although the ionic conductance and charge transfer at both interfaces change marginally between 90% and 30% SOC, at a low SOC such as 10%, the size of the third DRT peak increased.

The time constant of each process can be determined from the characteristic frequency, f_c corresponding to the local maxima of the peaks in Figure 3.7(c) via $\tau_{DRT} = 1/2\pi f_c$. While the DRT analysis is useful to separate the polarisation processes in the Nyquist plots, this empirical analysis has one limitation when applied to batteries. The boundary conditions for the DRT calculation require the complex impedance to tend to zero at high and low-frequency extremes.[317] As shown in Figure 3.7(a), the spectra show an increasing impedance modulus due to diffusion at low frequencies. Pre-processing of the impedance data is, therefore, necessary to subtract the low-frequency branch due to the diffusive behaviour of the cell before evaluating the spectra with the DRT method.[317] Due to this limitation, a simple expression is used to estimate the characteristic time due to diffusion, τ_{diff} in the PE:[216]

$$\tau_{\text{diff}} = \frac{d_{\text{pos}}^2}{D_{\text{Li}}(x_{\text{Li}})}, \tag{3.16}$$

where d_{pos} is the thickness of the PE and $D_{\text{Li}}(x_{\text{Li}})$ is the experimentally measured diffusion coefficient.

Table 3.1 The attribution of semi-circles to the possible physical mechanisms: the calculated time-constants show that the two processes identified by Iriyama *et al.*[211] as ionic conductance and charge-transfers happen between the microseconds and milliseconds timescale

Frequency range [Hz]	Time-constant,τ_{DRT} [s]	Possible cause
$10^6 - 10^4$	2.0×10^{-6}	Ionic conductance in the SE
$10^4 - 630$	7.5×10^{-5}	Charge-transfer at the Li-LiPON interface
$630 - 1$	9.8×10^{-4}	Charge-transfer at the LiPON-LCO interface

Figure 3.7(c) shows the comparison between Z_{imag} to the DRT spectrum. While only two semi-circles are apparent from Figure 3.7(a), the DRT analysis reveals the third semi-circle at 162 Hz. Figure 3.7(d) illustrates DRT spectra at different SOCs. Figure 3.7(d) shows that the peaks of the DRT spectra vary only marginally with the SOC. A small fourth peak can be observed towards the end of discharge. Because this peak has a maximum value ($R_{\text{pol}} \approx 10\,\Omega\,\text{cm}^2$), the contribution of this polarisation resistance is not considered in the present study.

Iriyama *et al.*[211] has previously assigned the first semi-circle to the electrolyte resistance in LiPON and the second semi-circle to the charge-transfer resistance at the Li|LiPON interface, based on the impedance measurement of the Pt|LiPON|Pt symmetric blocking cell and the Li|LiPON|Li symmetric non-blocking cell. They attributed the third semi-circle with the diffusion tail to the charge transfer at the LiPON|LCO interface and the diffusion tail in the LCO by using the full cell Li|LiPON|LCO impedance measurement.[211] Here, the same association is made. Table 3.1 summarises the frequency range and time-constant corresponding to each electrochemical process. The calculated time-constants show that the interfacial kinetics occur between the microseconds and milliseconds timescale.

This result implies that the double-layer capacitance effects are negligible for pulses above 0.2 s. This experimental finding can be correlated to Ong and Newman's modelling result,[252] who have modelled the double-layer capacitance in a dual Li-ion insertion cell. They showed that the double-layer capacitance shorts only the surface overpotential at milliseconds. After this short time, the potential continues to change due to the strong dependence of U on Li's local concentration in the electrode. Unlike an inorganic SE where only the cations are mobile, the electrolyte used by Ong and Newman to study the double-layer capacitance is PC + 1 M $LiClO_4$, in which both the cations and anions are mobile and accumulate at the interfaces.[252] Therefore,

the electrochemical model in this Chapter was extended to evaluate the effects of double-layer capacitance on the performance of solid-state lithium-metal batteries.

A detailed discussion on how the space-charge formation affects the performance of solid-state Li-metal cells can be found in Appendix F. While the space-charge effects are found to be negligible at low current densities, the instantaneous voltage drop corresponding to the space-charge contributions could cause an initial voltage drop approaching 0.18 V under 5C discharge at 25 °C. Nevertheless, as the operating temperature increases to 45 °C, the magnitude of initial voltage drop decreases, indicating that the space-charge formation is less significant due to a more homogenous charge distribution at high temperatures. The instantaneous voltage drop caused by the space-charge formation was found to occur in less than one second in the space-charge cell model. Above this short time-constant, the space-charge effects do not affect the cell performance under different operating conditions evaluated in the model (0.1C to 5C discharge for an operating temperature window from 25 °C to 45 °C), corroborating the conclusions obtained by Ong and Newman (*i.e.*, the capacitive effects short the surface overpotential at very short time-constant).[252]

3.3.3 Model parametrisation

Most of the electrochemical parameters used in this model to describe the pulse behaviour in the solid-state Li-metal cell were estimated based on experimental measurements. The Complex Non-Linear Least Squares (CNLS) algorithm was used in conjunction with the DRT analysis to fit the measured impedance spectra. The resulting equivalent-circuit model has three R-CPE pairs (Figure 3.8(a)), in which the time constants and frequency ranges of each R-CPE pair correspond approximately to the characteristic frequency and range of the DRT peaks. After estimating the semi-circle size, these were used as the starting conditions for the equivalent-circuit model to calculate the resistance of each semi-circle. By using the values obtained from the CNLS fitting, an impedance simulation was also performed to ensure that the semi-circles representing each electrochemical process do not cross (Figure 3.8(a)). The parameters estimated with the PEIS measurements are the exchange current densities, the ionic conductivity of the SE and diffusion coefficients in the non-porous PE. These parameters were calculated with Equations (3.17 - 3.23). The calculated parameters are shown in Figure 3.8c and Table 3.2.

3.3.3.1 OCV as a function of lithium content

Because Li is used as the NE, and its voltage is 0 V vs Li/Li^+, the equilibrium voltage of the cell is the equilibrium voltage of the PE. At equilibrium, the rate of the forward reaction is equal to the rate of the backward reaction. The electrode potential is then the electrochemical potential of electrons in equilibrium with the reactant and the product species.[81] When the open-circuit voltage of the cell is measured, the amount of Li intercalated into the PE can be deduced.

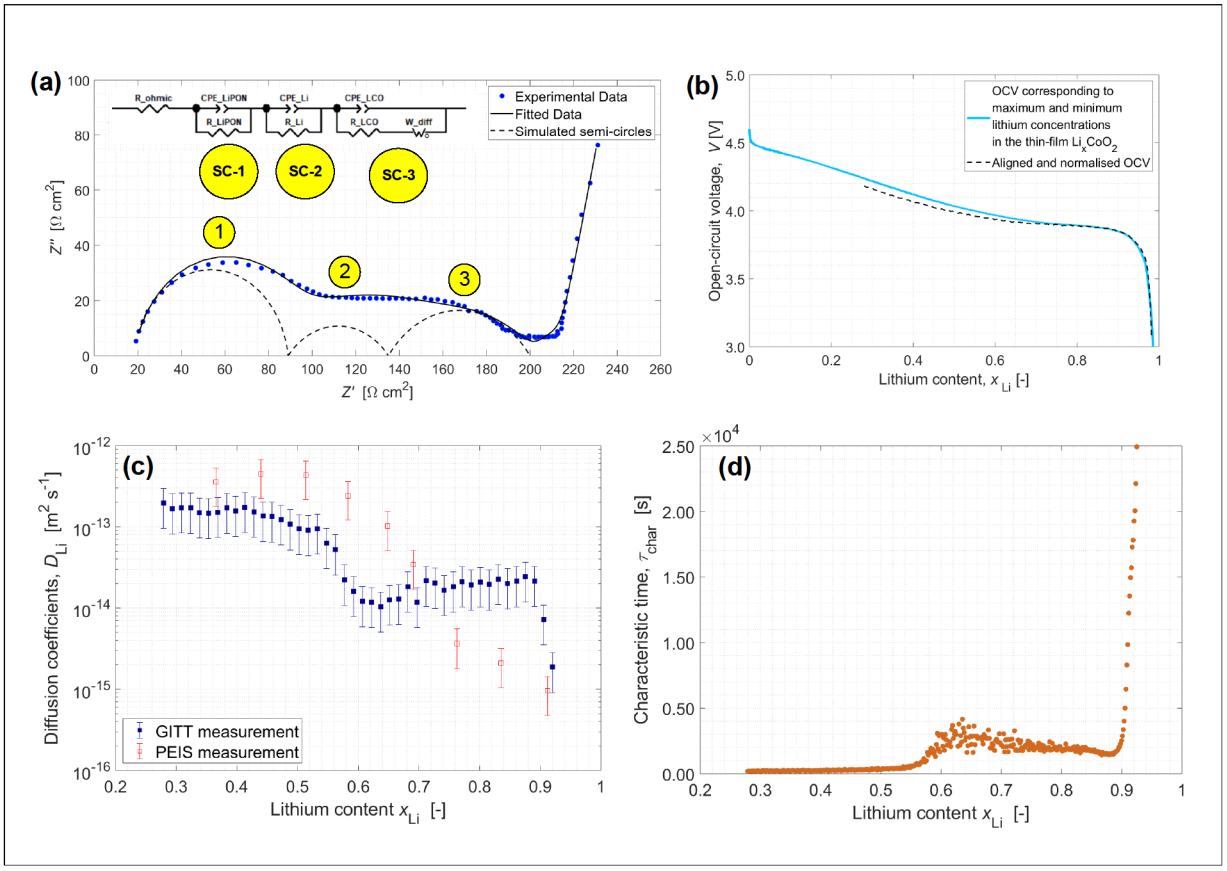


Figure 3.8 Experimental parametrisation of the continuum model: (a) The proposed equivalent circuit model comprises three R-CPE pairs corresponding to the three peaks observed in the DRT analysis at PEIS 90% SOC. The black dashed line indicates the simulated impedance curve to ensure that the semi-circles representing the electrochemical processes do not intersect with each other. (b) Aligned and normalised OCV curves to estimate the Li content in the cell. The black dashed solid line indicates the OCV curve for the voltage window 4.2 V and 3.0 V and the solid blue line denotes the voltage window 4.5 V and 3.0 V. (c) Experimental measurement of diffusion coefficients in the non-porous PE. The dark blue plot indicates the GITT method's measurement, whereas the red plot denotes the measurement using the PEIS procedure.(d) The characteristic time, τ_{char} due to concentration-dependent solid diffusion in the non-porous PE.

By measuring the upper and lower voltage limit of the cell, the minimum and maximum Li uptake in the PE were estimated. A new cell was overcharged with a small current (C/10) beyond 4.2 V to estimate the upper voltage limit. The initial characterisation result shows that the cell reaches a maximum cell voltage at 5.0 V before a sharp drop. Also, the gradient of the voltage profile begins to increase sharply after 4.6 V, which indicates possible irreversible reactions at high voltage.[318] Hence, the upper voltage limit was estimated to be 4.5 V before this sharp gradient change (Figure 3.9(a)). Likewise, the cell was overdischarged with a small current (C/10) beyond 3.0 V to estimate the lower voltage limit. A voltage plateau can be observed around 1.25 V. In another experiment following the procedures described in Section 3.2, the cell's impedance was monitored during overdischarge. A significant change in the cell impedance can be observed when the cell voltage drops below 3.0 V (Figure 3.9(c)), indicating an unstable PE. Based on these initial characterisation results, the voltage window was set to

[3.0, 4.5 V]. Another new cell was cycled first between the voltage windows defined by the manufacturer $3.0-4.2$ V and then the initial voltage limits given in Figure 3.9.

The initial voltage-capacity curves obtained by cycling a new cell between the voltage limits of 4.2 V and 3.0 V and 4.5 V and 3.0 V at a C-rate of C/40 show that a hysteresis effect can be observed between the discharge and charge curves at 4.5 V and 3.0 V (see Figure 3.10). Due to the hysteresis effect observed after the first cycle, the voltage windows for the following experiments were set to 4.2 V and 3.0 V. These two voltage-capacity curves were then aligned, and the Li content of the cell for the voltage window between 4.2 V and 3.0 V could be estimated. Figure 3.8(b) shows the aligned and normalised OCV curve as a function of Li content. Fabre *et al.* assumed the PE operates between the Li stoichiometry at 0.5 and 1.[60] These series of experimental measurements have, however, showed that the bulk PE in a thin-film configuration could operate between 0.27 and 1 for the voltage window between 3 V and 4.2 V. This relationship between the OCV and the Li content was included in the continuum model.

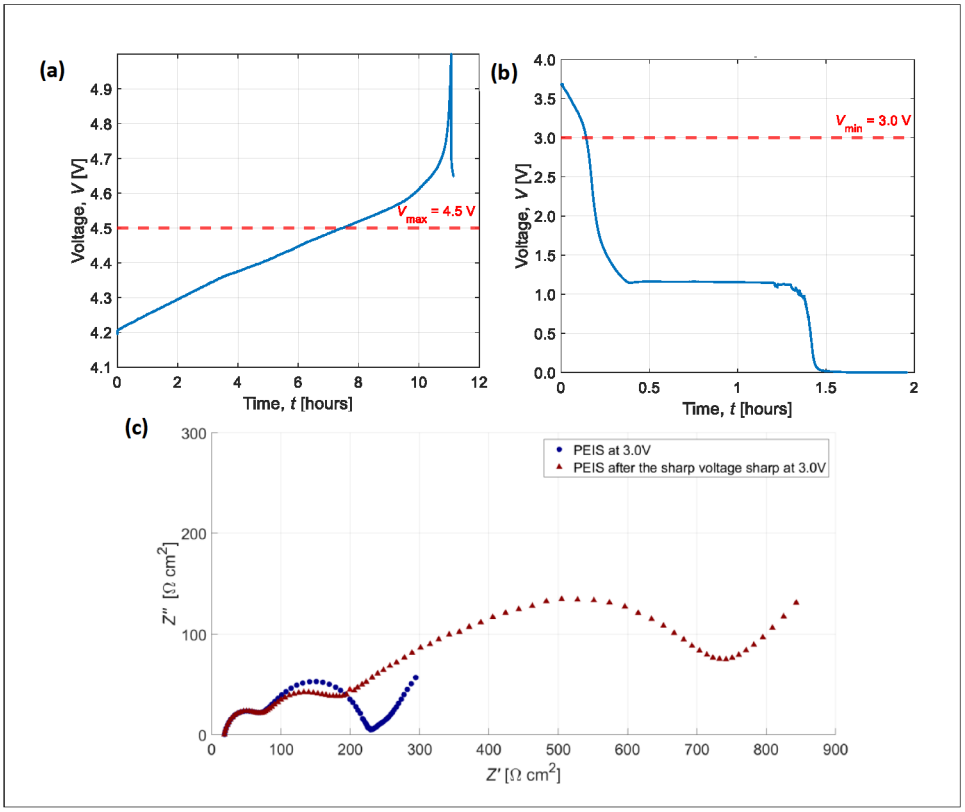


Figure 3.9 Initial overcharge (a) and overdischarge characterisation experiment (b) to estimate the upper and lower voltage limits of the cell, which are used as a basis to estimate the maximum and minimum Li content in the cell. (c) PEIS impedance measurement at the OCV of 3.0 V and 1.5 V.

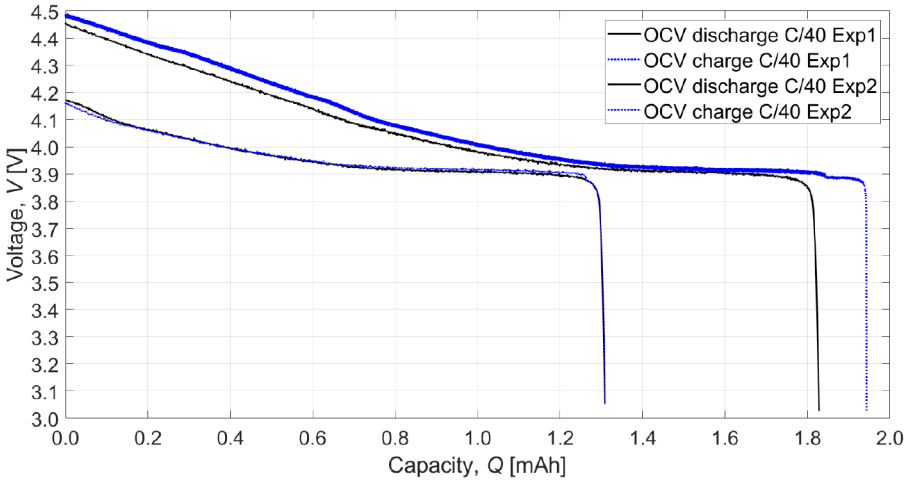


Figure 3.10 Cycling between the voltage limits of 4.2 V - 3.0 V (blue curve: discharge at C/40; red curve: charge at C/40) and 4.5 V - 3.0 V (black curve: discharge at C/40; blue curve: charge at C/40). The offset between the discharge and charge curves is the rest period between the discharge and charge sequence.

3.3.3.2 Ionic conductivity

The ionic conductivity of the SE was determined from the electrolyte thickness d_{elec}, surface area of the electrolyte A_{elec} and electrolyte resistance R_{elec}:[34]

$$\sigma_{\text{elec}} = \frac{d_{\text{elec}}/A_{\text{elec}}}{R_{\text{elec}}}. \tag{3.17}$$

3.3.3.3 Exchange current density

The exchange current density at the interface between the NE and the SE was estimated with:[60]

$$i_{0,\text{neg}} = \frac{R_{\text{gas}}T}{FR_{\text{ct,neg}}}, \tag{3.18}$$

where $R_{\text{ct,neg}}$ is the charge transfer resistance determined from fitting an equivalent circuit model to PEIS measurements. A high exchange current density implies that the surface overpotential is small, and the reaction is fast.[81]

3.3.3.4 Theoretical molar density of LCO

The theoretical molar density of LCO was estimated as follows:

$$c_{\mathrm{LCO,max}} = \frac{\rho_{\mathrm{LCO}}}{m_{\mathrm{LCO}}}, \tag{3.19}$$

where ρ_{LCO} is the density of the PE ($\rho_{\mathrm{LCO}} = 5050\,\mathrm{kg\,m^{-3}}$)[319] and m_{LCO} is the molar mass of LCO ($m_{\mathrm{LCO}} = 0.09787\,\mathrm{kg\,mol^{-1}}$).

3.3.3.5 Diffusion coefficients in the PE

The diffusion coefficients were determined from PEIS data based on the diffusion equations derived by Ho *et al.*[308] When the diffusion coefficient is large (*i.e.* $\omega \ll 2D_{\mathrm{Li}}/d_{\mathrm{pos}}^2$), the expressions for complex impedance follow:[308]

$$|Z|sin\beta = \left|\frac{V_{\mathrm{m}}(dU/dx_{\mathrm{Li}})}{zF\omega d_{\mathrm{pos}}A_{\mathrm{pos}}}\right|, \tag{3.20}$$

$$|Z|cos\beta = \left|\frac{V_{\mathrm{m}}}{zFA_{pos}}\left(\frac{dU}{dx_{\mathrm{Li}}}\right)\left(\frac{d_{\mathrm{pos}}}{3D_{\mathrm{Li}}}\right)\right|, \tag{3.21}$$

where V_{m} is the molar volume of LCO, U is the open-circuit voltage, x_{Li} is the Li content in LCO, ω is the radian frequency ($\omega = 2\pi f$), d_{pos} is the electrode thickness and A_{pos} is the surface area of the PE. The determination of D_{Li} based on Equation 3.20 and 3.21 assumes that the current is 90° out of phase with the voltage (*i.e.* $\beta = 90°$). The simutaneous solutions of these two equations yield the values for D_{Li} and dU/dx_{Li}.[308]

When the diffusion coefficient is small (*i.e.* $\omega \gg 2D_{\mathrm{Li}}/d_{\mathrm{pos}}^2$), the phase difference between the current and the voltage is equal to $\beta = 45°$.[308] In this case, the diffusion coefficient can be obtained from:[308]

$$|Z| = \left|\frac{V_{\mathrm{m}}(dU/dx_{\mathrm{Li}})}{zF\sqrt{D_{\mathrm{Li}}}A_{\mathrm{pos}}\sqrt{\omega}}\right|. \tag{3.22}$$

Diffusion coefficients can also be determined with the GITT measurement from:[320]

$$D_{\mathrm{Li}} = \frac{4}{\pi\tau_{\mathrm{pulse}}}d_{\mathrm{pos}}^2\left(\frac{\Delta V_{\mathrm{s}}}{\Delta V_{\mathrm{t}}}\right)^2. \tag{3.23}$$

The definitions of τ_{pulse}, ΔV_{s} and ΔV_{t} can be found in Figure 3.6(b). This equation is, however, only valid for short time constants ($\tau_{\mathrm{pulse}} \ll d_{\mathrm{pos}}^2/D_{\mathrm{Li}}$).[320] For the present cell, the smallest $d_{\mathrm{pos}}^2/D_{\mathrm{Li}}$ is 184 s. Therefore, another set of GITT experiments with $\tau_{\mathrm{pulse}} = 70\,\mathrm{s}$ was conducted for the measurement of the diffusion coefficients in the PE.

Table 3.2 Summary of parameters (a = Larfaillou *et al.*[63], b = Fabre *et al.*[60])

Parameters	Values	Estimated by	Literature values
Thickness of the SE, d_{elec}	$2\,\mu$m	value from literature[(a)]	$2-4\,\mu$m
Thickness of the PE, d_{pos}	$6\,\mu$m	value from literature[(a)]	$5-8\,\mu$m
Exchange current density at the Li|LiPON interface, $i_{0,\text{ neg}}$	$0.48\pm0.72\,\text{mA cm}^{-2}$	PEIS measurement	$1.5\,\text{mA cm}^{-2}$ [(b)]
Ionic conductivity, σ_{elec}	$(2.31\pm0.52)\times10^{-6}\,\text{S cm}^{-1}$	PEIS measurement	$1.2\times10^{-6}\,\text{S cm}^{-1}$ [(b)]
Theoretical molar density of LCO, $c_{\text{LCO, max}}$	$51599.06\,\text{mol m}^{-3}$	calculation	$50000\,\text{mol m}^{-3}$ [(b)]

Figure 3.8(c) shows the experimental measurements of diffusion coefficients in the PE using the PEIS (red marker) and the GITT method (dark blue marker). The experiments were repeated at a different cell with the same methods under the same conditions. The error bar, as shown in Figure 3.8(c) represents the deviations measured on two different cells and the instrumental errors of approximately 4%. From Figure 3.8(c), it can be seen that the diffusion coefficients in the PE is not constant, as assumed by Danilov *et al.*,[261] but decreases as the SOC decreases, as found also by Fabre *et al.*[60] The difference in the diffusion coefficients measured by the PEIS and GITT methods can be explained by considering the conditions, under which the experiments were conducted. As the PEIS experiment was carried out at the open-circuit voltage of each pulse, the diffusion coefficient estimated with this method was measured under quasi-equilibrium conditions, during which no net current passed through. On the other hand, the GITT method was implemented with a small current. Hence, the difference, as observed in Figure 3.8 implies that the diffusion behaviour in the PE has a more complex dependence on the cell history.[321–323]

As this work focuses on dynamic solid-state cell behaviour, diffusion coefficients estimated by the GITT method are chosen. The input interpolation diffusion was first fitted to the experimental pulse discharge data and subsequently compared with the GITT method's measurement. The concentration-dependent diffusion coefficient agrees very well with the GITT measurement for low SOCs. However, a deviation smaller than one magnitude of orders can be observed at high SOCs. The calculated characteristic time due to diffusion, τ_{diff}, as shown in Figure 3.8(d), increases sharply as the SOC decreases. This experimental analysis indicates that solid diffusion in the non-porous LCO could be the rate-limiting step for low SOCs.

The decrease in the diffusion coefficients in Figure 3.8(c) can be correlated to the structural change of the LCO electrode observed by Matsuda *et al.*[216] in the *in-situ* Raman spectra. They attributed their experimental observation to five phases: hexagonal I (H1) phase ($1 > x > 0.95$), two-phase region ($0.95 > x > 0.75$), hexagonal II (H2) phase ($0.75 > x > 0.55$), monoclinic phase ($0.55 > x > 0.45$) and hexagonal II' (H2') phase ($0.45 > x > 0.3$) (see Figure 3.11). The relationship between the phase change and diffusive behaviour of solid Li in LCO suggests that the phase transformation needs to be controlled to improve bulk mass transport.

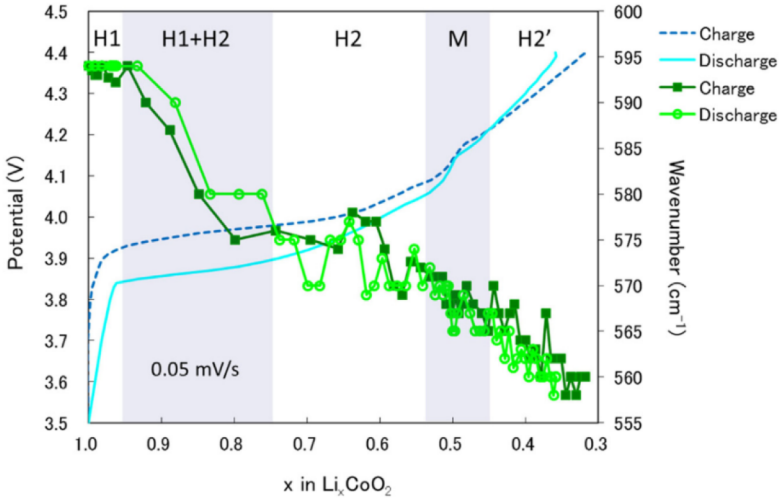


Figure 3.11 Five different phases were observed in the LCO electrode: hexagonal I (H1) phase ($1 > x > 0.95$), two-phase region ($0.95 > x > 0.75$), hexagonal II (H2) phase ($0.75 > x > 0.55$), monoclinic phase ($0.55 > x > 0.45$) and hexagonal II' (H2') phase ($0.45 > x > 0.3$). Reproduced with permission from Ref. 216, Copyright (2019), Elsevier.

Table 3.2 summarises the parameters used in this model. The charge transfer coefficients, α_{pos} and α_{neg} were assumed to be 0.5 in this model, assuming that the kinetic resistance between the charge and discharge of the cell is symmetric.[245] The variation of this parameter between 0 and 1 in the time-domain using Butler-Volmer equations as the boundary conditions does not affect the simulation results significantly.

3.4 Model-based overpotential analysis and cell design

3.4.1 Model validation

Figure 3.12(a) shows the simulated cell voltage for a pulse discharge at 0.1C compared to experimentally measured voltages. The pulse discharge curves change gradually from a linear profile at high SOCs to a concave profile at low SOCs. The change in the shapes of the voltage profiles, as observed in the experimental measurement, can only be reproduced in the model by using a concentration-dependent solid diffusion coefficient in the non-porous PE. As the diffusion coefficient of Li in the non-porous PE decreases for low SOCs, this mechanism can be the bottleneck in the cell performance when increasing the thickness of the PE to achieve a higher cell capacity. Nevertheless, it should also be noted that the OCV curve changes the most at the region towards low SOCs.

Pulse charging at 0.1C was also simulated to analyse the relaxation behaviour after charging. Figure 3.12(b) shows the simulated pulse charging profile at 0.1C compared to the

experimentally measured curves. Figure 3.12(c) shows the simulated and measured dynamic voltage profile of pulses at different C-rates (0.5C, 1C and 2C). The RMSE of the dynamic voltage prediction has a maximum deviation of approximately 4%.

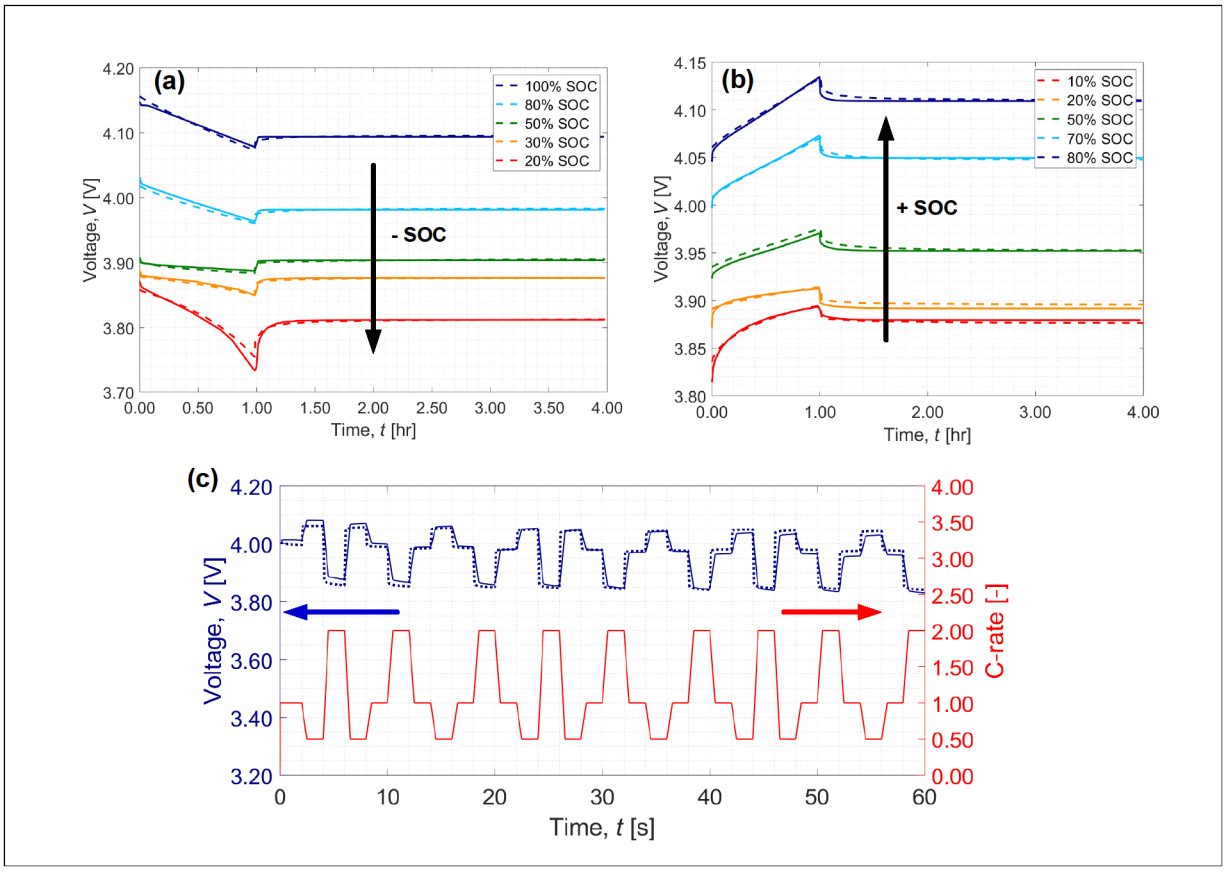


Figure 3.12 Comparison between model predictions (dashed lines) and experimental measurements (solid lines): (a) Pulse discharge (b) Pulse charging. (c) Dynamic pulses with different C-rates: the current profile (red) and the current profile (blue).

3.4.2 Quantification of solid diffusion overpotentials

The model was subsequently used to analyse the rate-limiting mechanisms inside the cell at different operating conditions. The rate-limiting mechanism was studied by analysing the overpotentials that caused the voltage losses in the cell.

Danilov *et al.*[261] have proposed four overpotentials: charge-transfer overpotentials at the PE and the SE interface, diffusion and migration overpotentials in the SE and the concentration overpotential in the PE. Due to a low transference number, it was implied in their model that the anion mostly provides ionic conductivity. The Li cation concentration gradient in the electrolyte would then occur due to the mobility of anions and their accumulation at the electrode surface.[248] As a result of this low transference number, the mass-transfer overpotential across the SE in Danilov's model includes a significant contribution from the diffusion overpotential. The transference number of 0.15 is in contradiction with the definition

established by Patterson[304] for SE and the material behaviour of ceramic-based SEs, in which only the Li-ions are mobile. This description corresponds to a transference number of 1, with no concentration overpotential in the SE. Secondly, in Danilov's model, a critical model parameter - the diffusion coefficient of solid Li in the PE - was not estimated based on experimental data and was assumed to be concentration-independent. The experimental measurement of solid diffusion in this work and the measurements by Fabre *et al.*[60] show that the solid diffusion in the non-porous electrode is concentration-dependent. A constant diffusion coefficient as assumed in the Danilov's model, leads to an underestimate of the role of Li diffusive behaviour in the electrode to the cell dynamic performance. These two discrepancies (non-unity transference number and non-concentration dependent solid diffusion) have been corrected in their most recent publication.[324] However, the implications of these inconsistencies on the overpotential analysis results in their previous works were not assessed.

In this work, voltage losses due to charge transfer at both interfaces, the ohmic drop in the SE and the solid diffusion overpotential in the non-porous PE are considered. Unlike Danilov's overpotential analysis, on the basis of unity transference number in the SE,[304] there is no concentration overpotential in the SE, and therefore, only the overpotential due to the ohmic drop is considered in the SE of this model. The solid diffusion overpotential in the non-porous PE was calculated based on the concentration-dependent solid diffusion estimated from the experimental measurements. The overpotentials were calculated as follows:[325]

$$\eta_{\text{pos/neg}}|_{z=0,\, z=d_{\text{elec}}} = \phi_{\text{s}} - \phi_{\text{elec}} - U, \tag{3.24}$$

$$\eta_{\text{ohm}} = \frac{1}{i_{\text{tot}}} \int_0^{d_{\text{elec}}} a \frac{i_{\text{loc}}^2}{\sigma_{\text{Li}^+}} dx, \tag{3.25}$$

$$\eta_{\text{diff}} = U_{\text{LCO}}(c_{\text{Li}}) - U_{\text{LCO}}(\bar{c}_{\text{Li}}), \tag{3.26}$$

in which $\eta_{\text{pos/neg}}$ indicates the charge transfer overpotentials, η_{ohm} denotes the ohmic drop in the SE and η_{diff} represents the solid diffusion overpotential in the PE. $\bar{c}_{\text{Li}}$ is the average Li concentration in the non-porous PE.

Figure 3.13(a) and (b) show the overpotential profiles for SOCs 80% and 30% at a current density of 0.69 A m^{-2} (corresponding to 0.1 C-rate). Under pulse operating conditions, the overpotentials have similar magnitudes at high SOCs, with the solid diffusion overpotential in the non-porous PE slightly larger than the other overpotentials, followed by the ohmic drop and the charge transfer overpotentials. However, as the SOCs decreases, solid diffusion overpotential in the non-porous PE increases significantly from 35% to 75% (Figure 3.13(b)). Based on these results, it can be concluded that the solid diffusion overpotential is the rate-limiting mechanism

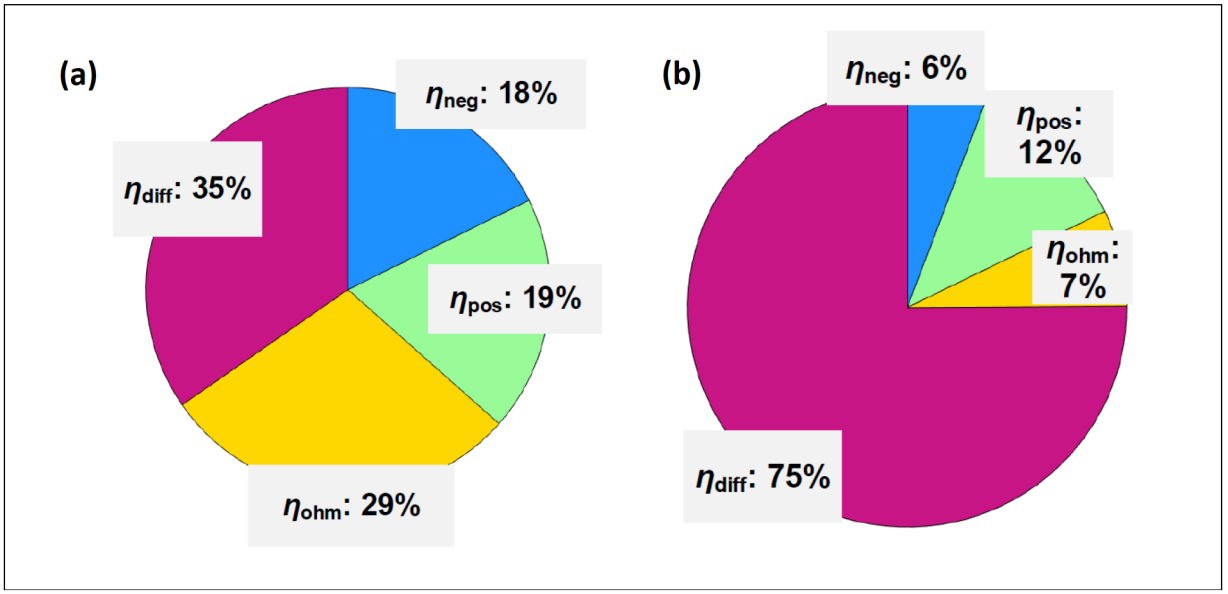


Figure 3.13 (a) Comparison of calculated voltage losses for SOCs more than 50% in (a) and for SOCs less than 30% in (b) based on the experimental pulse discharge profiles ($i_{\text{pulse}} = 0.69\ \text{A/m}^{-2}$ and $\tau_{\text{pulse}} = 1\ \text{hr}$). The solid diffusion overpotential represented in this work denotes the overpotential losses due to the diffusion in the non-porous PE.

for lower SOCs. This conclusion reflects the trend visible in Figure 3.7(a) between low and high SOCS.

Figure 3.14(a) shows the computed overpotentials as a function of current densities at 80% SOC under pulse operating conditions. The model prediction shows that solid diffusion in the PE has the most significant contribution in the power loss (27.87 mW m^{-2}) followed by the ohmic drop in the SE (16.71 mW m^{-2}). The predicted dependence of overpotentials on current densities at low SOCs is shown in Figure 3.14(b). At low SOCs, the range of allowed pulse currents without reaching the cut-off voltage decreases. Within this range of current densities, power losses are clearly dominated by solid diffusion in the non-porous PE (36.48 mW m^{-2}). When more Li is intercalated into the LCO, solid diffusion becomes the rate-limiting mechanism, followed by charge transfer at the PE interface.

Depending on the operating conditions and cell architecture, it should be noted that the performance limiting mechanisms in batteries are highly dynamic. For instance, Raijmakers *et al.*[40] found that ohmic overpotential across the SE is most dominant, followed by the diffusion overpotential at the end of discharge when the operating conditions are changed from pulses to a constant-current discharge mode. However, the interfacial reaction kinetics rather than the electrode solid diffusion could be limiting the cell performance for two additional scenarios: (i) under high C-rate discharge such that the reaction rate is higher than the equilibration rate; (ii) when the non-porous PE is replaced by a composite PE that consists of many particles.[326] All these studies have not considered degradation impacts such as Li creep, the formation of SEI layers, interfacial delamination or voids formation, which could add

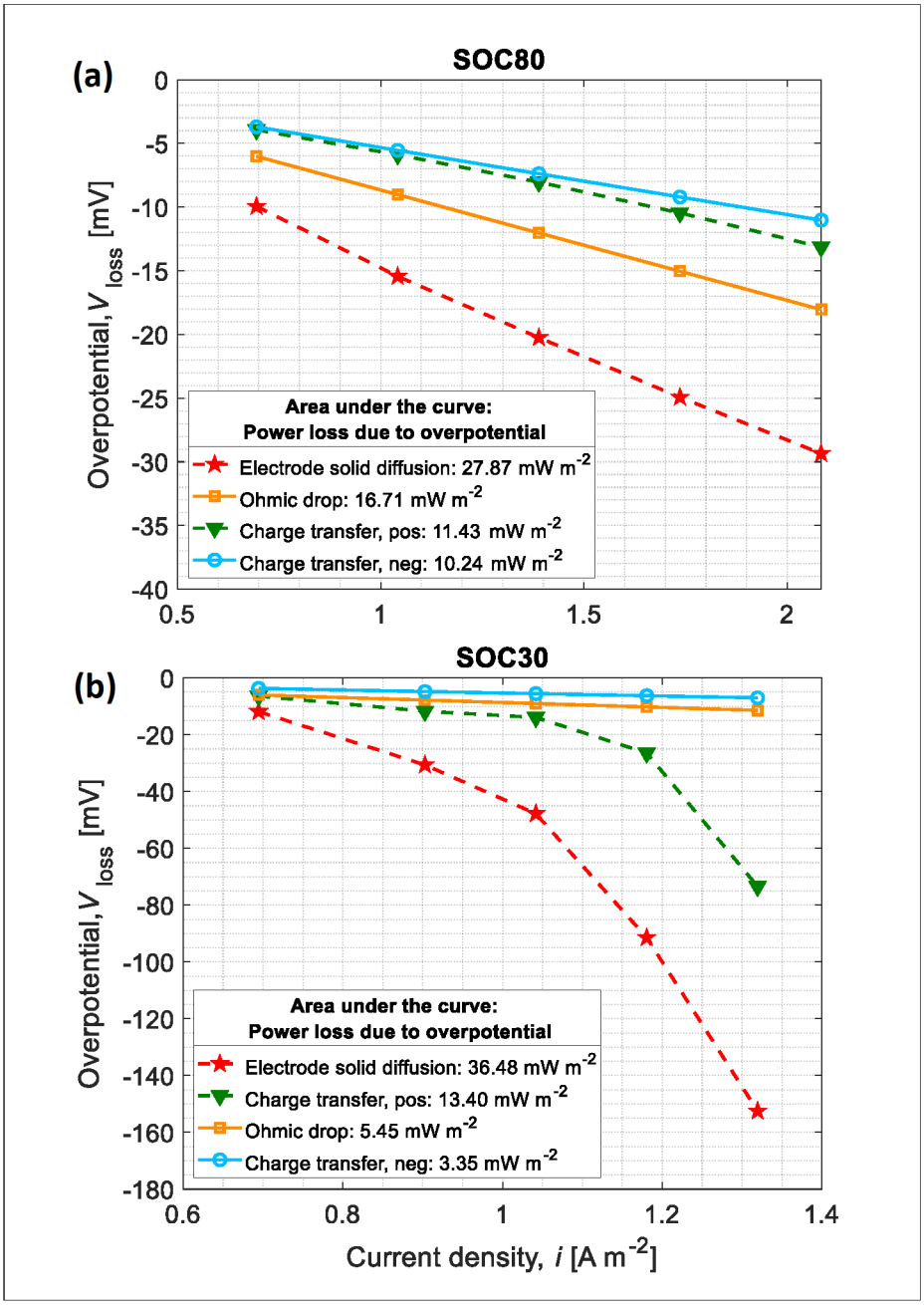


Figure 3.14 (a) The impact of operating current density on the various contributions to power loss due to overpotentials at SOC 80% and (b) at SOC 30%.

further complexity to understanding the performance limiting mechanisms under different operating conditions.

3.4.3 Model-based cell design

Based on the performance-limiting mechanisms discussed in Section 3.4.2, critical thickness of the PE and a critical ionic conductivity that minimises the voltage loss due to the solid diffusion in the non-porous PE and ohmic drop across the SE was calculated for the pulse operating conditions. Figure 3.15 shows the influence of different cell designs on cell performance and

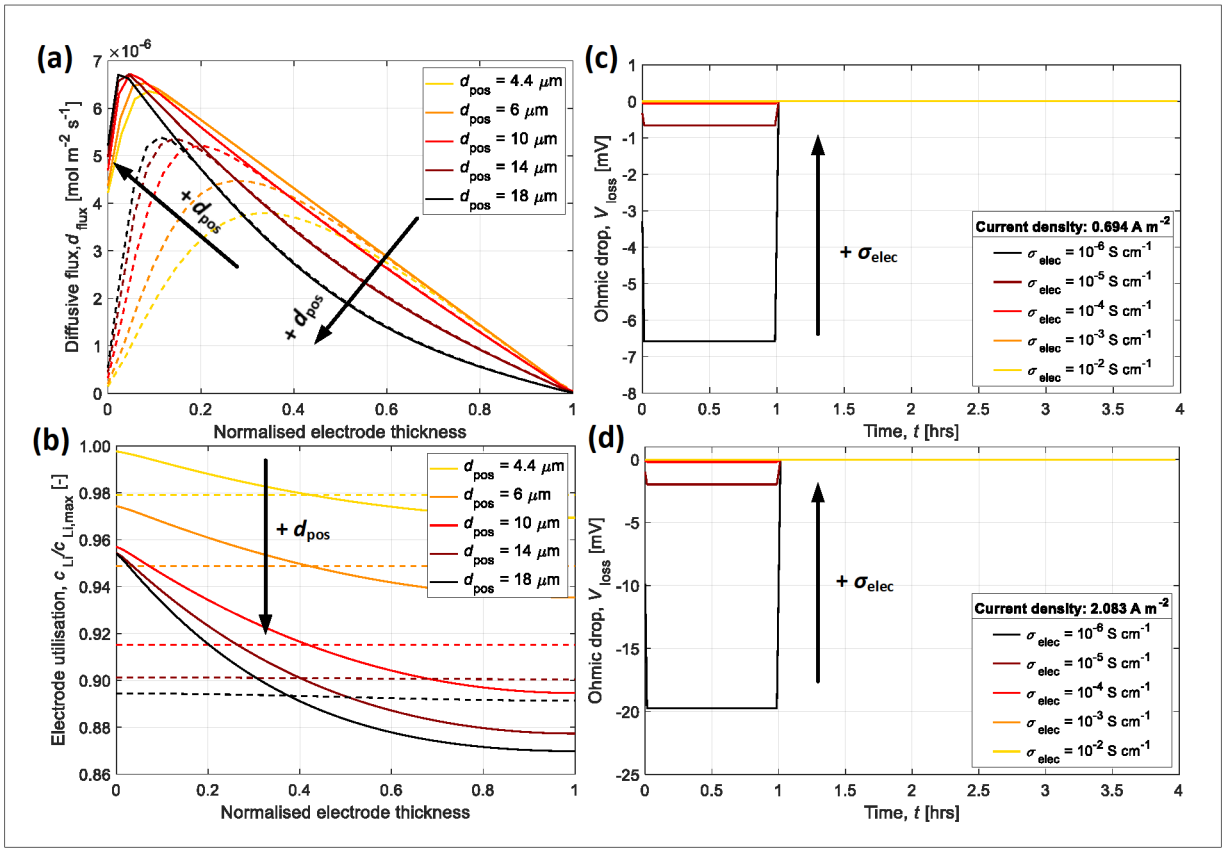


Figure 3.15 (a) Diffusive flux in the PE as a function of normalised electrode thickness: the solid lines indicate the diffusive flux at $t = 3600$ s whereas the dotted lines indicate the diffusive flux at $t = 3650$ s ($i_{\text{pulse}} = 0.694$ A m^{-2}, $\tau_{\text{pulse}} = 1$ hr, $\sigma_{\text{elec}} = 10^{-6}$ S cm^{-1}) (b) Ratio of electrode utilisation as a function of normalised electrode thickness: the solid lines indicate model evaluation at $t = 3600$ s whereas the dashed lines indicate the evaluation at time after the electrode achieves the equilibrium ($t = 14340$ s) ($i_{\text{pulse}} = 0.694$ A m^{-2}, $\tau_{\text{pulse}} = 1$ hr, $\sigma_{\text{elec}} = 10^{-6}$ S cm^{-1}) (c) Calculation of ohmic drop in the SE with different ionic conductivities for $i_{\text{pulse}} = 0.694$ A m^{-2}. (d) Ohmic drop in the SE with different ionic conductivities for $i_{\text{pulse}} = 2.083$ A m^{-2}.

losses. A thicker electrode is commonly suggested in the literature as a solution to increasing the capacity of the cell.[327,328] In a cell in which bulk LCO is used as the PE, increasing its thickness will achieve a higher capacity only if the operating current is low.[60] The model prediction shows that the critical thickness of the PE under the pulse operating condition ($i_{\text{pulse}} = 0.694$ A m^{-2}, $\tau_{\text{pulse}} = 1$ hr, $\sigma_{\text{elec}} = 10^{-6}$ S cm^{-1}) is 4.4 μm. After the interruption of discharge current at 3600 s, solid Li continues to diffuse into the inner part of the electrode. Figure 3.15(a) shows the diffusive flux in the PE across the electrode at time $t = 3600$ s (solid lines) and $t = 3650$ s (dotted lines) respectively. The z-axis is normalised to the electrode thickness. The position between the PE and the SE is denoted by $z = 0$. When the electrode thickness increases beyond the critical thickness, the diffusive peaks at $t = 3600$ s and $t = 3650$ s shift towards the interface with the SE. This result indicates that less percentage of the electrode will be utilised, as shown in Figure 3.15(b). When the electrode thickness is increased to 18 μm, the model prediction shows that less than 90% of the electrode is used after the cell relaxes and reaches the equilibrium. As a result, the solid diffusion overpotential increases from 9.6 mV to 26.3 mV and the cell internal

resistance increases from 194 $\Omega\,cm^2$ to 433 $\Omega\,cm^2$ when the electrode thickness is increased from 4.4 μm to 18 μm. This analysis demonstrates the importance of using a model-based procedure to calculate the optimum thickness of the electrode given the operating conditions. Making the electrode as thick as possible does not necessarily lead to an increase in the usable capacity of the cell.

Likewise, the influence of the electrolyte ionic conductivity on the ohmic drop in the SE is also analysed (Figure 3.15(c) and (d)). Various materials and designs of SEs with improved ionic conductivity have been proposed in the literature.[329] Table 3.3 illustrates selected examples of SEs. As the ohmic drop in the SE was shown to be dependent on the current density, the ohmic drop as a function of ionic conductivity was evaluated at two different current densities in this model (0.69 A m^{-2} and 2.08 A m^{-2}). Improving the ionic conductivity from 10^{-6} S cm^{-1} to 10^{-5} S cm^{-1} would reduce the ohmic drop by approximately 90% and further improvement of the ionic conductivity from 10^{-5} S cm^{-1} to 10^{-4} S cm^{-1} would reduce the ohmic drop by another 90%. However, the simulation result shows that the ohmic drop in the SE is no longer limiting the cell performance for both pulse current densities if the ionic conductivity is improved beyond 10^{-4} S cm^{-1}. Hence, there is no benefit in using inorganic SEs with the ionic conductivity above 10^{-4} S cm^{-1} if bulk LCO continues to be used as the PE.

Table 3.3 Other selected examples of SEs. (Reproduced with permission from Ref. 329, Copyright (2018), Elsevier)

Types of SE	Composition	Ionic conductivity in S cm^{-1}
Argyrodite (Li_6PS_5Cl)	Li_6PS_5Br	$10^{-3} - 10^{-2}$
	Li_6PS_5Cl	1.33×10^{-3}
Garnet ($Li_7La_3Zr_2O_{12}$)	$Li_{6.75}La_3(Zr_{1.75}Nb_{0.25})O_{12}$	8×10^{-4}
Perovskite ($Li_{3x}La_{2/3-x}TiO_3$)	$Li_{3/8}Sr_{7/16}Ta_{3/4}Hf_{1/4}O_3$	3.8×10^{-4}
NASICON ($LiTi_2(PO_4)_3$)	$LiTi_2(PO_4)_3$-0.2Li_3BO_3	3×10^{-4}
Sulfide (Li_4GeS_4)	75Li_2S-25P_2S_5 glass	2×10^{-4}
	$Li_{4.25+\delta}(Ge_{0.75-\delta}Ga_{0.25})S_4$	6.5×10^{-5}
LISICON (γ-Li_3PO_4)	$Li_{4-x}Si_{1-x}P_xO_4$(x = 0.5, 0.6)	1×10^{-6}

3.5 Conclusions

The conclusions of this chapter are reviewed against the research question outlined in Section 1.3:

Which mechanisms are limiting the performance of solid-state Li-metal batteries under pulse operating conditions?

A combination of experimental and numerical methods was used to study the pulse behaviour observed in the solid-state Li-metal cell. The experimental pulse voltage measurements show that solid-state Li-metal cell has a high internal resistance of $\approx 200\,\Omega\,\mathrm{cm}^2$ and it increases for low SOCs to $\approx 450\,\Omega\,\mathrm{cm}^2$. This magnitude of internal resistance could affect cell performance significantly if the cell were scaled to achieve a higher capacity. By comparing the PEIS measurements at different SOCs, the significant increase in the internal resistance at the end of SOC is attributed to the decrease in the solid diffusion coefficient. Based on the model presented here, future work aiming to improve solid-state battery performance should focus on the design of the PE for solid-state Li-metal cells to improve the mass transport of solid Li in the electrode and hence reduce the diffusion impedance and internal resistance. By calculating the time constant of different electrochemical processes using the DRT method, the experimental results show that ionic conductance and charge transfer kinetics happen in the timescale between microseconds and milliseconds. Comparing these time constants to the pulse discharge and charging duration shows that if the pulse duration exceeds milliseconds, the space charge effects at either interface is not the primary mechanism governing the pulse voltage response of solid-state Li-metal cells.

In the model-based overpotential analysis section, solid diffusion in the non-porous LCO is shown to be the rate-limiting mechanism followed by the ohmic drop at high SOCs. For low SOCs, the electrode solid diffusion and charge transfer overpotential at the PE interface are the two dominant voltage losses. Based on these rate-limiting mechanisms at different pulse operating conditions, the simulations using different thicknesses of the PE show that the solid diffusion overpotential would increase by more than 150% if the electrode thickness were increased from the critical thickness to 18 μm. This result implies that if decreasing diffusion coefficients at high Li concentrations in the non-porous PE is not addressed in the future cell design, increasing the thickness does not necessarily lead to increases in the usable capacity. Lastly, the present research proposes that an ionic conductivity of SE of $10^{-4}\,\mathrm{S\,cm}^{-1}$ is good enough for applications if bulk LCO continues to be used as the PE, as further improvement in the ionic conductivity is shown to yield a marginal overall cell performance gain. This study demonstrates that two popular trends in solid-state batteries research are not as productive as they might seem. Increasing the non-porous PE thickness, or increasing the ionic conductivity of the SE as much as possible, on their own, can only give a limited performance increase. Instead, a holistic model-based approach to cell design for optimum performance would be beneficial.

Acknowledgements and author contributions

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Chapter 4

Thermally coupled modelling of large-format solid-state cell stacks

Although solid-state Li-metal batteries provide potential solutions to the critical safety issues faced by conventional Li-ion batteries such as flammability,[4,10,330,331] solid-state Li-metal batteries have not been implemented for large-scale applications such as powertrain electrification due to scaling and manufacturing limitations.[13,332] Capacity of a single-layer cell is insufficient to meet the power demands. Therefore, overcoming the up-scaling and manufacturing barriers is an absolute prerequisite to enable the large-scale applications of solid-state Li-metal batteries. One possible method to increase the total power and energy output of solid-state Li-metal batteries is to scale and stack each unit cell in series or in parallel. In series stacking, each unit cell is connected by the Bipolar Plates (BP), whereas in parallel stacking, the Current Collectors (CC) and tabs of each unit cell are connected to form a stack. Toyota built the prototype of bipolar solid-state cell stack and showed that it is possible to obtain a maximum voltage of 16.26 V by stacking four layers of single unit cells.[333] Gambe *et al.*[334] have also developed a bipolar stack based on quasi-solid-state electrolyte and demonstrated a stack voltage experimentally up to 12 V. Ito *et al.*[335] have constructed a parallel solid-state cell stack by stacking three double-coated unit cells to achieve a capacity of 1 Ah.

While bipolar and parallel stack configurations have been proposed and measured experimentally, no systematic comparison between these two configurations is available regarding their advantages and limitations. A model-based approach is proposed to study the effects of upscaling parallel and bipolar stacks by identifying the scaling factor from a system of dimensionless governing equations. Based on the Ragone analysis, the volumetric and the gravimetric energy and power densities of both stack profiles are compared. Current collectors'

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impact in a single-layer cell is negligible due to their high electronic conductivity and negligible mass. However, as the number of unit cells in the stack increases, the current collectors' mass and volume ratio can significantly determine the stack's energy and power density. This study demonstrates that the choice of current collectors is critical in optimising the stack performance.

The heat generation in a single-layer cell is insignificant due to the large surface-to-volume ratio. However, the impacts of heat generation in a stack can be significant and affect the stack performance. Toyota has confirmed that their prototyped all-solid-state stack can be operated at a temperature of 100 °C.[333] The effects of such high operating temperature on the internal heat generation and electrochemical stack performance of the bipolar and parallel configurations have not been studied. Recently, Bock *et al.*[97] proposed an analytical stack model comprising 24 cells to study the temperature distribution at the stack centre and outer boundary. However, the analytical thermal model was not coupled with the electrochemical model. As a result, the values for the heat sources used in the thermal model were not calculated from the electrochemical model, and the stack performance also did not account for the impacts of heat generations. This gap is addressed by proposing a coupled electrochemical stack model with a two-dimensional thermal model, enabling the comparison for the impact of heat generation and temperature gradients for stacks of different configurations.

4.1 Model development

4.1.1 Temperature-dependent single-layer cell model

The one-dimensional single-layer model developed in Chapter 3 was improved to provide a framework to study the effects of different operating temperatures on the heat generations. Figure 4.1 illustrates the model domain of a single-layer cell. The temperature dependence is included in the following parameters: the Open-Circuit Potential (OCP) of the cell, ionic conductivity in the Solid Electrolyte (SE), exchange current densities at the electrode-electrolyte interfaces and solid diffusion in the Positive Electrode (PE). Secondly, due to the relatively small surface overpotential at the Negative Electrode (NE) and SE interface,[7] the Butler-Volmer expression describing the kinetics at this interface is linearised to[81,336]

$$i = i_{0,\mathrm{neg}}(\overline{T})\frac{(\alpha_\mathrm{a}+\alpha_\mathrm{c})F}{R_\mathrm{gas}\overline{T}}\eta_\mathrm{neg} \tag{4.1}$$

where $i_{0,\mathrm{neg}}(\overline{T})$ is the temperature-dependent exchange current density at the NE interface, α_a and α_c are the charge-transfer coefficient ($\alpha_\mathrm{a} = \alpha_\mathrm{c} = 0.5$), F is the Faraday's constant ($F = 96,485\,\mathrm{C\,mol^{-1}}$), R_gas is the universal gas constant ($R_\mathrm{gas} = 8.314\,\mathrm{J\,K^{-1}\,mol^{-1}}$), $\overline{T}$ is the

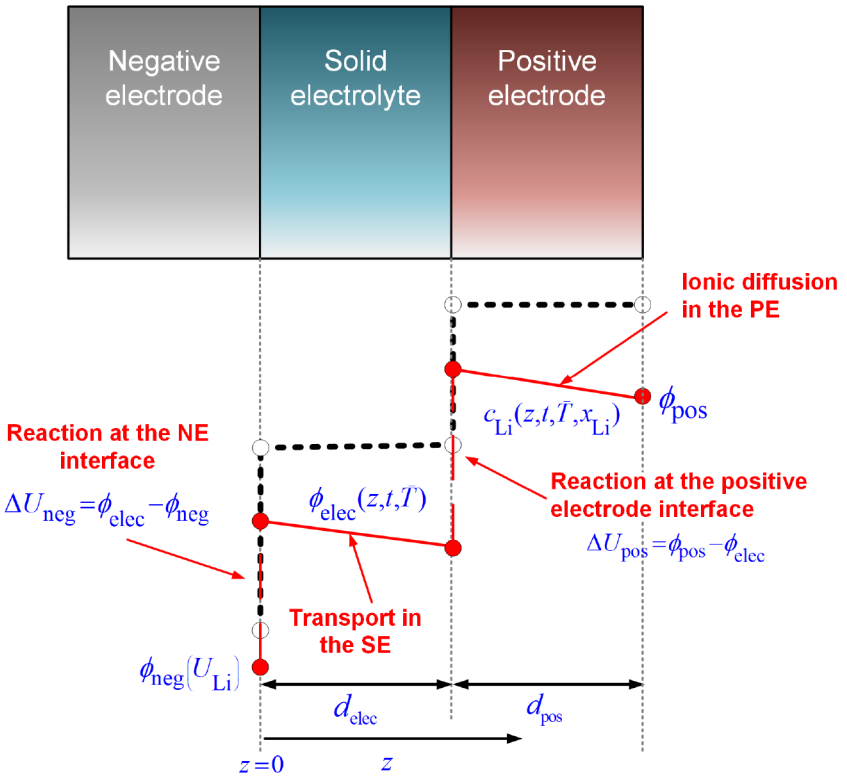


Figure 4.1 Illustration of the temperature-dependent single-layer model domain in the z-direction, where z denotes the spatial variation, t represents time, $\overline{T}$ indicates the temperature dependence and c_{Li} represents the concentration of Li^+ in the Positive Electrode (PE). The dashed lines and empty circles indicate the open-circuit states, whereas the red solid lines and filled circles denote the computational states under load. The potential differences due to interfacial charge-transfer kinetics are given by ΔU_{neg} and ΔU_{pos}. ϕ_{elec} denotes the electrolyte potential, whereas ϕ_{neg} and ϕ_{pos} represent the Negative Electrode (NE) and PE electrode potentials, respectively. U_{Li} is the equilibrium potential of Li-metal.

average temperature in Kelvin evaluated from the two-dimensional thermal model (see Section 4.1.4.4) and η_{neg} is the overpotential at the NE interface.

The overpotential at the PE side is higher than at the NE interface.[7] For example, as shown by the impedance spectrum in Figure 3.8(a), the size of the semi-circle due to the SE-LCO charge transfer kinetics is larger than the SE-Li charge transfer kinetics, which is also consistent with the impedance measurements obtained by Iriyama *et al.*[211] and Fabre *et al.*[60] Secondly, in the cell model computed using the full Butler-Volmer's equation (Chapter 3), the model results show that the negative charge transfer overpotential is smaller compared to the positive charge transfer overpotential at both high and low SOC (Figure 3.13). Thirdly, on the basis of unity transference number with Li^+-ions as the only mobile cations across the SE, the oxidative contribution to the reversible kinetics given in the Butler-Volmer's Equation will be smaller in contrast to the reduction kinetics at the interface. Therefore, the kinetics can be considered as irreversible, represented here by the Tafel equation[81,336]

$$i = -i_{0,\mathrm{pos}}(\overline{T})\left(\frac{c_{\mathrm{Li,surf}}}{c_{\mathrm{bulk}}}\right)\exp\left(\frac{-\alpha_{\mathrm{c}}F\eta_{\mathrm{pos}}}{R_{\mathrm{gas}}\overline{T}}\right), \tag{4.2}$$

where $i_{0,\mathrm{pos}}$ is the concentration and temperature-dependent exchange current density, given by:

$$i_{0,\mathrm{pos}} = Fk_{\mathrm{pos}}(\overline{T})\left(\frac{c_{\mathrm{LCO,max}} - c_{\mathrm{bulk}}}{c_{\mathrm{LCO,max}}}\right)^{0.5}\left(\frac{c_{\mathrm{bulk}}}{c_{\mathrm{LCO,max}}}\right)^{0.5} \tag{4.3}$$

The exchange current density can be defined as the current density at equilibrium, under which the rate of the forward reaction is equal to the rate of the backward reaction.[81] Therefore, c_{bulk} represents the average bulk Li concentration and can be calculated by averaging the concentration distribution within the PE domain ($c_{\mathrm{bulk}} = \overline{c}_{\mathrm{Li}}$). However, as the current density described by the Tafel's equation is irreversible, the inclusion of concentration-dependence to the PE kinetics should be further assessed by comparison to additional experiments in the future. $c_{\mathrm{LCO,max}}$ is the theoretical molar density of the LCO PE ($c_{\mathrm{LCO,max}} = 51599.06\ \mathrm{mol\ m^{-3}}$).[7] k_{pos} is the temperature-dependent rate-constant, and η_{pos} is the overpotential at the PE-SE interface. The term ($c_{\mathrm{Li,surf}}/c_{\mathrm{bulk}}$) in Equation 4.2 accounts for the contribution of the concentration gradient due to the diffusion in the PE to the rate of Li flux between the SE and the PE. Figure 4.6 compares this ratio for three current densities (0.1C, 1C and 5C). For low current densities ($\leqslant 1C$), this term can be approximated as unity. The flux of Li between the SE and the PE is driven predominantly by the charge-transfer reaction. However, as the current densities increase, the rate of Li flux is controlled by both charge-transfer and diffusion mechanisms, and the contribution of the solid concentration gradient cannot be neglected. The derivations of the Butler-Volmer's equation, linear Butler-Volmer's equation and cathodic Tafel's equation can be found in Appendix G.

A summary of the modified governing equations can be found in Appendix B. The model predictions for the single-layer cell with temperature-dependent parameters were first compared with the experimentally measured discharge curves at four operating temperatures. The model was then scaled for a stack by adjusting the electrode active area. This scaling approach was derived based on the experimental work of Ito *et al.*,[335] in which they scaled a pelletised cell to a practical size. The surface area is chosen based on a commercial Li-ion polymer battery (EiG C020).[337] Through the dimensionless governing equations, it is shown in Appendix C that scaling the electrode active surface area only affects the current density. The system of governing equations was non-dimensionalised (detailed in Appendix C) to identify the scaling factor and assess the influence of scaling the electrode active area on the model parameters. If the materials, electrode composition and the manufacturing process are the same for the small-scale and large-scale cells, Kim *et al.* demonstrated that the model parameters used for

small-scale cells could be used for large-scale cells.[338] Therefore, the nominal current of the single-layer scaled cell, $I_{\text{cell,scaled}}$, can be determined from

$$I_{\text{cell,scaled}} = i_{\text{cell,ref}} \times A_{\text{ref}}, \tag{4.4}$$

in which $i_{\text{cell,ref}}$ is the reference current density of the experimental cell and A_{ref} is the surface area of our reference cell.

4.1.2 Working principles of bipolar and parallel stacks

A stack comprises multiple single-layer cells. Generally, there are two types of stacks: bipolar and parallel,[334,339–341] as shown in Figure 4.2.

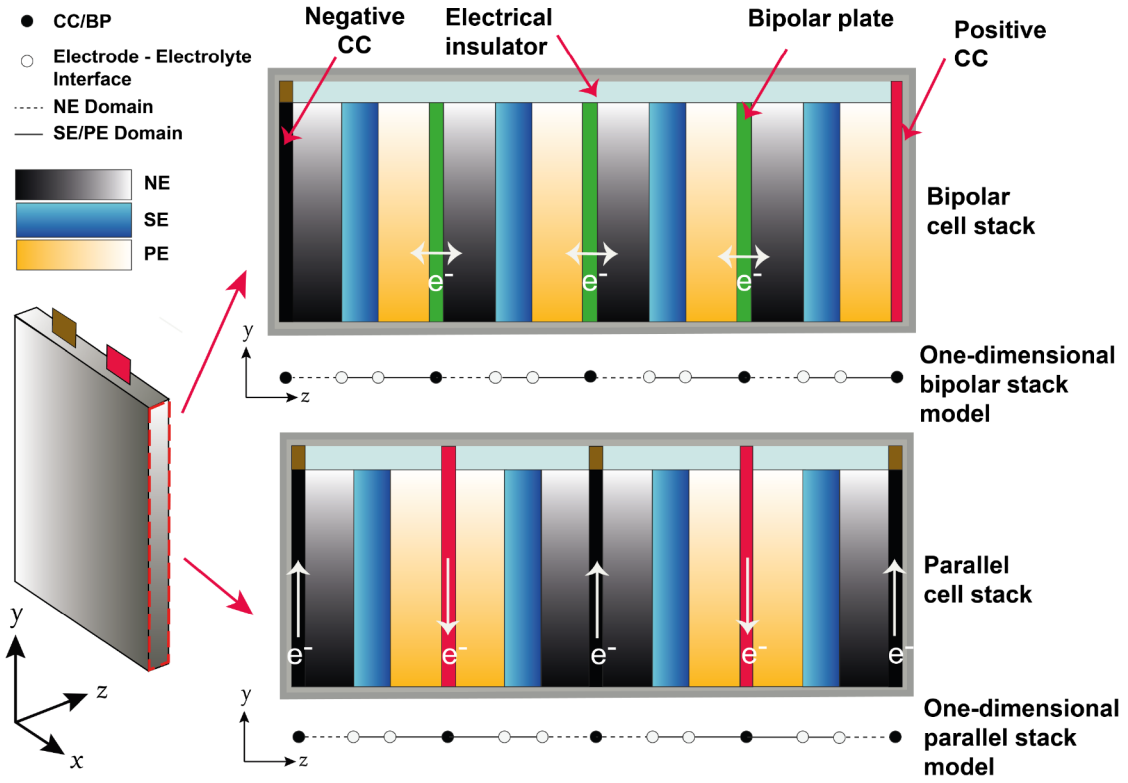


Figure 4.2 Configurations of the bipolar (top) and parallel stack (bottom) inside the pouch. In a bipolar stack, the electrical current flows from one unit cell to the adjacent unit cell through the bipolar plates, whereas in a parallel stack, the electrical current flows in-plane along the current collectors to the external tabs. The one-dimensional bipolar stack model is constructed by stacking the SE and PE domains (solid lines). The NE domain (dashed line) is represented by an interfacial point between the NE and the SE. The one-dimensional parallel stack model consists of the double-coated cells arranged in parallel. The filled circle symbols represent the bipolar plates in the bipolar stack model and current collectors in the parallel stack model, whereas the empty circles denote the electrode-electrolyte interfaces.

In a bipolar stack, each unit cell is connected in series through the bipolar plates, with the PE material coated to one side of the plate and the NE material coated to the opposite side of the plate. An electrical insulator such as the fluoroelastomer seal is used to separate the adjacent bipolar plates from direct contact and to prevent an internal short-circuit.[339,342] In addition, the bipolar plates must be free from pinholes to prevent a short between the electrode materials on both sides.[339,343] However, the bipolar plates must have high electronic conductivity to allow the flow of electrical current between adjacent cells and be electrochemically inert at the same time to prevent any side reactions with the electrode materials on both sides. The bipolar plates must be ultrathin and lightweight in mechanical properties to minimise the stack overall volume and weight. The bipolar plates must also have a high mechanical strength to maintain the integrity of the cell under extreme operating conditions such as overcharge, overdischarge or high operating temperatures.[339] Examples of bipolar plate materials include aluminium foils,[340,342] modified titanium foils,[344] carbon composites,[339] copper/aluminium bimetallic substrates[345] and SUS stainless steels.[334,346,347]

In a parallel stack, each unit cell consists of PE and NE materials separated by the SEs with current collectors at both ends of the single unit cell. For a double-coated cell configuration, the PE material is coated to both sides of the positive current collector.

There are two streams of current flow in a cell operation, given by the migration of Li-ions (the ionic current) and by the transport of electrical charges (*i.e.* the electrical current).[341] In the bipolar stack, the electrical current of unit cells flows perpendicular through the bipolar plates. In the parallel stack, the ionic current flows perpendicular from the NE to the PE, whereas the electrical current of all cells flows perpendicular and in-plane along the current collectors to the external tabs.

4.1.3 Stack model

4.1.3.1 One-dimensional bipolar stack model

In a one-dimensional bipolar stack model, each single-layer scaled cell is stacked in series to achieve a bipolar configuration, as shown by Figure 4.3(a). The governing equation to describe the relationship between the stacked and unit cell voltage is Kirchhoff's voltage law. Assuming a negligible cell-to-cell variation in a perfect stack, the total stacked voltage can be calculated by multiplying the number of cells with the individual cell voltage. Therefore, the open-circuit voltage of the bipolar stack, $U_{\mathrm{stack,BP,OCV}}$ can be calculated by

$$U_{\mathrm{stack,BP,OCV}} = N_{\mathrm{BP}}(\phi_{\mathrm{pos}} - \phi_{\mathrm{neg}}), \tag{4.5}$$

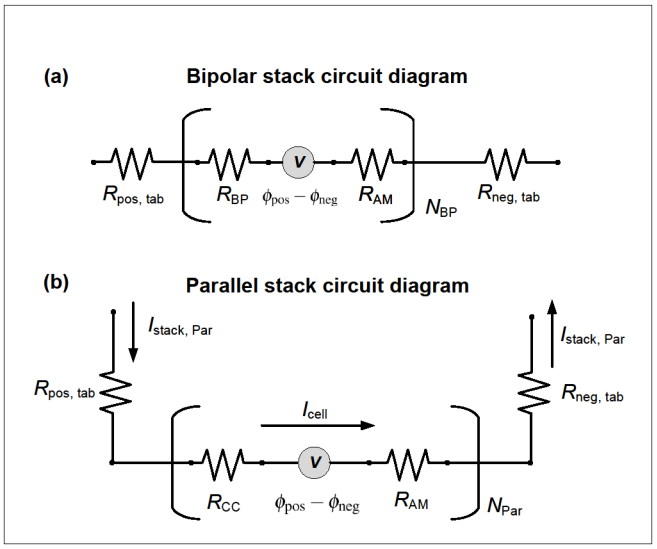


Figure 4.3 (a) Representative bipolar stack circuit diagram, where the ohmic resistances of the bipolar stack include a positive tab resistance ($R_{\mathrm{pos,tab}}$), a negative tab resistance ($R_{\mathrm{neg,tab}}$), ohmic resistances due to bipolar plates (R_{BP}) and ohmic resistances due to electronic transport across the electrodes (R_{AM}). (b) The parallel stack circuit diagram includes ohmic resistances from positive and negative tab resistances ($R_{\mathrm{pos,tab}}$ and $R_{\mathrm{neg,tab}}$), ohmic resistances due to the electronic transport in the current collectors (R_{CC}) and electrodes (R_{AM}).

where N_{BP} is the number of unit cells in a bipolar stack. Because the single-layer cells are connected in series and form part of the same circuit loop, the same current must flow through each unit cell, as given by

$$i_{\mathrm{stack,BP}} = i_{\mathrm{cell}}, \tag{4.6}$$

where i_{cell} is the current density of each unit cell.

The electrochemical behaviour of the stack was considered as a one-dimensional model in the z-direction (refer to Figure 4.2 for the definition of the coordinates). As shown by Yazdanpour *et al.*,[341] the in-plane current density $i = (i_{\mathrm{x}}, i_{\mathrm{y}}, 0)$ corresponds to the transport of electrons in the active materials and current collectors, whereas the through-plane current density, $i = (0, 0, i_{\mathrm{z}})$ denotes the transport of Li-ions. In this work, the ohmic losses due to electronic transport are lumped together and subtracted from the final stack voltage. The stack voltage, V_{BP} under load can be calculated by

$$V_{\mathrm{BP}} = N_{\mathrm{BP}}(\phi_{\mathrm{pos}} - \phi_{\mathrm{neg}}) - i_{\mathrm{stack,BP}} R_{\mathrm{stack,BP}}, \tag{4.7}$$

where $R_{\mathrm{stack,BP}}$ is the sum of all ohmic resistances in a bipolar stack:

$$R_{\mathrm{stack,BP}} = N_{\mathrm{BP}} R_{\mathrm{BP}} + N_{\mathrm{BP}} R_{\mathrm{AM}} + R_{\mathrm{tab,pos}} + R_{\mathrm{tab,neg}}. \tag{4.8}$$

As shown by Figure 4.2 and Figure 4.4(a), the current flows normal to the stack surface area in a bipolar stack and is distributed uniformly over them. Therefore, the ohmic resistance across the bipolar plates, R_{BP} can be calculated as follows:

$$R_{\mathrm{BP}} = \frac{d_{\mathrm{BP}}}{\sigma_{\mathrm{BP}} A_{\mathrm{BP}}}, \tag{4.9}$$

in which d_{BP} is the thickness of the bipolar plate, σ_{BP} is the electronic conductivity of the bipolar plate, and A_{BP} is the stack surface area. Because the current is flowing only in one direction through the bipolar plates in the middle of the stack, the calculation of the bipolar stack resistance can be simplified into a one-dimensional resistance, given by Equation 4.9. However, at the first and last unit cell of the bipolar stack, the current is flowing perpendicular and in-plane to the external tabs or vice versa. Due to the negligible impacts of the total resistance from the first and last current collectors, the current flow behaviour in these two current collectors is simplified into a one-dimensional electronic transport like all the other bipolar plates.

In Ref. 7, the ohmic resistance across both non-porous PE and NE was not considered in the single-layer model due to the relatively small size of the cell and a limited magnitude of applicable current densities. As a result, the voltage loss due to the electronic transport in both electrodes was found to be negligible. However, as the cell is scaled and stacked to model a large-format solid-state bipolar and parallel stack, the impacts of electronic transport resistance across both electrodes cannot be neglected. Hence, the ohmic resistance across the PEs and NEs, R_{AM} can be considered in the large-format stack models through

$$R_{\mathrm{AM}} = \frac{d_{\mathrm{neg}}}{\sigma_{\mathrm{neg}} A_{\mathrm{neg}}} + \frac{d_{\mathrm{pos}}}{\sigma_{\mathrm{pos}} A_{\mathrm{pos}}}, \tag{4.10}$$

in which d_{neg} is the thickness of the NE, σ_{neg} is the electronic conductivity of metallic Li, d_{pos} is the thickness of the PE and σ_{pos} is the electronic conductivity of LCO. The subscript AM represents the active materials in both electrodes.

Based on the direction of current flow into and out of the tabs, the ohmic resistance of the positive tab ($R_{\mathrm{tab,pos}}$) and negative tab ($R_{\mathrm{tab,\ neg}}$) can be calculated as follows:

$$R_{\mathrm{tab,pos}} = \frac{L_{\mathrm{tab,y}}}{\sigma_{\mathrm{tab,pos}} A_{\mathrm{tab,cross}}}, \tag{4.11}$$

$$R_{\mathrm{tab,neg}} = \frac{L_{\mathrm{tab,y}}}{\sigma_{\mathrm{tab,neg}} A_{\mathrm{tab,cross}}}, \tag{4.12}$$

where $L_{\mathrm{tab,y}}$ is the height of the tabs; $\sigma_{\mathrm{tab,pos}}$ and $\sigma_{\mathrm{tab,pos}}$ are the electronic conductivities of the positive and negative tabs; $A_{\mathrm{tab,cross}}$ is the cross-sectional area of the tab. It should be noted that only the first and last unit cells of the bipolar stack have positive and negative tabs. Because the tab resistance is calculated based on the current flow in the y-direction, but the voltage loss due to tab ohmic resistances is subtracted from the one-dimensional stack model in the z-direction, Equation 4.11 and Equation 4.12 are approximated 1D in-plane resistances. However, as shown by the computed 2D effective resistance compared to the 1D in-plane resistance in Appendix E, the difference between the 2D effective resistance and the 1D in-plane resistance can be considered negligible.

4.1.3.2 One-dimensional parallel stack model

Figure 4.3(b) shows the representative circuit diagram of the parallel stacking configuration of the single-layer cells. As the cells are arranged in parallel, all unit cells have the same voltage:

$$U_{\mathrm{stack,Par,OCV}} = (\phi_{\mathrm{pos}} - \phi_{\mathrm{neg}}). \tag{4.13}$$

The current of the parallel stack can be described by the Kirchhoff's current law. For an ideal stack with a negligible cell-to-cell variation, the relationship between cell and stack current can be described as follow:

$$i_{\mathrm{cell}} = \frac{i_{\mathrm{stack,Par}}}{2N_{\mathrm{Par}}}, \tag{4.14}$$

where N_{Par} is the number of unit cells stacked in parallel. The factor 2 indicates the double-coated configuration in each unit cell and is used to reproduce the experimental parallel stack measurements from Ito *et al.*[335] In real-world applications, a bipolar stack cannot be coated on both sides, whereas a double-coated configuration is often used for a parallel stack to reduce the gravimetric and volumetric contributions from inactive cell components.

Unlike a bipolar stack, each double-coated unit cell in a parallel stack has positive and negative tabs. While the cell voltage under load is identical, the sum of voltage loss due to positive and negative tabs must be subtracted using the stack current:

$$V_{\mathrm{stack,Par}} = V_{\mathrm{cell}} - i_{\mathrm{stack,Par}} R_{\mathrm{tab,neg}} - i_{\mathrm{stack,Par}} R_{\mathrm{tab,pos}}, \tag{4.15}$$

in which $R_{\mathrm{tab,neg}}$ and $R_{\mathrm{tab,pos}}$ are positive and negative tab resistance given by Equation 4.11 and Equation 4.12. Then, the cell voltage, V_{cell} can be calculated as follows:

$$V_{\text{cell}} = (\phi_{\text{pos}} - \phi_{\text{neg}}) - i_{\text{cell}} R_{\text{cell}}, \tag{4.16}$$

where R_{cell} is the sum of ohmic resistances in a unit cell:

$$R_{\text{cell}} = R_{\text{AM}} + R_{\text{CC,pos,eff}} + R_{\text{CC,neg,eff}}. \tag{4.17}$$

Due to the characteristics of a two-dimensional current flow in the current collectors of the parallel stack (see Figure 4.4b and Figure E-1a in the Appendix), a separate two-dimensional electrical model is solved to calculate the effective resistance of the positive and negative current collectors ($R_{\text{CC,pos,eff}}$ and $R_{\text{CC,neg,eff}}$). In this 2D electrical model, the potential drop in the current collector is assumed to be small such that the current distribution across the current collector remains uniform. The current collectors' thickness in the middle of the stack is also halved to account for the double-coated configuration. Table E-1 in the Appendix summarises the effective resistance computed using the 2D electrical model compared to the in-plane resistance calculated based on the resistivity and geometrical characteristics of the current collectors. The 1D in-plane resistance is found to be comparable to the 2D effective resistance, where the current boundary conditions are imposed on both sides of the current collectors.

4.1.3.3 Resistivity of electrode materials and current collectors

In principle, resistivity is a fundamental intrinsic material property, measuring the strength of a material in opposing the electric current flow with a uniform cross-sectional area. For a given material with an electronic conductivity, σ_{i}, the resistivity of the material, ρ_{i} can be represented by

$$\rho_{\text{i}} = \frac{1}{\sigma_{\text{i}}}. \tag{4.18}$$

Alternatively, the resistivity of a material can also be determined from

$$\rho_{\text{i}} = \frac{R_{\text{i}} A_{\text{i}}}{L_{\text{i}}}, \tag{4.19}$$

where R_{i} is the ohmic resistance of the material, A_{i} is the cross-sectional area and L_{i} is the length of the material. By rearranging Equation 4.19, the ohmic resistance of different cell components i in the bipolar and parallel stack model can be estimated. While resistivity is a fundamental intrinsic material property, the definition of the surface area, A_{i} and length, L_{i} depend on the direction of the current flow, as shown in Figure 4.4.

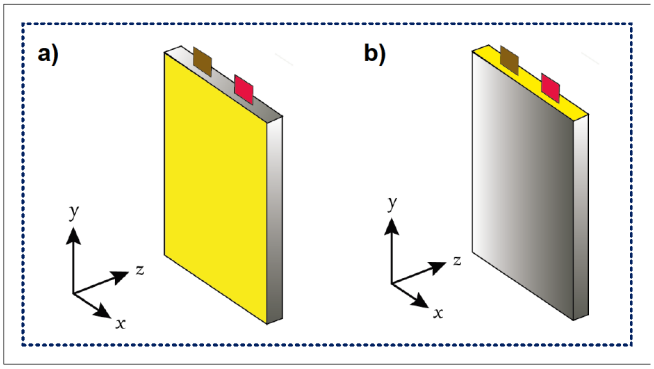


Figure 4.4 (a) The electrical current flows perpendicular to the stack surface area in a bipolar stack. (b) In a parallel stack, the electrical current flows perpendicular to the current collectors and then in-plane along the current collectors to the external tabs or vice versa. In both stack configurations, the cross-sectional area, A_i is defined by the surface normal to the current flow (yellow coloured area), whereas the length, L_i is defined by the dimension along the current flow.

Besides the stack geometrical characteristics, the impacts of current flow on the ohmic resistance of bipolar plates and current collectors are also considered through the parameter - electronic conductivity. While metallic conductors such as aluminium and Li have an isotropic electronic conductivity, anisotropic effects can become dominant for carbon composite materials. Depending on the matrix and fibre alignments in a carbon composite, the through-plane electronic conductivity of a carbon composite can be lower than the in-plane electronic conductivity by several orders of magnitude.[348–350] A parametric study was performed to assess the effects of different electronic conductivities of the carbon fibre bipolar plates on the gravimetric energy and power densities.

4.1.4 Two-dimensional thermal model

4.1.4.1 Energy balance

Chen *et al.*[351] have presented a detailed dimensional analysis of the conventional Li-ion thermal stack models by comparing the model accuracy and computational efficiency of the one-dimensional, two-dimensional and three-dimensional thermal models. The three-dimensional model is most accurate, but the computational time is $3000 - 11000$ times longer than the one-dimensional thermal model. They have shown that an in-plane two-dimensional model is able to capture the heat transfer behaviour of the stack with good accuracy and efficiency. Based on this analysis, a two-dimensional thermal model of the bipolar and parallel stacks is used, in which the heat generation is calculated from the one-dimensional electrochemical model. The heat transfer in the stack can be described by the following energy balance:[91]

$$\underbrace{\rho_{\text{eff}} C_{\text{p,eff}} \frac{\partial T}{\partial t}}_{\text{thermal energy storage}} = \underbrace{\frac{\partial}{\partial x}\left(k_{\text{x}} \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_{\text{y}} \frac{\partial T}{\partial y}\right)}_{\text{in-plane heat conduction}} + \underbrace{Q_{\text{gen,tot}}}_{\text{heat generation}} - \underbrace{Q_{\text{conv}}}_{\substack{\text{convective}\\ \text{heat}\\ \text{dissipation}}} - \underbrace{Q_{\text{rad}}}_{\substack{\text{radiative}\\ \text{heat}\\ \text{dissipation}}}, \tag{4.20}$$

where ρ_{eff} is the effective density of the stack, $C_{\text{p,eff}}$ is the effective specific heat capacity of the stack at constant pressure, T is the temperature, k_{x} and k_{y} are the effective thermal conductivities in the x and y directions respectively. $Q_{\text{gen,tot}}$ is the heat generation; Q_{conv} represents the heat dissipation by natural surface air convection and Q_{rad} denotes the heat dissipation by radiation. The effective in-plane thermal conductivity ($k_{\text{eff}} = k_{\text{x}} = k_{\text{y}}$) can be calculated as[95]

$$k_{\text{eff}} = \frac{\sum_{i=1}^{N_{\text{cell}}} v_{\text{i}} k_{\text{i}}}{v_{\text{cell}}}, \tag{4.21}$$

where N_{cell} is the number of cell components in each unit cell, $v_{\text{i}}/v_{\text{cell}}$ is the volume fraction and k_{i} is the thermal conductivity of each component. Equation 4.21 is derived assuming an ideal parallel conduction in each of the coplanar layers, which is only exact if the through-thickness is uniform.

For a parallel stack with the same layer-to-layer surface area across the stack, the effective thermal conductivity is given by[341]

$$\begin{aligned} k_{\text{eff,Par}} = \frac{1}{d_{\text{cell,Par}}} (&d_{\text{CC,pos}} k_{\text{CC,pos}} + d_{\text{CC,neg}} k_{\text{CC,neg}} \\ &+ 2d_{\text{pos}} k_{\text{pos}} + 2d_{\text{neg}} k_{\text{neg}} + 2d_{\text{elec}} k_{\text{elec}}), \end{aligned} \tag{4.22}$$

where $d_{\text{cell,Par}}$ is the thickness of the cell ($d_{\text{cell,Par}} = d_{\text{CC,pos}} + d_{\text{CC,neg}} + 2d_{\text{pos}} + 2d_{\text{neg}} + 2d_{\text{elec}}$). $d_{\text{CC,pos}}$ and $k_{\text{CC,pos}}$ are the thickness and thermal conductivity of the positive current collector; $d_{\text{CC,neg}}$ and $k_{\text{CC,neg}}$ are the thickness and thermal conductivity of the negative current collectors; d_{pos} and k_{pos} are the thickness and thermal conductivity of the PE, d_{neg} and k_{neg} are the thickness and thermal conductivity of the NE; d_{elec} and k_{elec} are the thickness and thermal conductivity of the SE.

To date, only Xu *et al.*[92] have measured the cross-plane thermal conductivity of the LiPON SE. In conventional liquid-based Li-ion batteries, Maleki *et al.* showed that the in-plane thermal

conductivity can be larger than the cross-plane thermal conductivity by a factor between 6-13.[96] Therefore, a parametric study was performed to analyse the effects of using different SEs thermal conductivities on the surface temperature of both stacks (see Figure 4.15(d)). Due to the dominant thermal conductivities from other cell components such as bipolar plates, the effects of using different SEs thermal conductivities on the stack average surface temperature were found to be negligible.

Similarly, the effective in-plane thermal conductivity of a bipolar stack can be estimated by

$$k_{\mathrm{eff,BP}} = \frac{1}{d_{\mathrm{cell,BP}}}(d_{\mathrm{BP}}k_{\mathrm{BP}} + d_{\mathrm{pos}}k_{\mathrm{pos}} + d_{\mathrm{neg}}k_{\mathrm{neg}} + d_{\mathrm{elec}}k_{\mathrm{elec}}), \tag{4.23}$$

in which $d_{\mathrm{cell,\ BP}}$ is the thickness of the bipolar unit cell ($d_{\mathrm{cell,\ BP}} = d_{\mathrm{pos}} + d_{\mathrm{elec}} + d_{\mathrm{neg}} + d_{\mathrm{BP}}$); d_{BP} and k_{BP} are the thickness and thermal conductivity of the bipolar plate.

The density, ρ_{eff}, and specific heat capacity, $C_{\mathrm{p,eff}}$, of the stacks can be estimated as:[351]

$$\rho_{\mathrm{eff}}C_{\mathrm{p,eff}} = \frac{\sum_{i=1}^{N_{\mathrm{cell}}} v_{\mathrm{i}}\rho_{\mathrm{i}}C_{\mathrm{p,i}}}{v_{\mathrm{cell}}}, \tag{4.24}$$

where ρ_{i} and $C_{\mathrm{p,i}}$ are the density and specific heat capacity of each component layer of the cell. Mei *et al.*[352] had calculated the effective specific heat capacity of the cell by defining the volume average of a mass-based property. If the effective density and specific heat capacity from Equation 4.24 need to be calculated separately, a mass average instead of a volume average should be used, as shown by

$$C_{\mathrm{p,eff}} = \frac{\sum_{i=1}^{N_{\mathrm{cell}}} m_{\mathrm{i}}C_{\mathrm{p,i}}}{m_{\mathrm{cell}}}, \tag{4.25}$$

where m_{i} is the mass of each cell component and m_{cell} is the total mass of the cell.

4.1.4.2 Calculation of heat generations

Generally, the heat generation in a battery, $Q_{\mathrm{gen,tot}}$ can occur irreversibly (Q_{irrev}) and reversibly (Q_{rev}):

$$Q_{\mathrm{gen,tot}} = Q_{\mathrm{irrev}} + Q_{\mathrm{rev}}. \tag{4.26}$$

In an all-solid-state Li-metal stack, the irreversible heat generation, Q_{irrev} can be attributed to losses due to the ionic transport in the SE (Q_{ohm}), reaction current at the SE-electrode interface

(Q_{ct}), solid Li transport in the non-porous bulk electrode (Q_{diff}) and electronic transport in the active materials and current collectors (Q_{CC}):

$$\begin{aligned} Q_{\mathrm{irrev,stack,BP/Par}} = I_{\mathrm{stack,BP/Par}}(\eta_{\mathrm{ohm}} + \eta_{\mathrm{neg}} + \eta_{\mathrm{pos}} + \eta_{\mathrm{diff}}) \\ + I^2_{\mathrm{stack,BP/Par}} R_{\mathrm{ohm,BP/Par}}, \end{aligned} \tag{4.27}$$

where η_{ohm} is the ohmic overpotential in the SE; η_{neg} and η_{pos} are the charge transfer overpotentials due to interfacial reaction kinetics at the respective interface; η_{diff} is the solid diffusion overpotential. The expressions to calculate these overpotentials can be found in Appendix B. The total thickness of both stacks is calculated from the sum of the stack thickness, the estimated volume change due to Li metal and the thickness of the pouch (see Table D-2 in Appendix D). The tab thickness is estimated based on literature values from Zhao *et al.*[353] and Hales *et al.*[354]

For a bipolar stack, $R_{\mathrm{ohm,BP}}$ is the sum of ohmic resistances of the active materials and bipolar plates in a bipolar stack ($R_{\mathrm{ohm,BP}} = R_{\mathrm{AM}} + R_{\mathrm{BP}}$). On the other hand, $R_{\mathrm{ohm,Par}}$ is the sum of ohmic resistances of the active materials and current collectors in a parallel stack ($R_{\mathrm{ohm,Par}} = R_{\mathrm{AM}} + R_{\mathrm{CC}}$). The irreversible heat dissipation due to Joule heating at both tabs, $Q_{\mathrm{irrev,tab}}$ can be calculated by

$$Q_{\mathrm{irrev,tab,BP/Par}} = I^2_{\mathrm{stack,BP/Par}} R_{\mathrm{tab,BP/Par}}, \tag{4.28}$$

in which $R_{\mathrm{tab,BP/Par}}$ is the ohmic resistance of both tabs in the bipolar and parallel stack.

The reversible heat generation, Q_{rev} occurs due to structural change of the PE and can be calculated as follows:[355]

$$Q_{\mathrm{rev,stack,BP/Par}} = \frac{I_{\mathrm{stack,BP/Par}} \overline{T} \Delta S}{nF}, \tag{4.29}$$

where n is the number of electrons and ΔS is the entropy of the stack, which can be estimated experimentally from the entropic heat coefficient (see Section 4.2.2).

4.1.4.3 Thermal boundary conditions

The convective heat dissipation in the two-dimensional thermal model can be defined as[95]

$$q_{\mathrm{conv}} = \left[\frac{1}{h} + \frac{d_{\mathrm{pouch}}}{k_{\mathrm{pouch}}}\right]^{-1} (T_{\mathrm{amb}} - T), \tag{4.30}$$

Table 4.1 Summary of stack geometrical and thermal parameters

Parameters	Positive electrode (LCO)	Solid electrolyte (LiPON)	Negative electrode/ Current collector (Li)	Reference
Thickness, d	$6\,\mu$m	$2\,\mu$m	$10\,\mu$m	[13, 63]
Surface area, A_{ref}	$0.0244\,\mathrm{m}^2$	$0.0244\,\mathrm{m}^2$	$0.0244\,\mathrm{m}^2$	[341]
Density, ρ	$3121\,\mathrm{kg\,m^{-3}}$	$2680\,\mathrm{kg\,m^{-3}}$	$534\,\mathrm{kg\,m^{-3}}$	[92, 95, 96]
Electronic conductivity, σ	$3100\,\mathrm{S\,m^{-1}}$	-	$1.1\times10^{7}\,\mathrm{S\,m^{-1}}$	[356, 357]
Thermal conductivity, k	$53.6\,\mathrm{W\,m^{-1}\,K^{-1}}$ (in-plane)	$1.4\,\mathrm{W\,m^{-1}\,K^{-1}}$	$81.8\,\mathrm{W\,m^{-1}\,K^{-1}}$	[92, 95, 98]
Specific heat capacity, C_{p}	$602\,\mathrm{J\,kg^{-1}\,K^{-1}}$	$1400\,\mathrm{J\,kg^{-1}\,K^{-1}}$	$3582\,\mathrm{J\,kg^{-1}\,K^{-1}}$	[92, 95, 96]

Parameters	Aluminium bipolar plate/ Current collector	Aluminium tab	Copper tab	Reference
Thickness, d	$10\,\mu$m	-	-	[13]
Surface area, A_{ref}	$0.0244\,\mathrm{m}^2$	$7\times10^{-4}\,\mathrm{m}^2$	$7\times10^{-4}\,\mathrm{m}^2$	[338, 341]
Tab distance from the edge, d_{edge}	-	$3\times10^{-3}\,\mathrm{m}$	$3\times10^{-3}\,\mathrm{m}$	[338]
Tab thickness, d_{tab}	-	0.2 mm	0.2 mm	[353, 354]
Density, ρ	$2700\,\mathrm{kg\,m^{-3}}$	$2700\,\mathrm{kg\,m^{-3}}$	$8960\,\mathrm{kg\,m^{-3}}$	[95]
Electronic conductivity, σ	$3.78\times10^{7}\,\mathrm{S\,m^{-1}}$	$3.78\times10^{7}\,\mathrm{S\,m^{-1}}$	$5.96\times10^{7}\,\mathrm{S\,m^{-1}}$	[341, 357]
Thermal conductivity, k	$238\,\mathrm{W\,m^{-1}\,K^{-1}}$	$238\,\mathrm{W\,m^{-1}\,K^{-1}}$	$398\,\mathrm{W\,m^{-1}\,K^{-1}}$	[95, 341]
Specific heat capacity, C_{p}	$897\,\mathrm{J\,kg^{-1}\,K^{-1}}$	$897\,\mathrm{J\,kg^{-1}\,K^{-1}}$	$385\,\mathrm{J\,kg^{-1}\,K^{-1}}$	[95]

in which h is the heat transfer coefficient ($h = 5\,\mathrm{W\,m^{-2}\,K^{-1}}$), d_{pouch} and k_{pouch} are the thickness and thermal conductivity of the pouch. The initial condition is given by the operating temperature and the ambient temperature is defined as 20 °C. By multiplying with the stack surface area, q_{conv} can be converted to Q_{conv} ($Q_{\mathrm{conv}} = q_{\mathrm{conv}} \times A_{\mathrm{ref}}$). Both stacks were cooled by natural air convection across the top surface of the stacks.

The parallel stack in the works of Ito *et al.*[335] was vacuum-sealed inside a laminated aluminium pouch. Therefore, the same material is modelled for both bipolar and parallel pouches in this work. Considering the surface emissivity of the laminated aluminium pouch, the radiative heat dissipation from the top and bottom of each pouch, Q_{rad} can be estimated by[351]

$$Q_{\mathrm{rad}} = \epsilon_{\mathrm{Al,top}}\sigma_{\mathrm{Boltz}}(T^4_{\mathrm{amb,top}} - T^4) + \epsilon_{\mathrm{Al,down}}\sigma_{\mathrm{Boltz}}(T^4_{\mathrm{amb,down}} - T^4), \tag{4.31}$$

where ϵ_{Al} is the surface emissivity of aluminium ($\epsilon_{\mathrm{Al,top}} = \epsilon_{\mathrm{Al,down}} = 0.09$) and σ_{Boltz} is the Stefan-Boltzmann's constant ($\sigma_{\mathrm{Boltz}} = 5.67 \times 10^{-8}\ \mathrm{W\,m^{-2}\,K^{-4}}$). Because the internal architecture of the stack is opaque, the radiative heat dissipation inside the stack is negligible.[351]

4.1.4.4 Electrochemical-thermal coupling

The heat generation in the thermal model was calculated from the electrochemical model, whereas the physical parameters in the electrochemical model were modified to include the temperature dependence, therefore coupling the electrochemical model to the thermal model two-ways. The notation $\overline{T}$ in the one-dimensional electrochemical model represents the surface-averaged temperature evaluated from the two-dimensional model:

$$\overline{T} = \frac{1}{A} \iint T dA. \tag{4.32}$$

The system of DAEs were solved in COMSOL Multiphysics® V5.4. A summary of the model parameters is given in Table 4.1.

4.2 Experimental parameterisation

A similar parameterisation procedure and a testing rig are used as in Chapter 3. The temperature was controlled with the Peltier element and measured with the thermocouples type K. The corresponding voltage and impedance profiles of the STMicroelectronic cell were recorded with Gamry Interface 1000. PEIS measurements at the open-circuit voltage of each pulse were taken at 25 °C, 35 °C, 45 °C and 55 °C to extract two of the temperature-dependent model parameters: the ionic conductivity in the SE and the exchange current densities at the NE and SE interface. The estimation of the temperature-dependent diffusion coefficient in the non-porous PE is discussed in Section 4.2.1, and the measurement of the entropic heat coefficient in Section 4.2.2.

Figure 4.5(a) shows the PEIS measurements at the four surface controlled temperatures. The ionic conductivity and charge transfer at both interfaces change marginally with SOC within the voltage window of 3.0 V and 4.2 V under isothermal operating conditions.[7] However, as the temperatures increase, the electrolyte resistance decreases from 72.56 Ω cm^2 to 6.71 Ω cm^2. The charge transfer resistances at the negative and PEs also decrease from 18.27 Ω cm^2 and 52.42 Ω cm^2 to 0.75 Ω cm^2 and 3 Ω cm^2, respectively.

The Distribution Function of Relaxation Times (DRT) analysis is used to distinguish the various contributions to the voltage loss at different operating temperatures.[315] The DRT analysis reveals four polarisation peaks at 25 °C and three peaks at 35 °C, at 45 °C and at 55 °C. A small shift in the DRT peaks is observed with increasing temperatures. Due to the different PEIS signals observed in this work compared to the PEIS measured in Ref. 7, 63, 60, a log-normal statistical analysis was used to quantify this variability by measuring the initial cell impedance

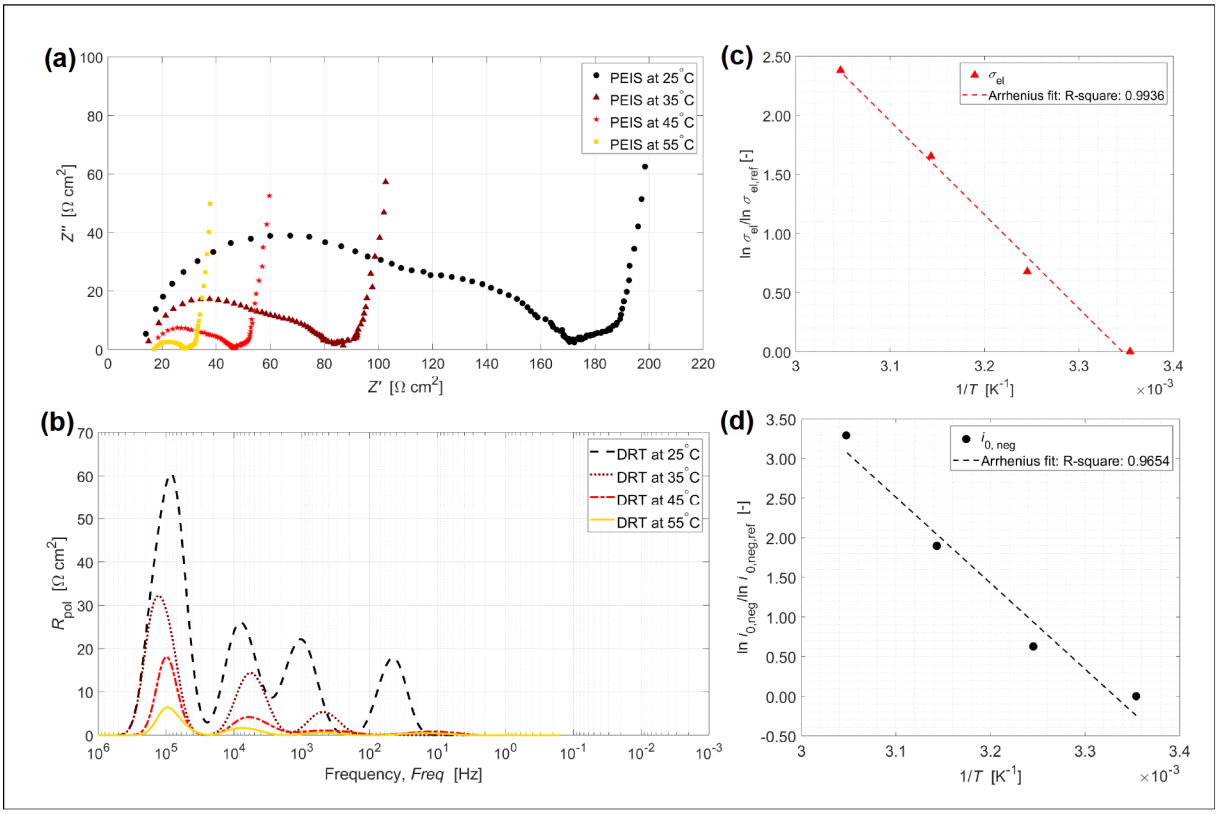


Figure 4.5 Experimentally measured cell impedance at four surface controlled temperatures: (a) An increase in the temperature from 25 °C to 55 °C reduces the electrolyte resistance by a factor of 10, the charge transfer resistance at the Li|LiPON interface by a factor of 24 and the charge transfer resistance at the LiPON|LCO interface by a factor of 17. (b) Corresponding DRT profiles. (c) The ionic conductivity estimated based on PEIS measurements obey the Arrhenius relationship ($R^2 = 0.9936$). (d) The temperature-dependent exchange current density at the Li|LiPON interface can also be described with the Arrhenius relation ($R^2 = 0.9654$).

of 23 cells after the formation cycling (three cycles of constant-current charge and discharge) at ambient temperatures (see Figure 4.8).

Two sets of parameters were estimated from the PEIS measurements: the ionic conductivity of the SE, σ_{elec} and the exchange current density, $i_{0,\text{neg}}$. The temperature-dependence of these parameters can be described by Arrhenius expressions:[246]

$$\sigma_{\text{elec}} = \sigma_{\text{elec,ref}} \exp\left[-\frac{E_{\text{a,elec}}}{R_{\text{gas}}}\left(\frac{1}{T} - \frac{1}{T_{\text{ref}}}\right)\right], \tag{4.33}$$

$$i_{0,\text{neg}} = i_{0,\text{neg,ref}} \exp\left[-\frac{E_{\text{a,i0}}}{R_{\text{gas}}}\left(\frac{1}{T} - \frac{1}{T_{\text{ref}}}\right)\right], \tag{4.34}$$

where $\sigma_{\text{elec,ref}}$ and $i_{0,\text{neg,ref}}$ are the ionic conductivity and exchange current density measured at the reference temperature, E_{a} is the activation energy and T_{ref} is the reference temperature defined as 298.15 K. By rearranging Equations 4.33 and 4.34 to

$$\ln\left(\frac{\sigma_{\text{elec}}}{\sigma_{\text{elec,ref}}}\right) = -\frac{E_{\text{a,elec}}}{R_{\text{gas}}}\left(\frac{1}{T}\right) + \frac{E_{\text{a,elec}}}{R_{\text{gas}}}\left(\frac{1}{T_{\text{ref}}}\right), \tag{4.35}$$

$$\ln\left(\frac{i_{0,\text{neg}}}{i_{0,\text{neg,ref}}}\right) = -\frac{E_{\text{a,i0}}}{R_{\text{gas}}}\left(\frac{1}{T}\right) + \frac{E_{\text{a,i0}}}{R_{\text{gas}}}\left(\frac{1}{T_{\text{ref}}}\right), \tag{4.36}$$

the values of $E_{\text{a,elec}}$ and $E_{\text{a,i0}}$ can be determined from the gradients of the curve.

The temperature-dependent OCP can be described by

$$U_{\text{cell}}(T) = U_{\text{cell,ref}} + (T - T_{\text{ref}})\frac{\partial U(x_{\text{Li}})}{\partial T}, \tag{4.37}$$

where $U_{\text{cell,ref}}$ is the OCP at 25 °C and $\partial U(x_{\text{Li}})/\partial T$ is the experimentally measured entropic heat coefficient, detailed in Section 4.2.2.

4.2.1 Measurement of temperature-dependent diffusion coefficients in the Positive Electrode (PE)

Concentration-dependent diffusion coefficients at 25 °C, 35 °C, 45 °C and 55 °C were obtained from the GITT data, following the procedures in Ref. 7. Figure 4.6(a) shows the concentration and temperature-dependent diffusion coefficients. For low Li content in the non-porous PE, the temperature does not affect the diffusion coefficients significantly. However, as the Li concentration in the PE increases, and an increase in the diffusion coefficient of a factor of 50 can be observed when the operating temperatures increases from 25 °C to 55 °C. The increase in the operating temperature reduces the mass transport barrier in the PE for low SOCs. The concentration and temperature-dependent diffusion coefficient can be approximated by

$$D_{\text{Li}} = D_{\text{Li,25 °C}}(x_{\text{Li}}) \times \exp\left[-\frac{E_{\text{a,diff}}}{R_{\text{gas}}}\left(\frac{1}{T} - \frac{1}{T_{\text{ref}}}\right)\right], \tag{4.38}$$

where $E_{\text{a,diff}}$ is an estimated activation energy ($E_{\text{a,diff}} = 20\,000\,\text{J mol}^{-1}$).

4.2.2 Measurement of entropy as a function of concentrations

A change in entropy is an indicator of a change in Li ordering and phase changes in the electrodes during charge and discharge.[264,358] The insertion of Li atoms into the lattice of the PE induces structural change and increases the disorder of atoms on the lattice. The entropy change under discharge must be identically opposite (negative in value) compared to its value under charge.[358]

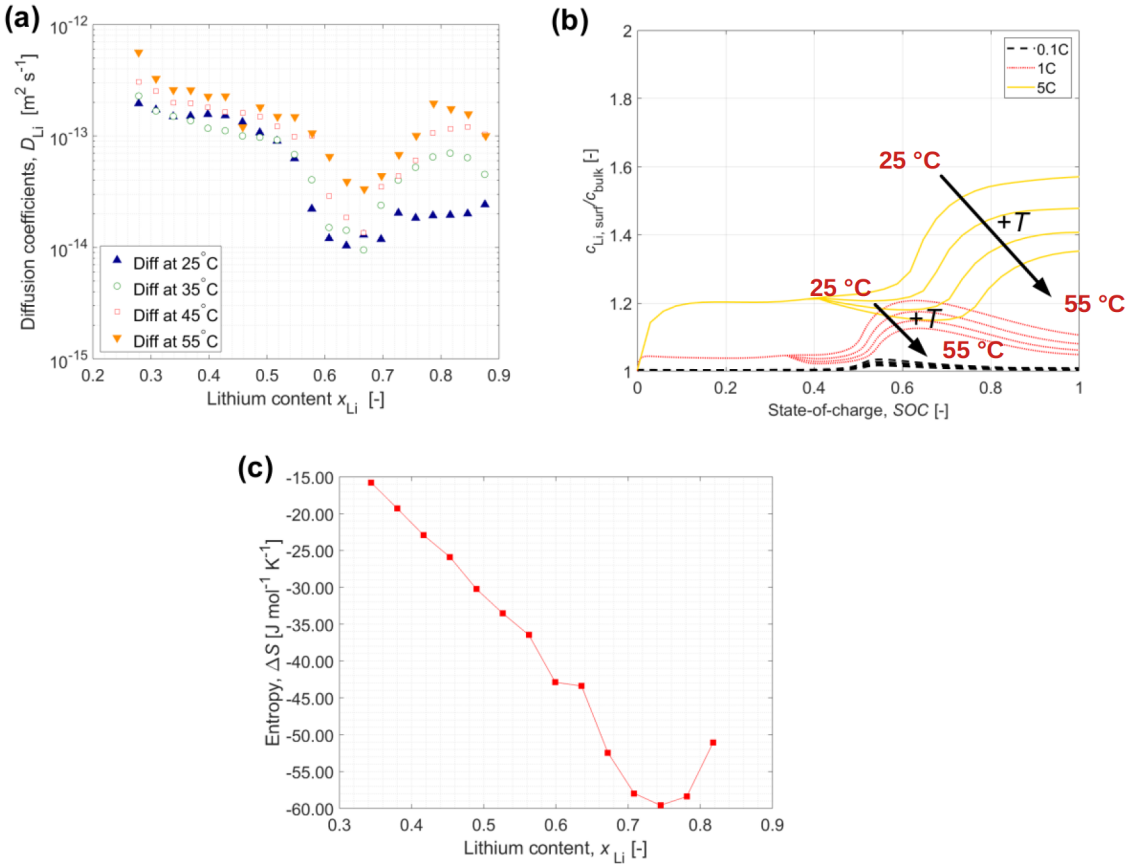


Figure 4.6 (a) Experimentally measured solid diffusion in the PE at four different operating temperatures: The impact of higher operating temperature improves the solid diffusion for low SOCs. (b) Comparison of the ratio $c_{\mathrm{Li,surf}}/c_{\mathrm{bulk}}$ for three C-rates: 0.1C, 1C and 5C. (c) Entropy of reaction in the LCO measured between 95% and 25% SOC.

The entropy, ΔS is proportional to the entropic heat coefficient, $\partial U(x_{\mathrm{Li}})/\partial T$ as follows:[264]

$$\Delta S = \left[nF \frac{\partial U(x_{\mathrm{Li}})}{\partial T} \right]_{\mathrm{SOC,p}}, \tag{4.39}$$

where n is the number of electrons and F is the Faraday's constant ($F = 96,485\,\mathrm{C\,mol^{-1}}$). ΔS is determined with the potentiometric method by measuring the change of OCP with respect to temperature at a fixed SOC. This method is preferred to the calorimetric method for thermally thin cell.[358] Zhang *et al.* have proposed a discontinuous measurement with a shortened voltage relaxation time to approximate the entropic heat coefficient ($\approx \partial U(x_{\mathrm{Li}})/\partial T$). Nevertheless, a relative error of 2% compared to the full discontinuous measurement method requiring long voltage relaxation was reported with this method in the temperature range between 20 °C and 30 °C.[264] As the temperature window in this model ranges from 25 °C to 55 °C, the full discontinuous measurement of $\partial U(x_{\mathrm{Li}})/\partial T$ was used to minimise this uncertainty.

Thomas *et al.*[358] have developed experimental procedures to measure the entropic heat coefficient for a temperature range between 21 °C and 29 °C. These procedures were adapted in this work for a wider temperature range from 25 °C to 55 °C. The cell was first charged with a constant current of 1 mA to 4.2 V at 25 °C and then held at the constant voltage of 4.2 V until the current dropped to 0.1 mA. Then, the cell was rested for 30 min before being discharged with C/10 until 5% of the nominal capacity is removed. A step-like temperature profile of 25 °C, 35 °C, 45 °C and 55 °C was applied to the cell, during which the cell was allowed to relax for 3 h before each temperature change. The experimental procedures were repeated to remove an incremental 5% of the cell's initial capacity until the SOC reached 25%. The overpotential of the cell for SOCs smaller than 25% is so dominant such that the OCP of the cell continues to change even after 10 h of relaxation per temperature. Therefore, the entropic heat coefficient was measured for the SOC window between 95% and 25%. Figure 4.6c shows the experimental estimated entropy of reaction in the non-porous bulk LCO electrode. The entropy of reaction becomes more negative with decreasing SOCs, which can be attributed to increasing lattice disorder.[358]

4.2.3 Variability statistical analysis

Figure 4.7 shows the initial impedance spectra and the capacity measurement after three formation cycles at 1 mA of constant-current charge and discharge. The change in the shape of impedance signal (for example, PEIS-1 and PEIS-23) implies that some degradations may had already occured during cell manufacturing or storage. As shown by Figure 4.7, all of the PEIS measurements were first normalised by excluding the influence from the contact resistance (*e.g.* all of the semi-circles begin from the [0,0] point). One drawback and future improvement potential of this work is the creation of a systematic database and cell labelling to record the experiments from different cells. While both Figure 4.7(a) and Figure 4.7(b) show a significant variability in terms of initial impedance and capacity measurements, it was unclear which impedance measurement from Figure 4.7(a) corresponded to the capacity measurement in Figure 4.7(b).

Figure 4.8(a) shows the log-normal statistical analysis to quantify the variability of 23 cells by the initial PEIS measurements from Figure 4.7(a). These variations were also observed in the experimental results by Fabre *et al.* and Larfaillou *et al.*,[60,63] in which three semi-circles in the EIS measurements were observed by Fabre *et al.*[60] and four semi-circles were proposed by Larfaillou *et al.*[63] on different cells of the same chemistry. Figure 4.8(b) illustrates the corresponding boxplot of the statistical analysis. From the boxplot, the first quartile, median and third quartile can be determined, which are 128 Ω, 152 Ω and 183 Ω respectively. Based on the dataset from 23 measurements, the variability corresponding to the first and third quartile is 42.97%. Therefore, an initial cell screening is necessary to minimise this variability. Because of the relatively large variability, the number of cells used for the experiments in this Chapter

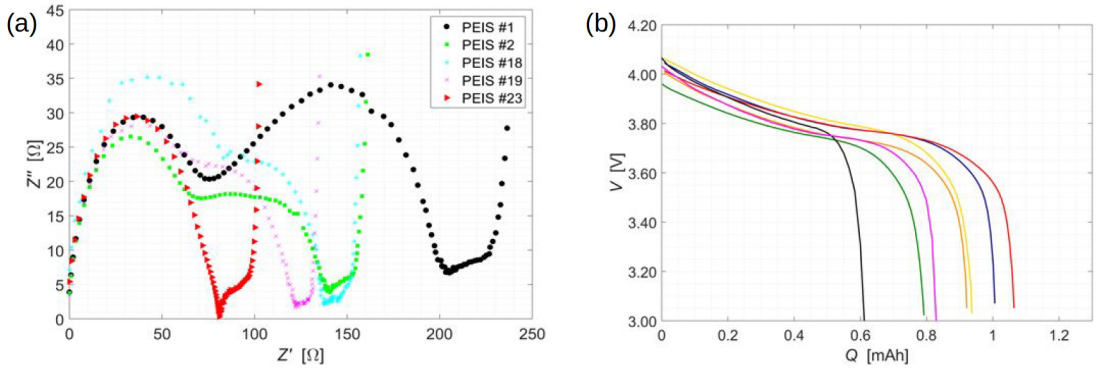


Figure 4.7 The initial impedance spectra and the capacity measurement after three formation cycles at 1 mA of constant-current charge and discharge.

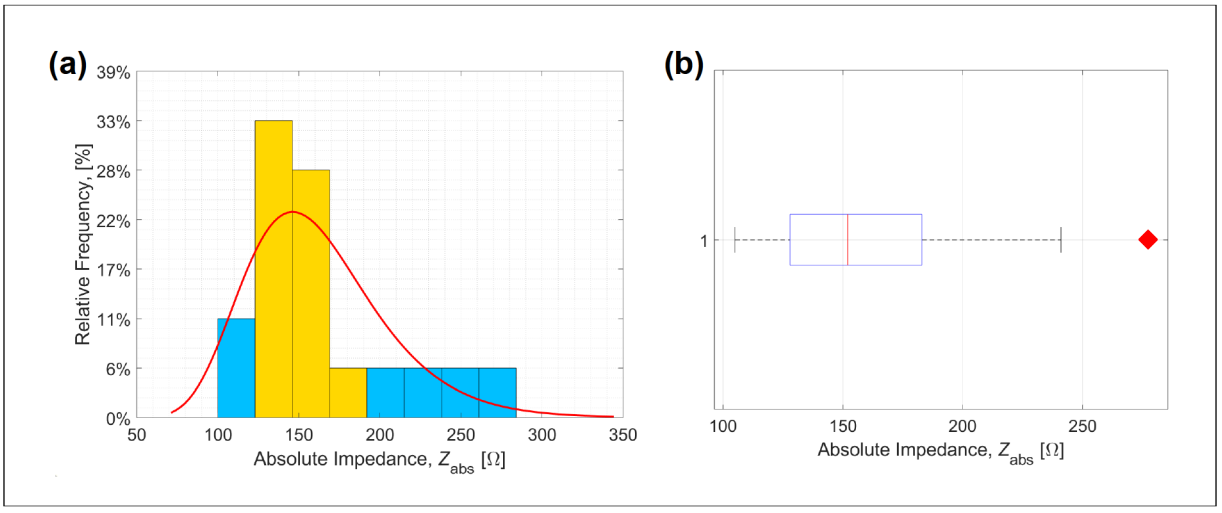


Figure 4.8 (a) A log-normal statistical analysis to quantify the initial impedance variability of 23 cells: The highlighted yellow bars corresponds to the interquartile range of the boxplot. (b) A representative boxplot of the statistical analysis.[‡]

was reduced to minimise the effects of inherent variability. While these deviations could be caused by manufacturing or synthesis conditions, another possible reason could be the effects of calendar ageing due to the transport and storage conditions.[359,360]

4.2.4 Fitting functions and parametric studies

Figure 4.9(a) shows the fitted rate-constant as a function of temperature. The rate constant increases with increasing temperatures, but the rate of increase decreases with temperature. Figure 4.9(b) and Figure 4.9(c) illustrate the effect of this parameter on the cell discharge voltage

[‡]The test bench was moved into a new laboratory, in which the air-conditioning system was not functioning for a period of time. To minimise the external noise due to fluctuating ambient temperature, a ventilator was placed in front of the test bench for these specific measurements.

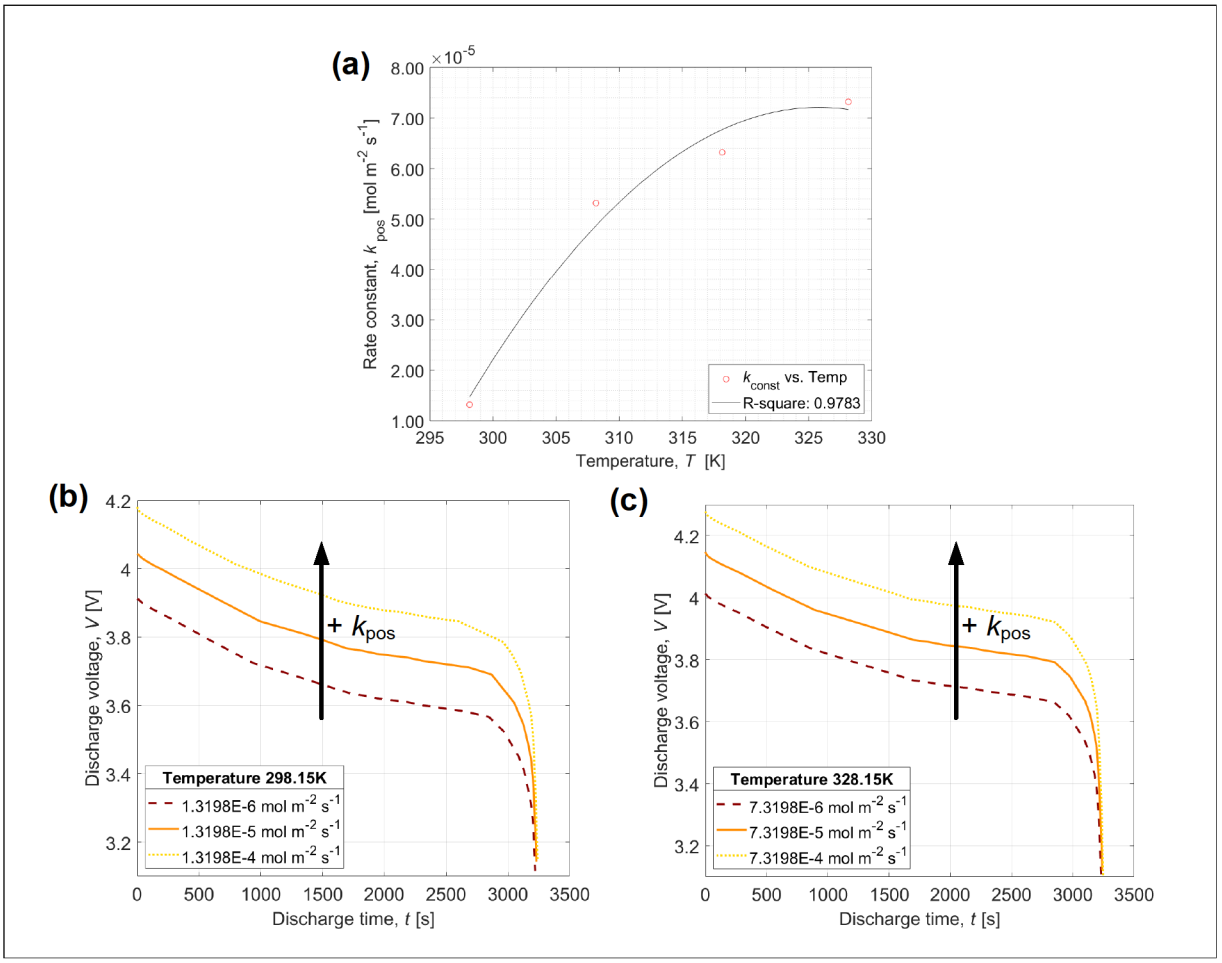


Figure 4.9 (a) The fitted rate-constant, k_{pos} as a function of operating temperature. The effect of k_{pos} on the cell discharge voltage curve at 25 °C in Figure 4.9(b) and at 55 °C in Figure 4.9(c). The solid orange lines correspond to the model parameter values chosen in this work.

at 25 °C and 55 °C. The simulated cell voltages were found to be sensitive to this parameter. The cell voltage changes significantly when k_{pos} is modified by one magnitude of order. Future works are required to study the impact of this sensitivity on different model predictions. Due to the decoupling of different possible rate mechanisms at the interface, estimating this parameter from experimental measurement is challenging. One possible method to quantify the interfacial rate constants is by using DFT-calculations, as demonstrated by Kurchin and Viswanathan.[361]

4.3 Qualitative model validations

Figure 4.10a shows the simulated and the experimentally measured voltage profile for current discharged at a cell temperature of 25 °C, 35 °C, 45 °C and 55 °C. While most model parameters were estimated from experimental measurements, k_{pos} was used as a fitting parameter in this work (Figure 4.9). As shown by Figure 4.10a, the cell performance improves with increasing operating temperatures, which can be attributed to the decreasing electrolyte and interfacial impedance (Figure 4.5) as well as higher diffusion coefficients (Figure 4.6a).

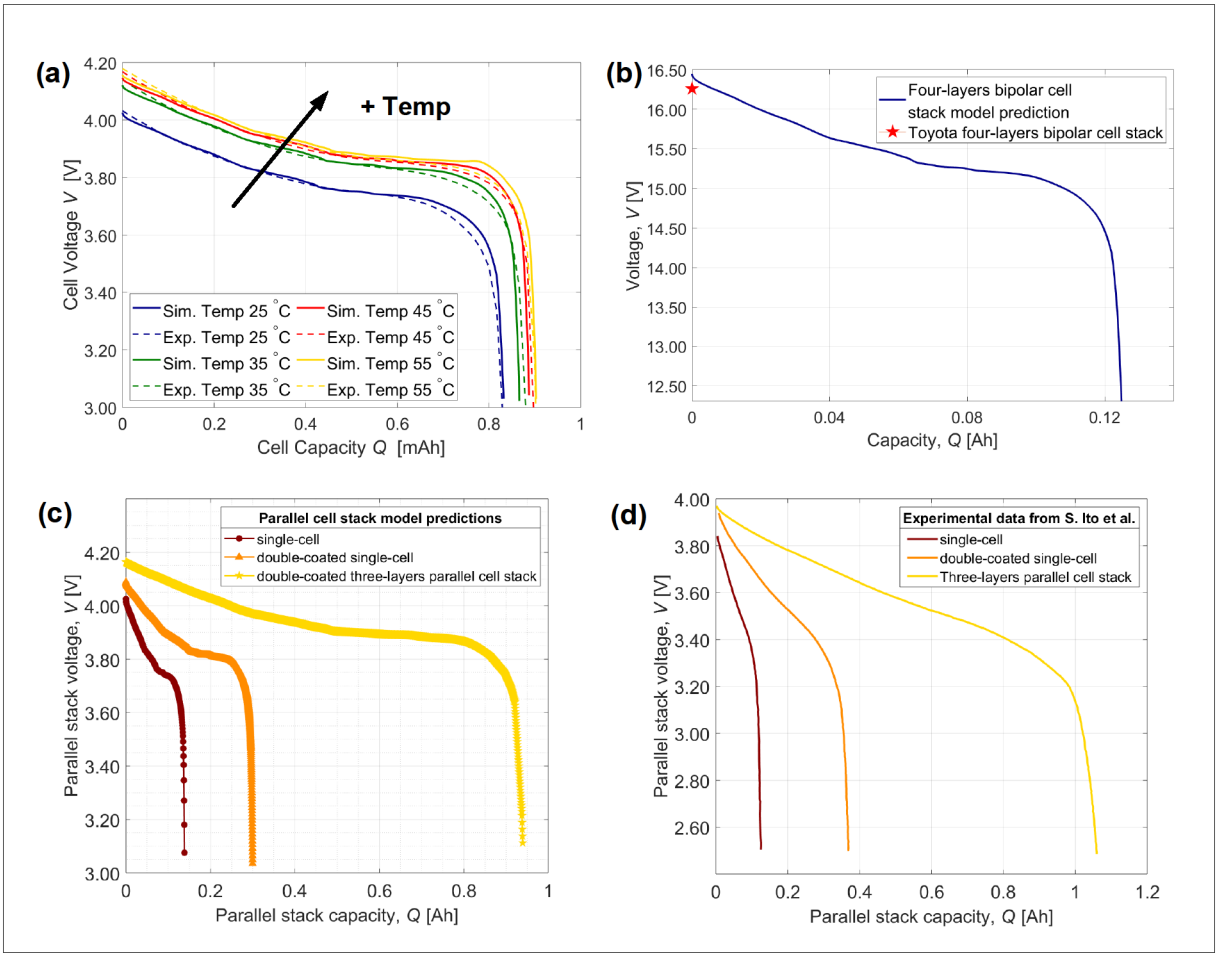


Figure 4.10 (a) Comparison of simulated constant-current discharge profiles of the single-unit cell model to experimental measurements at four different operating temperatures. (b) Qualitative validation of simulated bipolar stack voltage profile (4 cells) with the maximum experimental stack output voltage from Toyota.[333] Terminal voltage for a 0.1C discharge from the single-cell, double-coated single-cell and 3-cell parallel stack, (c) as predicted by the model and (d) obtained experimentally from Ito *et al.*[335]

As discussed in Section 4.1.1, the single-unit cell model was then scaled up by adjusting the electrode active surface area. The scaled cell model was placed in series and in parallel to achieve bipolar and parallel stack configurations. Toyota[333] showed that the bipolar stack could output a stack voltage of 16.26 V (indicated by the red star in Figure 4.10b). Four single-layer scaled cells were stacked in series giving a predicted maximum output voltage of 16.45 V, close to that achieved by Toyota on a four-layer all-solid-state stack using LCO as the PE, sulfide as the SE and graphite as the NE.

Ito *et al.*[335] have developed a parallel stack with the nominal capacity of approximately 1 Ah by stacking three single-layer double-coated cells in parallel. The electrochemical cell had a Li_2O-ZrO_2 coated $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) PE, sulfide-based SE and graphite NE. Figure 4.10c and 4.10d compare qualitatively the model predicted parallel stack profile with their experimental stack result. The single-cell model in Figure 4.10c uses a factor of 1 instead of 2 in Equation 4.14 and $N_{\mathrm{Par}} = 1$, whereas the double-coated single-cell model retains the factor

of 2 in Equation 4.14. N_{Par} is changed to three for the third discharge curve to model the three-layers parallel configuration.

4.4 Model-based stack design

4.4.1 Bipolar and parallel stack discharge

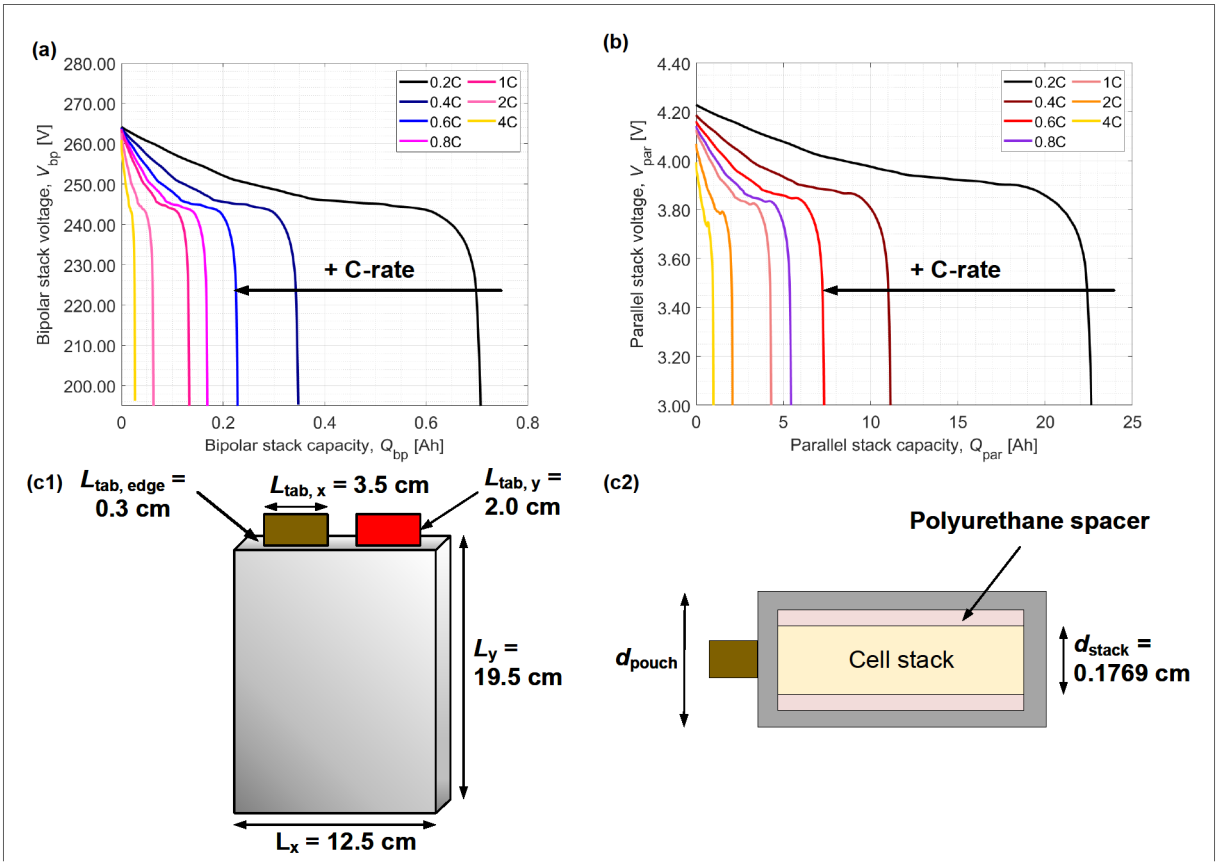


Figure 4.11 (a) With 63 cells stacked in series, a bipolar stack can achieve up to 265V with a limited stack capacity of less than 1Ah. (b) In a parallel stack, a high capacity of about 23 Ah can be obtained at a C-rate of 0.2 C with a maximum stack voltage of 4.2 V. (c1) The external dimensions of the pouch and tabs. (c2) Thickness of the pouch includes the stack thickness and the thickness of the polyurethane spacer used to reduce the internal volume deformation due to Li creep.

EiG C020 is chosen as the reference in the stack design of this work (cell chemistry: graphite|EC:DEC $LiPF_6$|$LiNiCoMnO_2$). The composite PE of the EiG C020 cell is 70 μm and the stack excluding the pouch case is 7.074mm thick.[341] In solid-state Li-metal cells, the thickness of a non-porous PE is limited by the slow diffusion of intercalated Li-ions, thus indicating a thinner PE would be used.[7] Moreover, instead of graphite, Li is used as the NE. The overall stack thickness assumed for this study is 0.1769 cm. Within the same stack volume for both bipolar and parallel stacks, the thickness of each component of the single unit cell was fixed, with values as given in Table 4.1. Therefore, the stack volume corresponds to 32

double-coated parallel cells or 63 cells in a bipolar configuration. Figure 4.11b and 4.11c show the simulated discharge stack profile for both bipolar and parallel configurations. As shown by Figure 4.11b, the bipolar stack can achieve a stack voltage up to 265 V with a stack capacity of 0.7 Ah, whereas the capacity of the parallel stack is 23 Ah, at a C-rate of 0.2 C.

Two common degradation mechanisms associated with the use of Li metal have been observed experimentally: (1) Li creep and (2) voids formation at the interface between the NE and the SE.[26,38,111,145] As discussed in Section 2.2.3 and Section 2.2.5, an external stack pressure is required to restrict the internal volume deformation due to Li metal.[26,38,111,145] Zhang *et al.*[362] have developed an in-situ instrument to track the volume change of Li metal electrode during lithiation and delithiation. They showed that a thickness change up to 23 μm is observed during cycling, even when the cell was placed under an external pressure of 850 kPa. Li *et al.*[363] proposed the use of polyurethane foam as a spacer (range of thickness $<$ 3.5 mm) to reduce the internal stress and strain inside the pouch of large-format Li-ion batteries. Based on the experimental observations of Ref. 362, it was inferred that a commercial large-format solid-state Li-metal stack could include internal spacers. By multiplying the total number of Li NEs and current collectors with the thickness change observed by Ref. 362, a spacer made of polyurethane foam of thickness 2.231 mm (parallel) and 1.426 mm (bipolar) between the stack and the pouch layer was included in this study. Therefore, the bipolar and parallel stacks have a projected volume of 84.06 cm^3 and 102.71 cm^3 respectively. As shown by Figure 4.13, the additional spacer decreases the gravimetric energy density by less than 5% for parallel and bipolar stacks due to the low density of the polyurethane ($35-40$ kg m^{-3}).[363] However, the polyurethane spacer can account for 43% - 53% of the stack volume if the spacer occupied the entire space between the stack and pouch. Table D-2 in the Appendix shows an example calculation of the mass and volume of a parallel stack that uses Li as the negative current collector and bipolar stack that uses aluminium as the bipolar plate. The calculated stack volume and mass for different current collectors and bipolar plate materials are summarised in Table 4.2.

4.4.2 Volumetric and gravimetric density

With the known mass and volume of the stacks, the energy and power density of the stacks can be estimated. Figures 4.12a and 4.12b show the simulated Ragone profiles of bipolar and parallel stacks compared to Sanyo 18650 Li-ion,[364] Sanyo prismatic Li-ion,[364] Li-sulfur[365] and supercapacitor LTO/LCO.[366] It should be noted that a typical Ragone profile comparing the power and energy density of different cell chemistries is C-rate dependent. The Ragone plots for bipolar and parallel stacks in this work were simulated with the discharge C-rates from 0.1 C to 5 C. 1C corresponds to 0.15 A for the bipolar stack and 9.6 A for the double-coated parallel stack. For a C-rate of 0.1, the volumetric energy density can reach up to 447.9 Wh L^{-1} for the parallel stack using Li as the negative current collectors (denoted as parallel Li stack) and 908 Wh L^{-1} for the bipolar stack using aluminium bipolar plates (denoted as bipolar aluminium stack). For

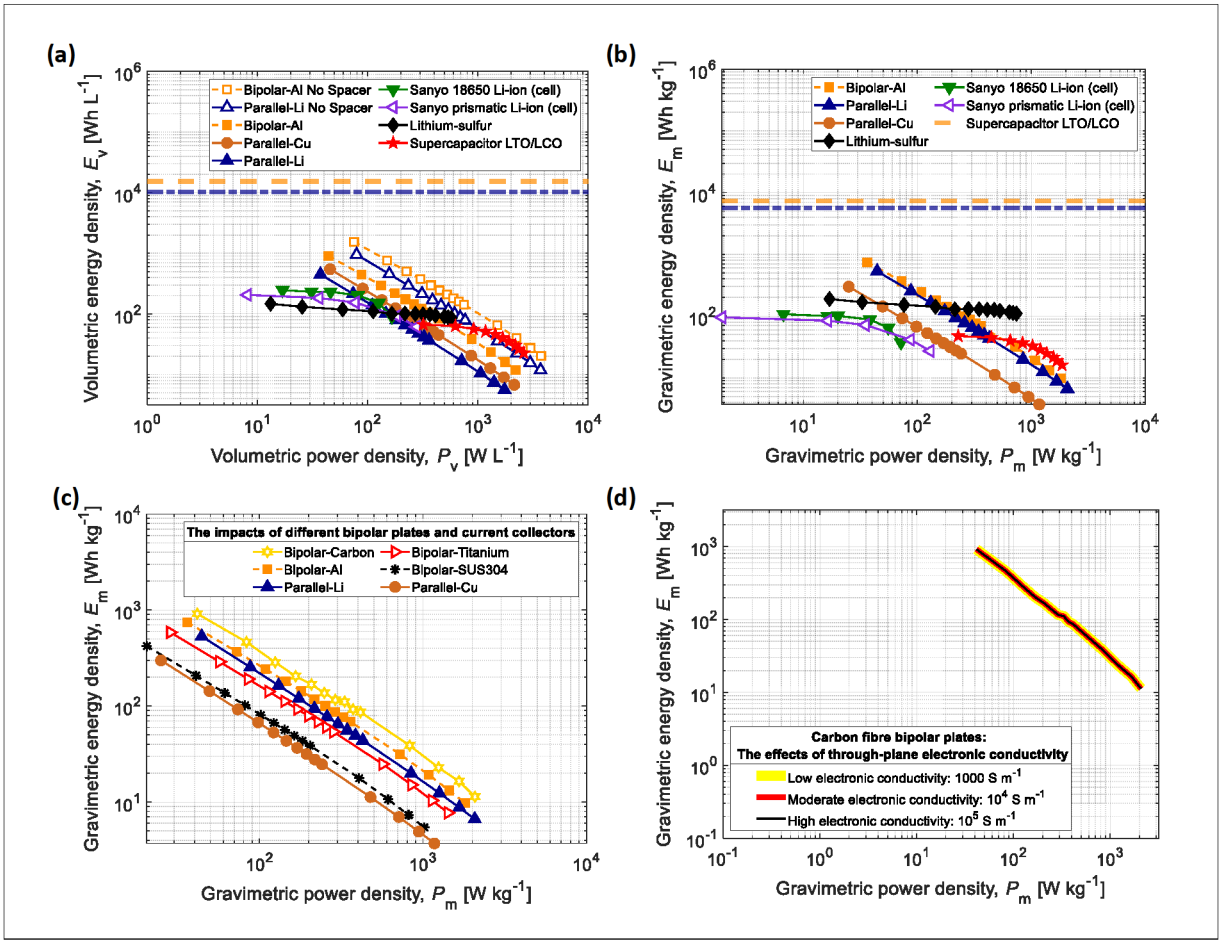


Figure 4.12 (a) Comparison of simulated volumetric Ragone profiles of the bipolar and parallel stack with aluminium bipolar plates (orange square), copper foils (brown circle) and Li foils (blue triangle) and without polyurethane spacer to Sanyo 18650 Li-ion (cell),[364] Sanyo prismatic Li-ion (cell),[364] Li-sulfur[365] and supercapacitor LTO/LCO.[366] (b) Simulated gravimetric Ragone profiles of bipolar and parallel stacks compared to literature values. The dashed lines in Figure (a) and (b) represent the theoretical maximum volumetric and gravimetric energy densities of bipolar Al and parallel Li stacks with negligible voltage losses (C-rate = 1/100). (c) Comparison of the gravimetric energy and power density of bipolar and parallel stacks made up of different types of current collectors: carbon composite, aluminium foils, Li foils, titanium foils, SUS304 stainless steel foils and copper foils. (d) The effects of different through-plane electronic conductivities of the carbon composite bipolar plates on the gravimetric energy and power densities of the bipolar stack.

stacks with polyurethane spacers, the bipolar aluminium stack has a higher volumetric energy density than a parallel copper stack and parallel Li stack. As shown in Figure 4.11, the bipolar stack is a relatively high-power cell with a discharge stack voltage of up to 265 V. As a result, the volumetric energy density of the bipolar aluminium stack is approximately two times higher than that of the parallel copper stack. The parallel copper stack has a higher volumetric energy and power density than the parallel Li stack due to the Li volume deformation inside the stack. If Li foil is used as the negative current collector, the total thickness change due to Li current collector and NEs can reach up to 2.231 mm. As a result, 53 vol-% of the spacer is required to reduce the internal stress and strain. However, because of the density of copper (8.960 g cm^{-3}) compared to Li (0.534 g cm^{-3}), the parallel Li stack has a higher gravimetric energy and power

Table 4.2 Calculated stack mass and volume for different parallel and bipolar stacks

Parallel stack		
Materials	Stack mass (g)	Stack volume (cm^3)
Lithium foil	86.499	102.708
Copper foil	153.629	84.208
Bipolar stack		
Carbon fibers	89.047	84.064
Aluminium foil	102.378	84.064
Titanium foil	130.216	84.064
Stainless steel	181.365	84.064

density than the parallel copper stack. If Li current collectors are substituted by copper foils, the volume fraction of the spacer can be reduced from 53% to 43%, but the mass ratio of the current collectors increases from 33% to 62%. Figure 4.13 illustrates the mass and volume fraction of the parallel Li and bipolar aluminium stack.

For an ideal stack without the volume deformation due to Li electrodes and current collectors, the volumetric power and energy density of bipolar aluminium stack without spacer can be 1.71 times higher than that of the bipolar aluminium stack with spacer. Similarly, the parallel Li stack's volumetric power and energy density of parallel Li stack without spacer can be higher than the parallel Li stack with spacer by a factor of 2.13.

The maximum volumetric energy density of parallel Li stack is 1.81 higher than the maximum of Sanyo 18650 Li-ion cylindrical cell, 3.05 times higher than the maximum of Li-sulfur reported by Mikhaylik,[365] 6.72 times higher than the maximum of LTO/LCO supercapacitor reported by DuPasquier *et al.*[366] Likewise, a factor of 3.68, 6.18 and 13.61 can be obtained with the bipolar aluminium stack. In a parallel stack using Li as both the NEs and the negative current collectors, due to the higher specific capacity of Li ($3860\,mAh\,g^{-1}$) compared to graphite NE ($372\,mAh\,g^{-1}$), the maximum gravimetric energy density of the parallel Li stack can be 4.95 times higher than Sanyo 18650 Li-ion cylindrical cell. However, if Li is used as the NE and copper is used as the current collector, this comparative factor reduces to 2.79. On the other hand, the maximum gravimetric energy density of the bipolar aluminium stack can be 6.93 times higher than Sanyo 18650 Li-ion cylindrical cell.

When the discharge C-rate increases, the energy density decreases but the power density increases. Only 83.39 Wh L^{-1} and 68.48 Wh kg^{-1} can be achieved with the bipolar aluminium stack and 36.78 Wh L^{-1} and 43.67 Wh kg^{-1} with the parallel Li stack when the stacks were discharged with 1C. The estimated volumetric and gravimetric power density at 1C for the bipolar aluminium stack are 439.21 W L^{-1} and 360.64 W kg^{-1}, respectively. Similarly, for the parallel Li stack, the corresponding volumetric and gravimetric power density are 360.8 W L^{-1} and 428.41 W kg^{-1}. The low energy density at 1C can be attributed to the limited thickness of the PE in each unit cell of the stack. For a non-porous PE, the increase in the thickness is limited by the slow diffusion in the electrode.[7] As a result, the active materials only account for 27% to 33% of the parallel and bipolar volume ratio. Also, the volumetric energy density was significantly affected by the possible volume deformation of Li. For an ideal scenario without deformation, the estimated volumetric energy density for the parallel Li and bipolar aluminium stack at 1C is 78.17 Wh L^{-1} and 142.19 Wh L^{-1} respectively. The maximum volumetric and gravimetric power density for bipolar aluminium stack at 5C is 2198 W L^{-1} and 1805 W kg^{-1}, which is close to the maximum volumetric and gravimetric power density for LTO/LCO supercapacitor (2608 W L^{-1}, 1860 W kg^{-1}) reported by DuPasquier and co-workers.[366] Finally, it is important to emphasise that this is a general electrochemical-thermal model that does not consider the impact of any stack failure, such as an internal short-circuit due to the propagation of Li filaments or interfacial decompositions.

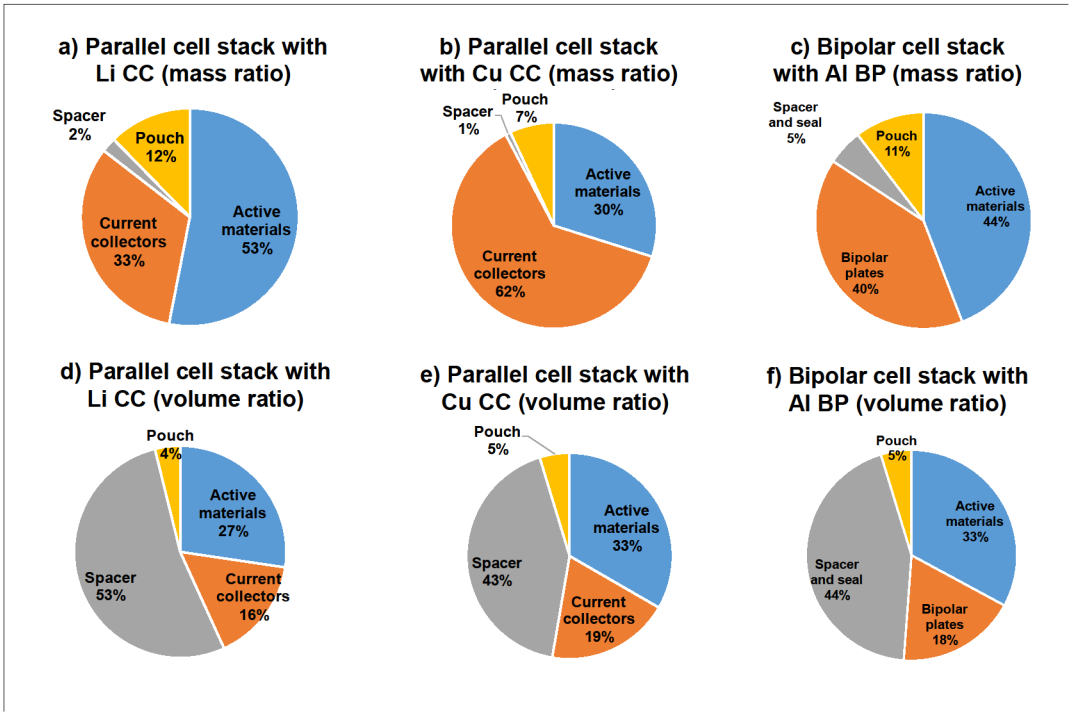


Figure 4.13 Mass and volume ratio of the parallel and bipolar stacks: (a) Mass ratio of the parallel Li stack. (b) Mass ratio of the parallel stack with copper foil as the negative current collector. (c) Mass ratio of the bipolar stack with aluminium foil as the bipolar plate material. (d) Contribution to the total volume of the stack by its various components: (d) Li current collectors and (e) copper current collectors in the parallel stack, (f) aluminium bipolar plates in the bipolar stack.

4.4.3 The effects of current collectors

The current collector materials have a significant impact on the gravimetric power and energy density of the stack. Four different materials are investigated in this work as potential bipolar plates for large-format bipolar solid-state Li-metal stacks, which include aluminium foil, titanium foil, carbon composite and SUS stainless steel. As for large-format parallel solid-state stacks, copper and Li foils as negative current collectors are compared in this study.

Liu *et al.*[340] have demonstrated that aluminium foil is stable as a bipolar plate material for sodium-ion cells. Aluminium foil is shown to exhibit a negligible parasitic current from 0 V to 5 V, while copper foil shows a sharp rise in current density from 3.6 V onwards, due to the copper oxidation at high potentials. They also demonstrated that there is no alloying reaction between aluminium foil and metallic sodium. In a separate study led by Fraunhofer IKTS, Wolter *et al.*[342] used the aluminium foil as the bipolar plate in a Li-based bipolar stack and showed that a stack voltage up to 9 V could be achieved with four unit cells. LaFollette and Utah[339] proposed a composite of long carbon fibres filled with carbon particles and fluoroelastomer as the bipolar plate for lead-acid batteries. Due to the carbon composite density compared to aluminium foil (see Table D-1), a gain factor up to 1.15 and 1.2 in the gravimetric power and energy density can be achieved when using a conductive carbon composite as the bipolar plate material. A modified titanium foil has been proposed by Lang *et al.*[344] as a possible candidate for bipolar plate, though they have investigated the material for a lead-acid battery only. The recent patent by Nagaya *et al.*[347] proposed the SUS stainless steel as the current collectors for solid-state cells. However, the model prediction shows that the gravimetric power density of the bipolar titanium and SUS stainless steel stack lag by a factor of 1.27 and 1.77 respectively, compared to the bipolar aluminium stack. Hence, on the basis of gravimetric power and energy density, carbon composite and aluminium foil are more suitable than titanium and stainless steel as bipolar plate materials.

While metallic conductors such as aluminium and Li have a relatively isotropic electronic conductivity, the through-plane electronic conductivity of a carbon composite can be several orders of magnitude lower than the in-plane electronic conductivity. As shown by Figure 4.2, the electrical current flows from one unit cell to the next unit cell through the bipolar plates. Figure 4.12(d) shows the simulated effects of through-plane electronic conductivity of carbon composite on the gravimetric energy and power densities. Due to a smaller magnitude of applied current densities and a larger stack surface area for the electronic transport in a bipolar stack, the gravimetric energy and power densities are found to be not sensitive to the variation in the through-plane electronic conductivity.

Copper has been used as the negative current collector in conventional parallel Li-ion stacks. It is possible to replace the copper foil with Li as the negative current collector when Li is used as the NE in a solid-state stack. In this work, the impact of Li and copper current collectors on

the parallel stack's gravimetric power and energy density is investigated. Here, the model shows that the simulated gravimetric power and energy density of the parallel Li stack can be 1.77 times higher than a parallel copper stack, which can be attributed to the higher mass ratio of active materials in parallel Li stack (53%) compared to parallel copper stack (30%) (see Figure 4.13).

4.5 Stack temperature profiles

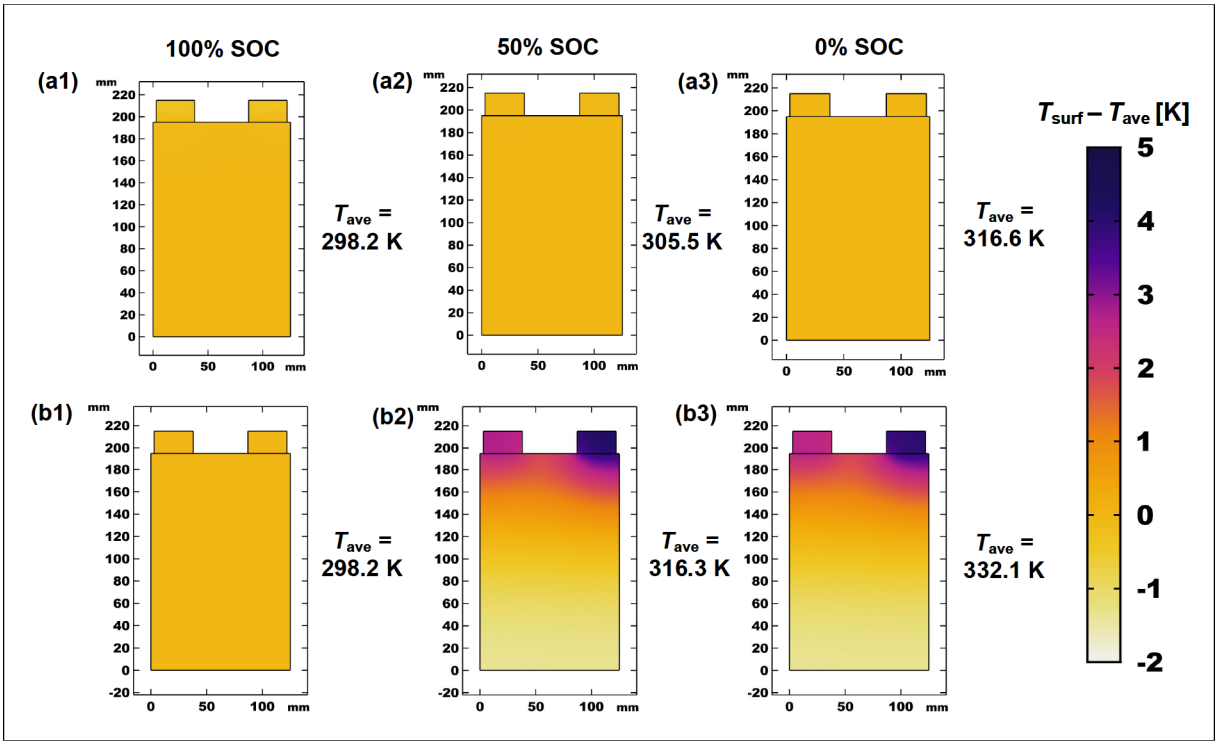


Figure 4.14 Temperature profile across the surface and tabs of the bipolar and parallel stack at the initial temperature of 298.15 K and 3C constant-current discharge. The temperature distributions are normalised by the average temperature at each time-step to compare the temperature gradients of two different stacks: (a1) Two-dimensional temperature profile of the bipolar stack at 100% SOC, where the average surface temperature is 298.2 K, (a2) at 50% SOC, where the average surface temperature is 305.5 K and (a3) at 0% SOC, where the average surface temperature is 316.6 K. (b1) Surface temperature profile of the parallel stack at 100% SOC ($T_{\text{ave}} = 298.2\,\text{K}$), (b2) 50% SOC ($T_{\text{ave}} = 316.3\,\text{K}$) and (b3) 0%SOC ($T_{\text{ave}} = 332.1\,\text{K}$).

Whilst the heat generation in a single-layer cell is insignificant because of the small and thermally thin cell, heat generations from a multilayer stack can significantly affect the stack performance. Figure 4.14 illustrates the model predicted temperature across the surfaces and tabs of the bipolar aluminium and parallel Li stacks under the operating conditions of 3C constant-current discharge from an initial temperature of 298.15 K. In the models, both stacks were cooled by natural air convection across the top surface of the stacks ($h = 5\ \text{W m}^{-2}\,\text{K}^{-1}$, air temperature = 20 °C) with additional heat dissipation by radiation from the top and bottom of the stacks.

The temperature gradients are normalised by the average temperature ($T_{\text{surf}} - T_{\text{ave}}$) at each time-step for ease in comparing.

As shown by Figure 4.14(a1) and Figure 4.14(b1), the bipolar and parallel stack show a negligible temperature gradient at the beginning of discharge. While the bipolar aluminium stack shows a negligible temperature gradient throughout discharge, the temperature gradients around the tabs of the parallel Li stack increase. The predicted temperature distribution is consistent with the experimental IR imaging result reported by Kim *et al.*, who recorded the highest temperature gradients near the tabs of a Li-ion polymer battery.[338] The parallel stack shows an average temperature rise of 33.91 K, whereas the average temperature rise of the bipolar stack is 18.51 K. For a large-format parallel Li-ion stack using liquid electrolytes, Yazdanpour *et al.*[341] showed through experimental measurements that the temperature increase could achieve up to 30 K under a high C-rate discharge. The significant temperature gradients and higher temperature rise of the parallel Li stack are caused by Joule heating due to tabs and current collectors (see Figure 4.15(b)).

The parallel stack has a total heat generation of 12.18 kJ whereas the bipolar stack has a total heat generation of only 4.99 kJ. For the given operating condition, the double-coated parallel stack has a higher nominal current than the single-sided bipolar stack, leading to a higher heat generation. As shown by Figure 4.2, a parallel stack also has external tabs at each unit cell, whereas a bipolar stack has only one positive and one negative tab at the two outermost unit cells. Both stack models neglect the contact resistance between the tabs and the external connectors, whose value is dependent on the experimental setup. In reality, the additional contact resistance would aggravate the Joule heating effects.[353]

4.6 Advantages and disadvantages of bipolar and parallel stacks

Although the bipolar stack shows significant advantages over the parallel stack in terms of higher energy densities and lower heat generations, a bipolar stack has a higher risk of stack failure. The failure of one unit cell, such as delamination or crack propagation, does not lead to an entire parallel stack's failure. On the other hand, failure in one unit cell will certainly cause the failure of the entire bipolar stack. Understanding the microscale's failure mechanisms will be critical for the successful commercialisation of bipolar solid-state Li-metal batteries for any medium to large scale application.

Secondly, as the total stack current for a bipolar stack is equal to one unit cell's current, the Couloumbic capacity of the stack does not scale with the number of unit cells inside the stack. In this work, the nominal capacity of 63 cells stacked in series is only 0.12 Ah. Therefore, a thick electrode design with an optimised mass transfer is required to improve the stack capacity. Table 4.3 summarises the advantages and disadvantages of bipolar and parallel cell stacks.

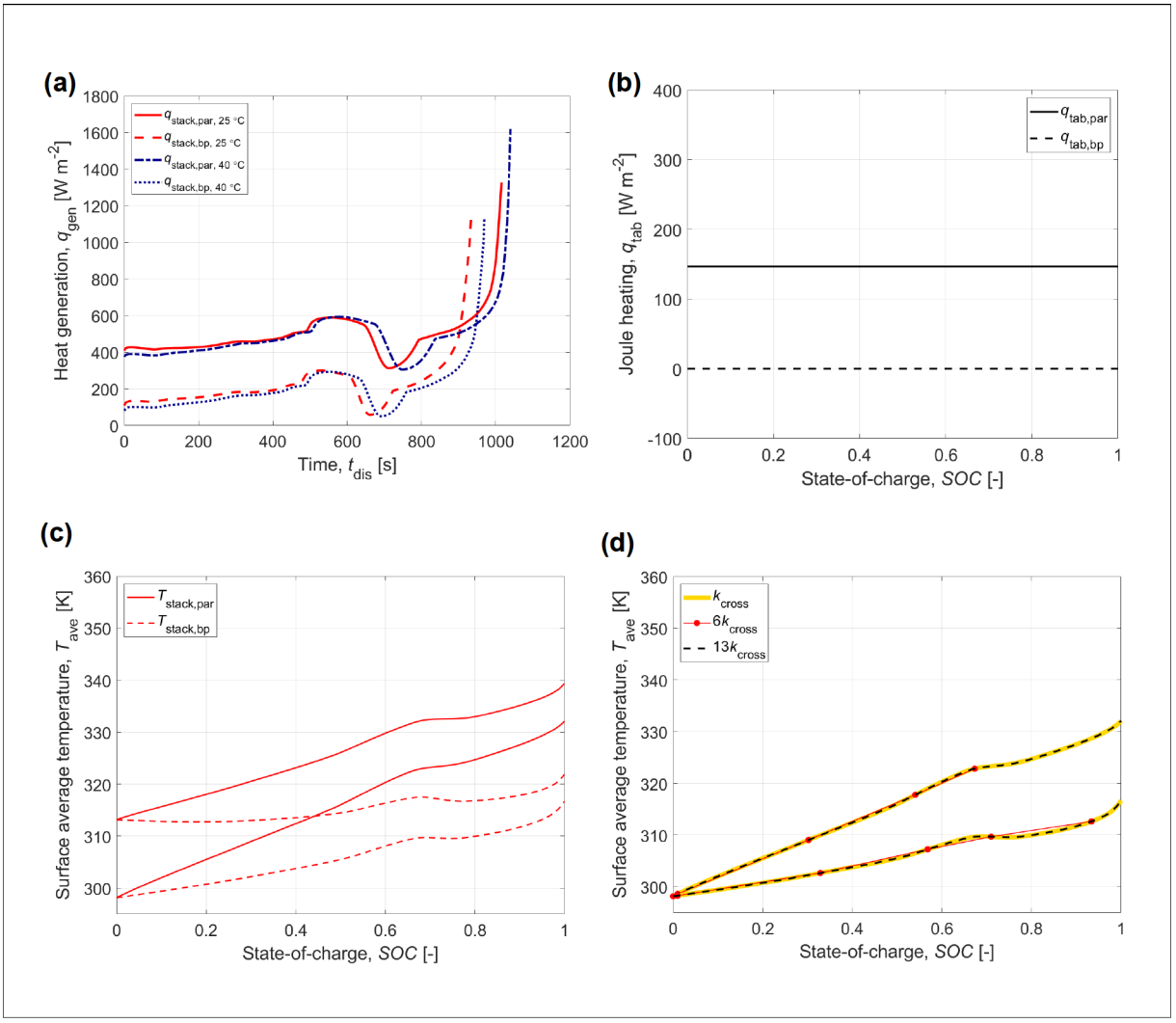


Figure 4.15 (a) The estimated heat generation in the bipolar aluminium stack and the parallel Li stack under 3C constant-current discharge from an initial temperature of $298.15\,\mathrm{K}$ and $313.15\,\mathrm{K}$. (b) The Joule heating effects in the parallel (solid black lines) and bipolar stacks (dashed black lines). (c) The temperature change profile of the parallel (solid red lines) and bipolar stacks (dashed red lines). (d) The effects of different SE thermal conductivity on the surface average temperature change.

Table 4.3 Advantages and disadvantages of bipolar and parallel stacks

	Bipolar stack	Parallel stack
Current homogeneity	More uniform current distribution can be achieved across the entire surface area. The bipolar stack uses the entire stack surface area to transfer current from one unit cell to the adjacent unit cell.	Current transferred through the external tabs of the parallel stack causes higher local current densities around the tabs.
Coulombic stack capacity	Limited stack capacity (0.12 Ah) due to the serial connection of each unit cell: A thick PE configuration with an optimised electrode design is necessary to improve the stack capacity.	A high nominal capacity (4 Ah) with a thin PE (6 μm) can be achieved by scaling the number of unit cells (32 double-coated unit cells) in a parallel configuration.
Power and energy density	The volumetric energy and power densities of the bipolar aluminium stack are higher than those of the parallel Li stack.	The temperature-dependent creep behaviour of Li metal implies that Li foils may not be used as the negative current collectors. If copper foils substitute Li foils as the negative current collectors, the gravimetric energy and power density decreases by a factor of 1.77.
Heat generations	The heat generation due to Joule heating in a bipolar stack is negligible (0.036 W m^{-2}).	Under a 3C constant-current discharge, Joule heating in a parallel stack can reach up to 146 W m^{-2}. A higher heat generation in the parallel stack suggests that an effective thermal management is required, which could further reduce the volumetric and gravimetric density of the battery modules at the system level.
Effects of unit cell failure	Reliable bonding of each unit cell is necessary as delamination in one unit cell will cause the failure of the entire bipolar stack.	Failure of one unit cell does not necessarily lead to failure of the entire stack.

4.7 Conclusions

By reviewing the research questions outlined in Section 1.3, the conclusions of this chapter can be summarised as follows:

How does upscaling of a single-layer cell affect the gravimetric and volumetric of large-format solid-state batteries?

A two-ways thermally coupled bipolar and parallel solid-state stack model was developed by scaling a single-layer cell model based on dimensionless governing equations and stacking the single-layer cell models in series and in parallel.

The parameter values of the single-layer cell model were obtained from experimental PEIS and GITT measurements at 25 °C, 35 °C, 45 °C and 55 °C. When increasing the operating temperature from 25 °C to 55 °C, the electrolyte resistance decreases by a factor of 10.8. In contrast, the charge-transfer resistance at the NE and PE interface can be reduced by a factor of 24.4 and 17.5, respectively. A higher operating temperature is shown to have a negligible impact on the diffusion coefficients for high SOCs, but an increase up to a factor of 50 can be observed for low SOCs.

By fixing each component's thickness in the single unit cell within the same stack volume for both bipolar and parallel stacks, the energy and power densities of both stack configurations can be compared. The stack model is used to study (1) the voltage discharge profiles of bipolar and parallel stacks, (2) the effects of Li volume deformation on stack volumetric power and energy densities, (3) the effects of different current collectors on gravimetric power and energy densities and (4) the effects of carbon composite through-plane electronic conductivities on the stack gravimetric power and energy densities. The bipolar stack can reach up to 265 V with 63 cells stacked in series, whereas a nominal capacity of 4.23 Ah is achievable with 32 double-coated cells stacked in parallel. A polyurethane spacer was included in the stack design to reduce the internal stress and strain due to Li metal's temperature-dependent creep behaviour. The bipolar aluminium stack has a higher volumetric energy and power density than the parallel Li stack due to the additional required spacer to suppress the volumetric deformation of the Li current collectors. In a parallel stack, if the Li foils are substituted by the copper foils as the negative current collectors in order to reduce volume change, the gravimetric energy and power densities drop by a factor of 1.77. By replacing the bipolar plates with different materials in the model, the model predicts that the bipolar stack with carbon composite and aluminium for bipolar plates has higher gravimetric energy and power density than the titanium and stainless steel bipolar stack because of lower densities of carbon composite and aluminium. The impacts of through-plane electronic conductivity of carbon composite bipolar plates on the gravimetric energy and power densities of the bipolar stack are found to be negligible due to a smaller magnitude of current densities and a larger stack surface area for the electronic transport in the

bipolar stack. In addition to the stack performance metrics determined by this study, cost and manufacturability must also be considered for practical applications in future works.

What are the thermal behaviour of large-format solid-state batteries? How does a bipolar stack solid-state battery differ from a parallel stack in terms of the heat generations and temperature gradients?

Through comparing the temperature profiles of the bipolar and parallel stacks under the operating conditions of 3C constant-current discharge from an initial temperature of 25 °C, the parallel stack shows an average temperature rise of 33.91 K, whereas the bipolar stack of only 18.51 K. While Joule heating in a bipolar stack is negligible, in a parallel stack, it can reach 146 W m^{-2}. Therefore, the bipolar stack is more advantageous than the parallel stack in terms of higher energy densities and lower heat generation rates. However, due to each unit cell's serial configuration, delamination or crack propagation in one unit cell will lead to the entire stack's failure. For this reason, an in-depth understanding of the failure mechanisms will be critical for the successful implementation of the bipolar solid-state Li-metal batteries.

Data availability

The electrochemical parameters measured in this work are available at `https://github.com/mc-git-code/Solid-State-Cell-Parameters`, `DOI:10.5281/zenodo.4281060`

Acknowledgements and author contributions

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Chapter 5

Mechanical behaviour of inorganic solid electrolytes

Due to the much higher impedance of inorganic solid electrolyte compared to liquid electrolyte (see Figure 1.8), increasing the conductivity of inorganic solid electrolytes to achieve an ionic conductivity comparable to that of liquid electrolytes ($10^{-2}\,\mathrm{S\,cm^{-1}}$) has become an important research target.[22,24,28,54,61–63] For a wide range of electrolytes, the ionic conduction often depends on the ionic diffusion coefficient. A higher diffusion coefficient increases the electrolyte conductivity. However, an independent measurement of both electrolyte conductivity and diffusion coefficient is challenging. Therefore, many existing studies use Nernst-Einstein's relation to estimate the ionic conductivity after the determination of the diffusion coefficient or vice versa.[54,116,236,261,324,367–372] However, the validity of this relation is questionable in describing the ionic mobility for many inorganic solid electrolytes.

In general, Nernst-Einstein's model relates the diffusion coefficient of an uncorrelated ion to the electrolyte's ionic conductivity. The failure of Nernst-Einstein's relation in modelling the ionic mobility was demonstrated by Marcolongo and Marzari.[374] Due to the high concentration of mobile ionic species in solid electrolytes, they showed that ionic correlations could act to increase the cooperative ionic motion and subsequently the ionic conductivity.[374,375] Therefore, the application of Nernst-Einstein's model without considering the ionic interactions leads to an underestimation of the ionic conductivity.[374] As a result, the Haven's ratio or the collective correlation factor were proposed to account for the ion-ion correlations.[375] However, these studies have not considered the physical meaning of the forces governing ionic mobility. How would the correlation factor change if the fundamental forces determining the ionic mobility for many inorganic solid electrolytes deviate from those assumed in the derivation of Nernst-Einstein's relation?

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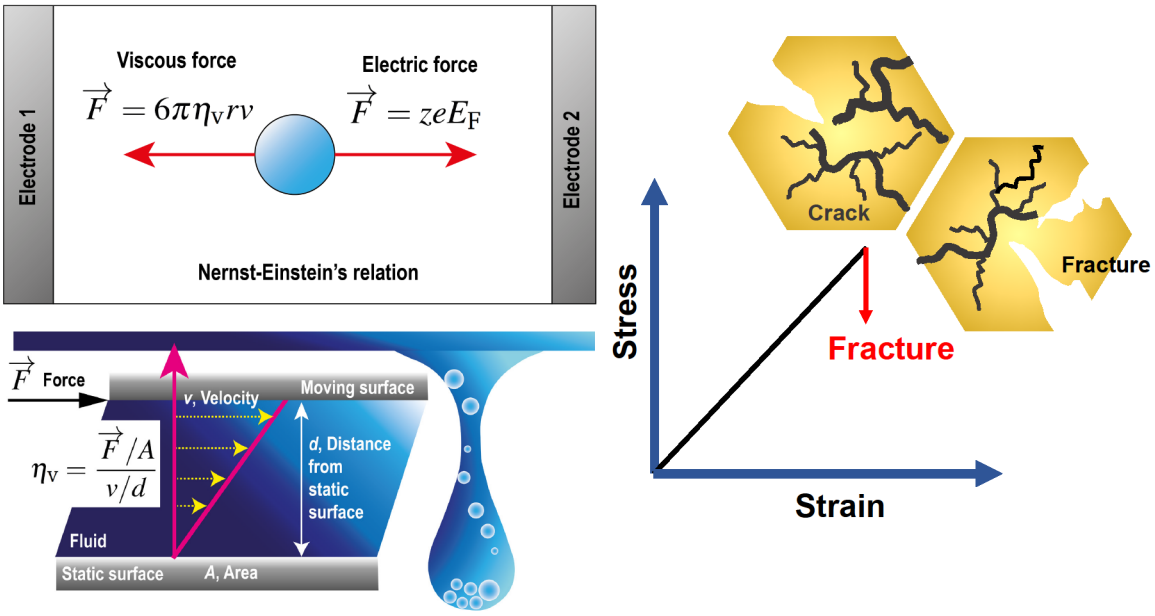


Figure 5.1 (Top left) Governing forces given by Nernst-Einstein's relationship, where the forward electric force is in a dynamic equilibrium with the backward viscous force. (Bottom left) The dynamic viscosity is a measure of the fluid resistance to flow. (Right) For brittle inorganic solid electrolytes characterised by cracks formation and electrolyte fracture, the stress-strain relationship before the electrolyte fracture can be approximated as linear. Reproduced with permission from Ref. 373, Copyright (2021), CC-BY.

By revisiting the original derivations proposed by Einstein[376] and later expounded by Brett *et al.*,[377] Feynman *et al.*[378] and Peskir,[379] the present research evaluates the fundamental assumptions of the Einstein's and Nernst-Einstein's relations as well as their validity in describing the ionic mobility for inorganic solid electrolytes. Despite the popular applications of these two relations in a wide range of electrolytes, in the absence of viscoelastic measurements as a function of temperatures, Nernst-Einstein's relation may not be directly transferable to model the ionic mobility for many inorganic solid electrolytes.

5.1 Fundamental physics of Nernst-Einstein's relation

The Einstein's relation shows that the diffusion coefficient, D, is directly proportional to the mobility, μ $[(\mathrm{m}^2\ \mathrm{mol})/(\mathrm{J\ s})]$:[81]

$$D = \mu R_{\mathrm{gas}} T, \tag{5.1}$$

where R_{gas} is the universal gas constant and T is the absolute temperature. By considering a displacement distribution function, the mean displacement of a suspended particle can be expressed as a function of the diffusion coefficient *via*[380]

$$\overline{x^2} = 2Dt, \tag{5.2}$$

where x represents the vector displacement of an atom, and $\overline{x^2}$ denotes the mean displacement over all possible routes in time t. Equation 5.2 was also derived by Smoluchowski and therefore, this equation is known as Einstein-Smoluchowski relation.[380] The relationship between $\overline{x^2}$ and t was later verified experimentally by Perrin, who measured the sedimentation equilibrium in a colloidal suspension.[380,381] Experiments were performed with different colloidal materials and solvent viscosities under various external conditions to demonstrate the kinetic theory of fluids.[381]

The diffusion coefficient, D, can be further related to the equivalent electrolyte conductivity, λ [(S cm^2)/equiv], through Nernst-Einstein's relationship given by[81]

$$\lambda = \frac{|z|F^2 D}{R_{\text{gas}} T}. \tag{5.3}$$

It should be noted that Equation 5.3 is only valid for non-interacting particles, *i.e.* when the ionic hopping are completely random.[382] If the hopping probability depends on the direction of the previous hops, the diffusion coefficient becomes correlated.[375,382] In this case, Equation 5.3 can be expressed as[382]

$$\lambda = \frac{|z|F^2 D}{R_{\text{gas}} T} \left(\frac{\partial \ln c}{\partial \mu} \right), \tag{5.4}$$

where c is the site fraction and μ is the chemical potentials of the particle.

The detailed derivations of the Einstein's, Einstein-Schmoluchowski and Nernst-Einstein's relation can be found in the works of Brett and co-worker,[377] Feynman *et al.*,[378] Islam[380] and Peskir.[379]

5.1.1 Governing forces in Nernst-Einstein's relation

Einstein[376] developed the theory of diffusion to describe the mobility of small particles in a fluid, where the fluid indicates either a liquid or a gas. The term diffusion denotes the collective motion of all Brownian particles in the fluid.[376] Einstein determined the diffusion coefficient of a suspended single particle from the dynamic equilibrium condition, which considers the superposition of two processes in opposite directions. In the absence of an external electric field, the first process describes the movement of a suspended single particle under the influence of a force, whereas the second process describes the diffusion due to the thermal molecular movement.[376] The force considered in Einstein's model is the viscous force, $\overrightarrow{F}$:[376]

$$\overrightarrow{F} = 6\pi\eta_{\mathrm{v}} r v, \tag{5.5}$$

where r [m] is the radius of the particle, η_{v} [Pa s] is the dynamic viscosity of the fluid and v [m s^{-1}] is the velocity vector of the single particle. The dynamic viscosity is a measure of the fluid resistance to flow (see the bottom left panel of Figure 5.1). By considering the dynamic equilibrium of the thermal molecular movement and molecular drift due to viscous force, Einstein demonstrated that the diffusion coefficient depends on the fluid viscosity and the size of suspended particle.[376]

In the presence of an external electric field, the backward viscous force is counterbalanced by the forward electric force:[377]

$$\underbrace{6\pi\eta_{\mathrm{v}} r v}_{\text{Viscous force}} = \underbrace{zeE_{\mathrm{F}}}_{\text{Electric force}}, \tag{5.6}$$

in which ze is the charge of each ion and E_{F} is the applied electric field between two metallic plates. The top left panel of Figure 5.1 illustrates the mobility of an isolated ion in an electric field between two parallel electrodes, where the movement of the ion is governed by a forward electric force and a backward viscous force. Therefore, the drift velocity of the single-particle can be described by[377]

$$v = \underbrace{\frac{ze}{6\pi\eta_{\mathrm{v}} r}}_{u} E_{\mathrm{F}}, \tag{5.7}$$

where u [(C m)/(N s)] is the proportionality coefficient between the velocity and electric field strength. u can be related to the ionic mobility, μ, from Equation 5.1 *via* $\mu = u/(zF)$, where F is the Faraday's constant.

5.1.2 Diffusion coefficients in gaseous media

For gaseous media involving the acceleration and collisions of gaseous molecules, Feynman *et al.*[378] demonstrated that the drift velocity of the gas particles could be derived by considering the drift due to an externally applied force, $\overrightarrow{F}$ [(kg m)/s^2]. In this case, the drift velocity becomes[378]

$$v = \mu_{\mathrm{gas}} \overrightarrow{F}, \tag{5.8}$$

where μ_{gas} [s/kg] is the constant of proportionality denoted as the gaseous mobility. This equation is derived based on the assumption that gaseous particles accelerate under the applied external force:[378]

$$\begin{aligned} v &= a\tau, \\ &= \frac{\overrightarrow{F}}{m}\tau, \end{aligned} \tag{5.9}$$

in which a [m/s^2] is the acceleration of the gaseous particles, τ [s] is the mean time between collisions and m [kg] is the mass of the gas molecule. By comparing Equation 5.8 and 5.9, the gaseous mobility is defined by τ/m. μ_{gas} can be further related to the diffusion coefficient ($D = \mu_{gas}kT$) through the kinetic theory of gases:[378]

$$\frac{1}{2}mv_{rms}^2 = \frac{3}{2}kT, \tag{5.10}$$

where v_{rms} [m/s] is the root-mean-square velocity of gas molecules and k [J/K] is the Boltzmann's constant ($k = R_{gas}/N_A$). Equation 5.10 can be derived from the ideal gas law under the assumption that the volume of gaseous molecules is negligible compared to the total volume, in which the gas is contained.

By examining the fundamental assumptions in these derivations, it is evident that the relationship between the diffusion coefficient and electrolyte conductivity can only be established in a viscous or a gaseous medium.

5.1.3 Diffusion measurements in inorganic solid electrolytes

Hayamizu and Aihara[383] have measured the diffusion coefficient and ionic conductivity of ^{7}Li-ion in sulfide-based solid electrolyte, $(Li_2S)_7(P_2S_5)_3$ using Pulse-Gradient Spin-Echo (PGSE) NMR method and AC impedance spectroscopy independently. By using the PGSE NMR method, the diffusion coefficient can be determined from the Stejskal and Tanner equation, where the echo attenuation depends on the gradient strength, g [T m^{-1}], interval between the leading edges of the gradient pulse, Δ [ms] and pulse duration, δ [ms].[383–385] The ^{7}Li-ion diffusion measured by the PGSE-NMR method is determined by the migration of the ^{7}Li-ion during a time interval Δ.[384] The first signal encodes the target ^{7}Li-ion, and the second signal detects the encoded species after an interval Δ.[384] The measured signal attenuations usually have a standard deviation of 2-5% for ^{7}Li-ion.[386,387]

Figure 5.2(a) shows the temperature-dependent diffusion coefficient between 303 K and 353 K. The apparent diffusion coefficient measured by the PGSE NMR method shows a qualitative

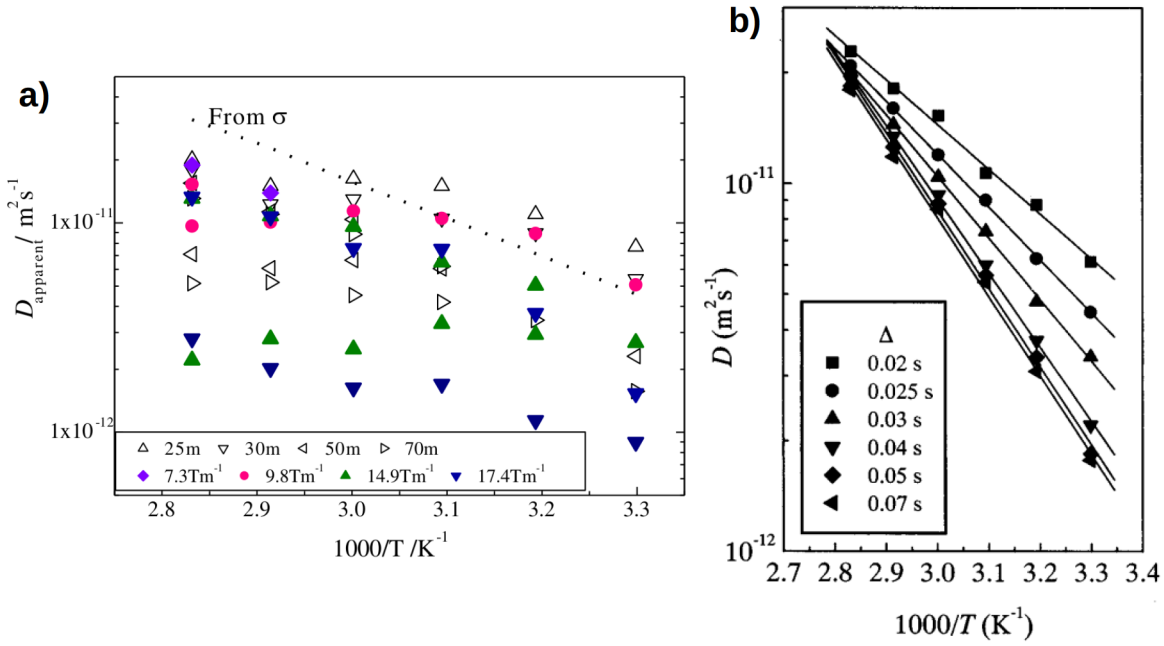


Figure 5.2 The degree of scattering observed in the Pulse-Gradient Spin-Echo (PGSE)-NMR diffusion measurements of (a) inorganic solid electrolytes and (b) solid polymer electrolytes. (a) The opened triangles represent the diffusion measurements using different intervals between two gradient pulses, Δ, whereas the filled triangles denote the diffusion measurements using different magnitudes of gradient strength, g. The standard notation to denote pulse delays of milliseconds (Δ) is "ms" instead of "m". The dotted line is the estimated diffusion coefficient from the ionic conductivity measurement using Nernst-Einstein's equation. The standard deviations of a typical ^{7}Li-ion PGSE-NMR measurement are between 2-5%.[386,387] Reproduced with permission from Ref. 383, Copyright (2013), Elsevier. (b) The temperature-dependent diffusion measurement as a function of Δ in solid polymer electrolytes. Reproduced with permission from Ref. 388, Copyright (2000), Elsevier.

agreement with the estimated diffusion coefficient from the measured ionic conductivity using Nernst-Einstein's relation (*i.e.* both measured and estimated diffusion coefficients become larger with increasing temperature). However, the diffusion coefficients measured with the PGSE NMR method deviate significantly from the estimated diffusion coefficient using Nernst-Einstein equation.

Due to the strong dependence on the g- and Δ-values, the PGSE-NMR measurement method shows no unique apparent diffusion coefficient in the sulfide-based solid electrolyte. For instance, Figure 5.2(a) shows that at the same gradient strength of $g = 14.9$ T m^{-1} and the same interval of $\Delta = 30$ ms, different diffusion coefficients were obtained for all temperatures.[383] Two modes of a fixed δ with varying g and a fixed g with varying δ yield different echo attenuation plots.[384] Such observations differ from the diffusion measurements taken in polymer electrolytes, organic solvents and ionic liquids, where the measured signal attenuations can be quantified reliably.[386,388–391] Figure 5.2(b) shows the diffusion measurement in solid polymer electrolytes. Unlike the strong degree of scattering observed in

the diffusion measurement of $(Li_2S)_7(P_2S_5)_3$ inorganic solid electrolytes (Figure 5.2a), the temperature-dependent diffusion coefficients do not scatter depending on measuring conditions.[388] The scattered ionic diffusions in $(Li_2S)_7(P_2S_5)_3$ (for example, the diffusion measurement at the gradient strength $g = 9.8\ \mathrm{T\,m^{-1}}$ denoted by the pink circles in Figure 5.2a) also reveal that the dependence of diffusion coefficients on ionic conductivity is non-linear.[383] Such behaviour is different from the estimated diffusion coefficient using Nernst-Einstein's relation, where the diffusion coefficient is predicted to be linearly proportional to the electrolyte conductivity. In contrast to the non-linear diffusion coefficients shown in $(Li_2S)_7(P_2S_5)_3$ inorganic solid electrolyte, the diffusion measurement performed in solid polymer electrolytes indicates a linear relationship between the diffusion coefficient and ionic conductivity.[388]

Even with a better-controlled measuring condition, Hayamizu *et al.*[384] showed that the simple application of Nernst-Einstein's equation in inorganic solid electrolytes is still questionable. They showed that a PGSE-NMR diffusion measurement with a longer time interval, Δ, could reduce the degree of scattering observed in inorganic solid electrolytes.[384] However, the diffusion coefficient calculated from Nernst-Einstein's equation is larger than the equilibrated diffusion coefficient obtained by the PGSE-NMR measurements.[384,385] As a result, the N_{carrier} calculated from the experimental ionic conductivity and equilibrated diffusion coefficient through Nernst-Einstein's relation were found to be higher than the values estimated by the molecular formula and experimental density.[384,385] In addition, an equilibrated measurement of the diffusion coefficient may not be representative of the fast ionic transport across the solid electrolyte.

By comparing the echo-attenuation plots obtained in single crystals and powders, grain morphologies were shown to cause such unusual diffusive behaviour in inorganic solid electrolytes.[385]

By comparing the echo-attenuation plots obtained in single crystals and powders, grain morphologies were shown to cause such unusual diffusive behaviour in inorganic solid electrolytes.[385] Nevertheless, another possible reason could be the lack of viscoelastic behaviour in an inorganic solid electrolyte. In reality, the viscosity, η_{v}, is an important parameter determining the ionic diffusion coefficient.[386,387,390,391] For instance, Hayamizu *et al.*[386] showed that the diffusion coefficients of 12 organic solvents are directly correlated to the inverse of viscosity. A good correlation can be found between the viscosity diffusion coefficient (D_η) and viscosity (η_{v}) according to Stokes-Einstein's equation:[386]

$$D_\eta = \frac{kT}{6\pi\eta_{\mathrm{v}} r}, \tag{5.11}$$

where r is the effective hydrodynamic radius. Figure 5.3 shows that the diffusion coefficient is inversely proportional to the viscosity for 12 organic solvents.[386]

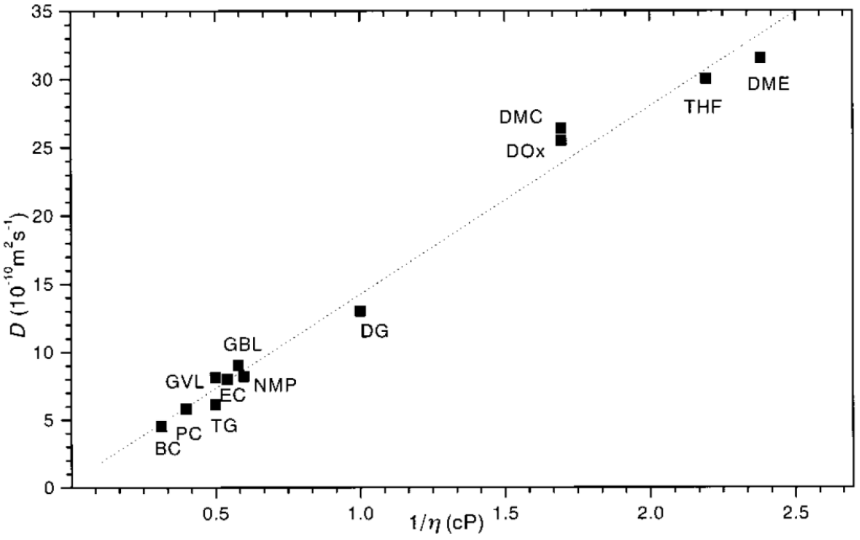


Figure 5.3 The relationship between the diffusion coefficient and viscosity of 12 organic solvents. Reproduced with permission from Ref. 386, Copyright (1999), American Chemical Society.

5.2 Mechanical behaviour of inorganic solid electrolytes

In a broad sense, the family of inorganic solid electrolytes consists of two sub-branches: (i) ceramic-based solid electrolytes and (ii) glassy solid electrolytes. By using Nernst-Einstein's relation to describe the mobility of Li^+ ions in inorganic solid electrolytes, one assumes that the transport of Li^+ ions through inorganic solid electrolytes can be described as viscous flow or viscoelastic behaviour. However, many of the existing experimental results measuring the mechanical behaviour of inorganic solid electrolytes usually indicate that inorganic solid electrolytes are brittle and ceramic-like rather than viscoelastic.[18,33,104–107]

5.2.1 Characteristics of brittle and viscoelastic solids

A brittle solid typically exhibits a linear stress-strain relationship with very few plastic deformation signs before a catastrophic crack or fracture (see Figure 5.1). This phenomenon is caused by the low capacity of ceramics in absorbing the applied energy before they fracture.[392,393] Unlike a viscoelastic solid, stress in a brittle material is independent of the rate of strain. This relationship before failure can be described by Hooke's law as

$$\sigma_{\mathrm{st}} = E\epsilon, \tag{5.12}$$

in which σ_{st} [Pa] is the applied stress, ϵ [−] is the corresponding strain, and E [Pa] is the proportionality constant known as Young's modulus. Figure 5.4(a) shows the stress-strain

relationship for brittle ceramics such as ZTA, Y-PSZ, Mg-PSZ and Syalon +BN.[392] Gogotsi[392] introduced a brittleness measure, χ, to characterise the elastic behaviour of ceramics. He considered a ceramic as linearly elastic if the brittleness measure $\chi = 1$ or inelastic if $\chi < 1$. While materials such as ZTA and Y-PSZ have a χ-value of 1, he showed that the mechanical behaviour of Mg-PSZ and Syalon+BN can deviate slightly from the linearly elastic regime.[392] Nevertheless, for a wide range of temperatures, the mechanical behaviour of brittle ceramics can be approximated with Hooke's law, as shown by Figure 5.4(b).

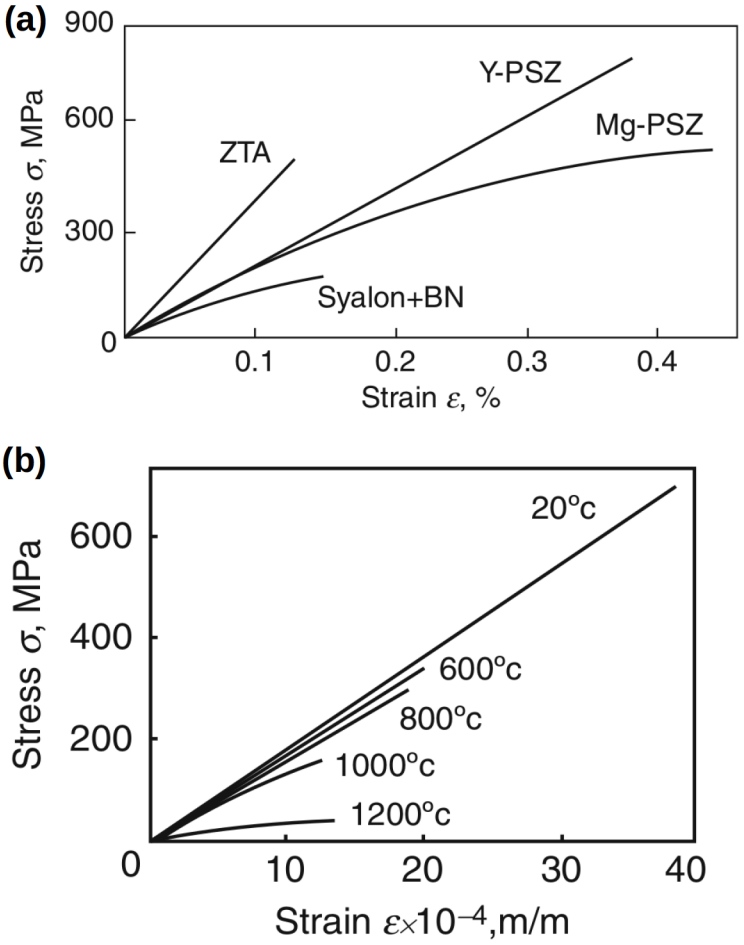


Figure 5.4 (a) Illustration of the stress-strain relationship for brittle ceramics: ZTA and Y-PSZ have a brittleness measure of 1, whereas Syalon + BN and Mg-PSZ have a brittleness measure of 0.70 and 0.44, respectively. (b) The stress-strain relationship for Y-PSZ ceramics at different temperatures. Reproduced from Ref. 392, Copyright (2014), with permission from Springer.

In contrast, viscoelastic solids such as polymers and Li metal exhibit mechanical behaviour, in which both solid-like and liquid-like characteristics are prevalent.[38,394–396] As a result, these materials can undergo significant deformations before failure (see the inset of Figure 5.6d). Stress is always proportional to the rate of strain, indicating a time-dependent deformation or a viscous behaviour. For an ideal viscous material, the stress-strain relationship can be represented by

$$\sigma_{st} = \eta_v \frac{\partial \epsilon}{\partial t}, \tag{5.13}$$

where η_v is the dynamic viscosity - a key parameter influencing the viscous force in Equation 5.5.

In Figure 5.5, Vincent[397] compared the stress-strain relationships for different mechanical behaviours. As shown by the top left panel in Figure 5.5, an elastic material will return to its original shape on removal of the load. However, due to dissipation of the deformation energy, a plastic material will not return to its original shape after the load is removed (see bottom left panel). While an elastic-plastic mechanical behaviour shows a combination of elasticity and permanent deformation, a viscoelastic material will return to its original shape on removal of the load. Nevertheless, compared to the pure elastic mechanical behaviour, a time-dependent deformation occurs due to the contribution of the viscous component to the viscoelastic response.[397]

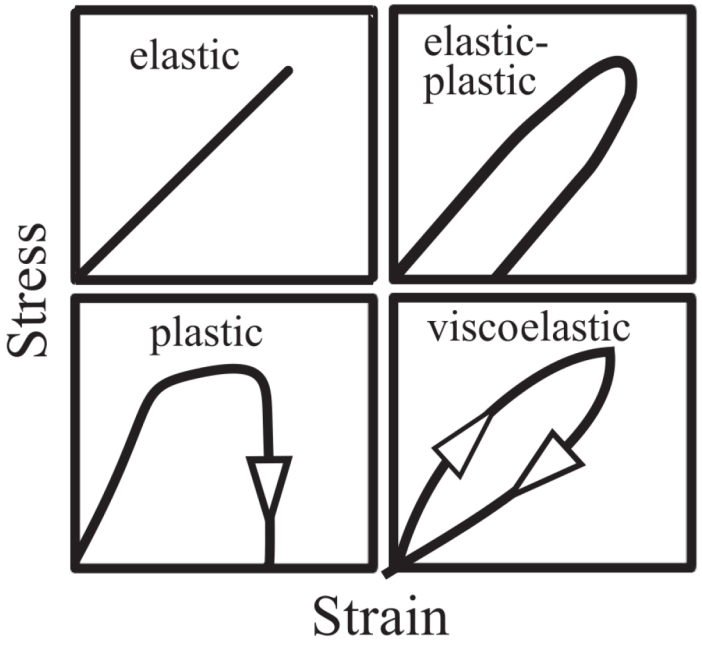


Figure 5.5 Illustration of stress-strain relationships for different types of mechanical behaviours: elastic, elastic-plastic, plastic and viscoelastic characteristics. Reproduced with permission from Ref. 397, Copyright (2012), Princeton University Press.

5.2.2 The effects of operating temperatures

Temperature plays a significant role in determining the viscoelastic behaviour of a solid. Brittle material such as inorganic solids also have different stress-strain relationships at room

temperature compared to at high temperature. While a linear stress-strain relationship is usually observed before an immediate crack or a fracture through the material at ambient room temperature, at high temperatures such as $200 - 400$ °C, the stress-strain relationship has been found to be non-linear even before a crack or fracture.[393]

Lewis *et al.*[33] illustrated the crack formation in the LAGP solid electrolyte captured by low-magnification cross-sectional SEM images (see Figure 5.6a), when the LAGP cells were cycled until failure at 0.1 mA cm^{-2} and 0.5 mA cm^{-2}. As the applied current densities increase, they showed that the horizontal cracks at the interface penetrated deeper into the bulk solid electrolyte. These images portray cracks propagating in the absence of plastic deformation signs, indicating that LAGP is brittle and has a ceramic-like mechanical behaviour.[33] Typical deformation behaviour is characterised by an irreversible change in volume in response to exerted forces, as portrayed in the inset of Figure 5.6(c). In Figure 5.6(b), Korte and Clegg[393] showed the fracture of ceramic micropillars into multiple fragments when compressed with a nano-indenter at room temperature, corroborating the conclusion that ceramic-like electrolyte is brittle. Nevertheless, when the same material was compressed at elevated temperatures such as 200 °C and 400 °C, considerable deformation rather than a brittle fracture was observed.[393] In contrast, Figure 5.6(c) shows that a viscoelastic solid such as Li metal deformed significantly even at room temperature when it was compressed.[38]

While high operating temperatures improve the ionic transport across the inorganic solid electrolyte, the temperature increment is capped by the (i) interfacial decomposition at high temperatures and (ii) the low melting point of Li metal. Firstly, due to the low interfacial stability, the rate of decomposition at both interfaces was shown to increase at high temperatures.[86,88,228] For instance, Wang *et al.*[86] showed that a solid-state cell cycled at 80 °C lost about 35% of the initial capacity after 250 cycles while the cell cycled at 25 °C maintained the same initial capacity. By using Transmission Electron Microscopy (TEM) and Scanning Transmission Electron Microscopy (STEM)-Electron Energy Loss Spectroscopy (EELS) analysis, they showed that the decrease in the capacity at 80 °C was caused by the decomposition reaction in the disordered $LiCoO_2$ layer at the interface.[86] Secondly, if pure metallic Li is used as the negative electrode to boost the gravimetric and volumetric energy density,[8] one should note that Li melts at 180 °C. This limitation indicates that a solid-state cell with a Li electrode cannot be operated at temperatures approaching 180 °C. Therefore, within this limited operating temperature range, ceramic-based inorganic solid electrolytes are expected to demonstrate a brittle rather than a viscoelastic mechanical behaviour.

5.2.3 Glassy solid electrolytes

However, due to different chemical compositions, structures and processing conditions, one should also note that the brittleness of inorganic solid electrolytes cannot be generalised for

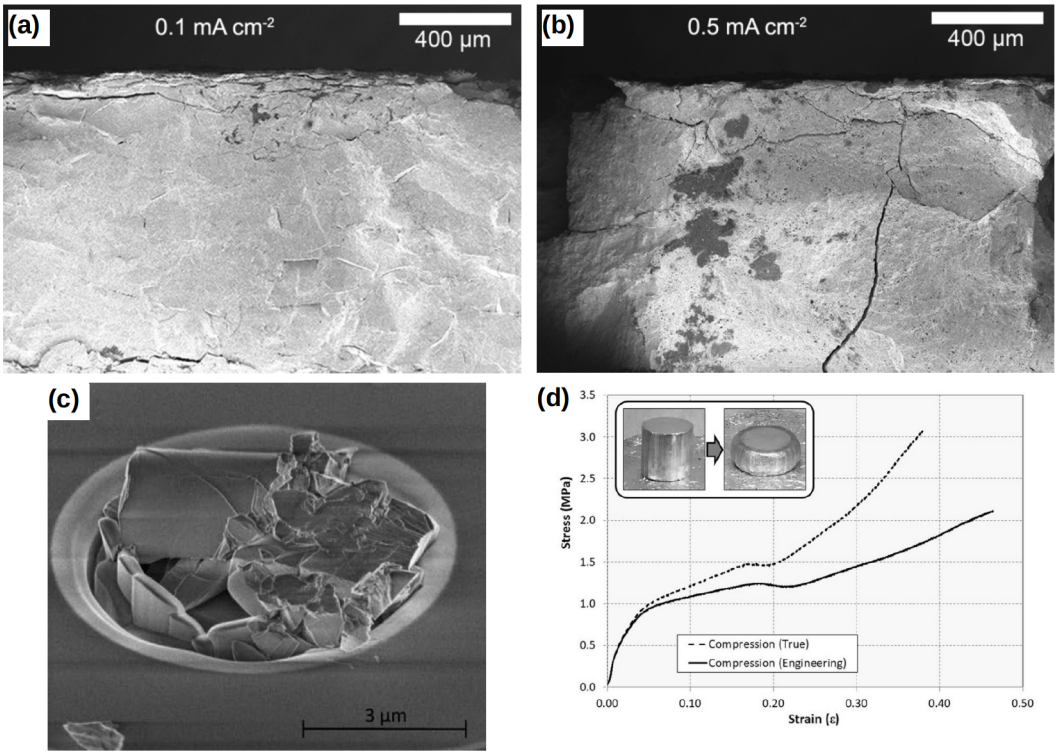


Figure 5.6 Comparison of the brittle and viscoelastic material behaviour: Cross-sectional SEM images of $Li_{1+x}Al_xGe_{2-x}(PO_4)_3$ (LAGP) solid electrolyte cycled until failure at (a) $0.1\,\mathrm{mA\,cm^{-2}}$ and (b) $0.5\,\mathrm{mA\,cm^{-2}}$ current densities. Reprinted from Ref. 33, Copyright (2019), with permission from American Chemical Society. (c) The fracture of ceramic micropillars upon compression with a nano-indenter at room temperature. Reprinted from Ref. 393, Copyright (2009), with permission from Elservier. (d) The compressive stress-strain behaviour of a solid Li at room temperature. The inset shows that Li metal deforms significantly when subjected to compressive stress, indicating that Li metal has viscoelastic mechanical behaviour.‡ Reprinted from Ref. 38, Copyright (2019), with permission from Springer Nature.

all different solid electrolytes. While solid electrolytes such as LLZO, LLTO and LATP have a low fracture toughness comparable to that of brittle inorganic materials ($\approx 1\,\mathrm{MPa\,m^{-2}}$) (see Figure 5.7(a)),[398] Kalnaus *et al.*[398] demonstrated recently that glassy solid electrolytes such as LiPON portrayed nanoscale ductility and time-dependent deformation behaviour. By using nanoindentation, they observed accommodation of stress *via* pile-up rather than by cracking in LiPON, as shown by Figure 5.7b.[398]

Unlike ceramics, glasses consist of network formers such as SiO_2 and network modifiers such as alkali oxides.[400] At high temperatures, a glass-forming melt behaves as a liquid and becomes a glassy solid upon cooling below the glass-transition temperature.[401] The viscosity of glasses depends strongly on the temperature, which has been usually described by the Vogel-Fulcher-Tamman's relation:[402]

‡For a compression test, one should note that the true stress should be smaller than the engineering stress due to a larger instantaneous cross-sectional area during compression.

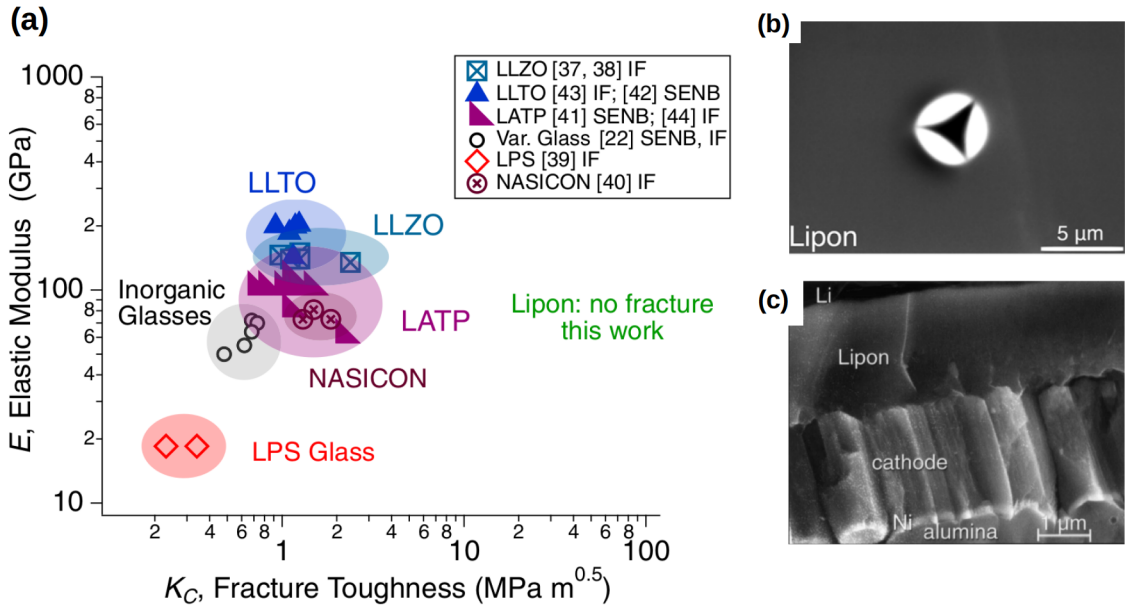


Figure 5.7 (a) **Stiffness versus fracture toughness of ceramic-based and glassy solid electrolyte.** The typical fracture toughness of brittle materials is approximately 1 MPa m^{-2}. When LiPON was subjected to the nanoindentation, no fracture was observed throughout the experiments. Reprinted from Ref. 398, Copyright (2021), with permission from Springer. (b) Under nanoindentation experiments, a significant pile-up instead of cracking was observed in LiPON. Reprinted from Ref. 398, Copyright (2021), with permission from Springer. (c) The micrograph of a fracture cross-section observed in LiPON. Reprinted from Ref. 399, Copyright (2000), with permission from Elsevier.

$$\eta_{\mathrm{v}}(T) = \eta_0 \exp\left(\frac{D_{\mathrm{frag}} T_0}{T - T_0}\right), \tag{5.14}$$

where η_0 is the constant, D_{frag} is the fragility index of glasses and T_0 is the temperature, at which the liquid ceases to flow. Glasses such as soda-lime glasses have very high glass-transition temperature at 840 K - 900 K.[403] As a result, the viscosity-temperature behaviour was determined for temperatures ranging from 793 K to 1772 K.[403]

Some glasses like oxide glasses are ionic conductors, which imply that their ionic conductivity can be measured by the impedance spectroscopy.[400] Mehrer *et al.*[400] measured the temperature-dependent diffusion coefficients of a soda-lime silicate glass for temperatures ranging from approximately 450 K to 1600 K (see Figure 5.8). In their works, the charge diffusion coefficient or sometimes also denoted as the conductivity diffusion coefficient, D_σ is the diffusion coefficient determined from Nernst-Einstein's relation, where the particles were assumed to be non-interacting (Equation 5.3). They obtained the tracer diffusion coefficient of radioisotopes ^{22}Na and ^{45}Ca with the radiotracer technique.[400] By comparing the conductivity diffusion coefficient to the tracer diffusion coefficient of ^{22}Na and ^{45}Ca radioisotopes, they

concluded that the ionic conductivity of a soda-lime glass is caused predominantly by the mobility of Na ions.[400] They also determined the viscosity diffusion coefficient by Stokes-Einstein's relation (Equation 5.11), which corresponded to the mobility of the network-forming units.[400] Nevertheless, as discussed in Section 5.2.2, operating temperatures ranging from 450 K to 1600 K are not feasible for an inorganic solid-state Li-metal batteries. Therefore, future works are required to quantify the viscoelastic behaviour of glassy solid electrolytes and the interplay with their ionic conduction mechanisms at ambient temperatures.

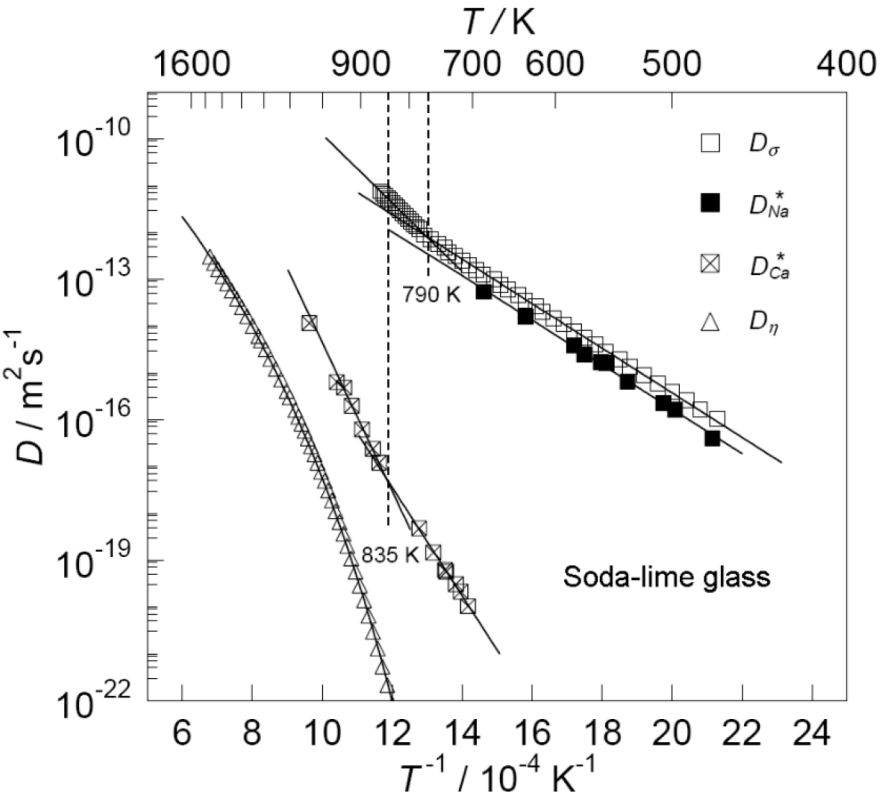


Figure 5.8 The temperature-dependent charge diffusion coefficient (D_σ), tracer diffusion coefficients of ^{22}Na (D^*_{Na}) and ^{45}Ca (D^*_{Ca}) and viscosity diffusion coefficient (D_η) for a soda-lime silicate glass. Reproduced from Ref. 400, Copyright (2008), with permission from IOP Publishing.

5.2.4 Loss tangent measurements

Although the nanoscale micrograph of LiPON reveals the accommodation of stress *via* pile-up, the value of fracture toughness for LiPON remains unknown.[398] Moreover, a fracture cross-section was observed in another micrograph of LiPON (Figure 5.7c),[399] thus suggesting that LiPON may have different mechanical behaviour at different length scales. It is also worth noting that not all glassy materials exhibit time-dependent deformations. While metallic glasses are

likely to yield plastically under an opening stress, oxide glasses have a very low fracture toughness ($< 1\,\mathrm{MPa\,m^{1/2}}$) and were shown to exhibit brittle cracks.[404,405]

Since the viscoelastic behaviour is a time- and frequency-dependent deformation, the value of the loss tangent can be used as the indication of a viscoelastic characteristic.[394,406] In a viscoelasticity measurement, the material is perturbated with a small oscillating strain and the resulting stress is measured.[397] Figure 5.9 illustrates the sinusoidal applied strain and the resultant stress response observed in an elastic and a viscoelastic material.[397] If the material depicts a linearly elastic mechanical behaviour, the strain will be proportional to the stress, as shown by Figure 5.9(a).[397] However, if the material behaves in a viscoelastic manner, a phase shift between the applied strain and resultant stress will be observed, as illustrated by Figure 5.9(b).[397] The loss tangent, $\tan\delta$, is then the ratio between the loss modulus E'' [Pa] and the storage modulus E' [Pa]:[407,408]

$$\tan\delta = \frac{E''}{E'}, \tag{5.15}$$

where

$$\begin{aligned} E' &= \frac{\sigma_{\mathrm{st},0}}{\epsilon_0}\cos\delta, \\ E'' &= \frac{\sigma_{\mathrm{st},0}}{\epsilon_0}\sin\delta. \end{aligned} \tag{5.16}$$

Here, $\sigma_{\mathrm{st},0}$ and ϵ_0 are the peak amplitudes of stress σ_{st} and strain ϵ, whereas δ is the phase shift between stress and strain.[407] An elastic solid has a loss tangent of zero, indicating that the applied stress and the resulting strain are in phase. In contrast, a viscoelastic solid such as polymers and rubbers can have a loss tangent exceeding unity.[395,396,406,409,410] Although the loss tangents of inorganic solid electrolytes have not been measured experimentally, similar behaviour can be expected from them as measured in other ceramic materials such as alumina, which has a loss tangent of 9×10^{-4} at room temperature.[406] Compared to the loss tangent of polymers and rubbers, this low magnitude of loss tangent shows that ceramic-based materials exhibit a negligible viscoelastic behaviour at room temperature.

However, as discussed in Section 5.2.3, due to a large variation in the chemical compositions of inorganic solid electrolytes,[54] it should be noted that the brittle behaviour cannot be generalised for different types of these solid electrolytes. Different classes of inorganic solid electrolytes may exhibit different mechanical behaviour, which requires an individual mechanical characterisation.

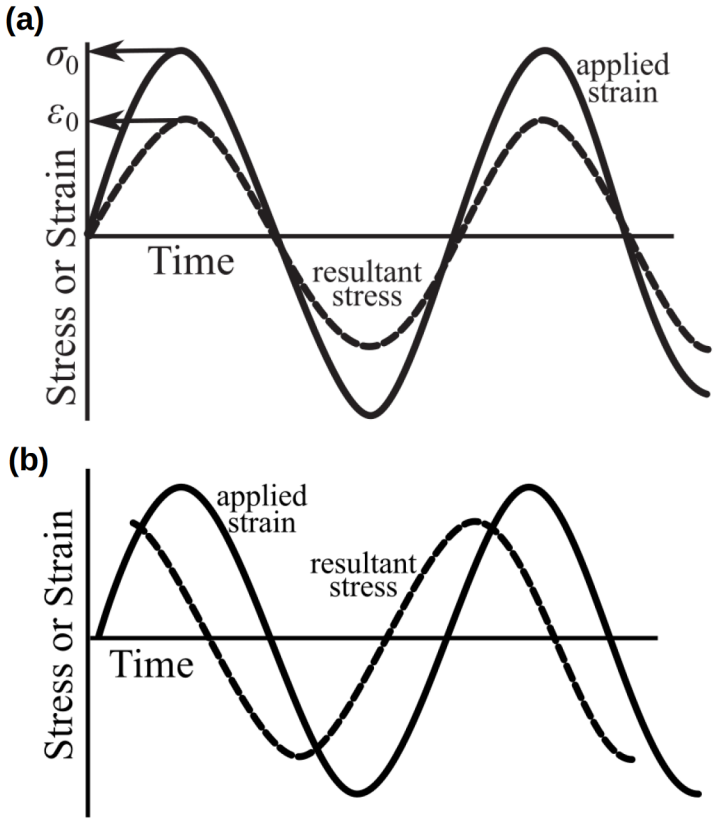


Figure 5.9 Sinusoidal applied strain and the resultant stress response observed in (a) an elastic material and (b) a viscoelastic material. Reproduced with permission from Ref. 397, Copyright (2012), Princeton University Press.

5.3 Alternatives to Nernst-Einstein's relation

By using time-resolved *operando* neutron depth profiling methods, Han *et al.*[31] measured the Li concentration profiles in three different representative classes of inorganic solid electrolytes (*e.g.* LiPON, c-LLZO and Li_3PS_4) at different temperatures. Their experimental measurements showed a near-zero concentration gradient across the bulk solid electrolytes (see Figure 2.15). A near-zero concentration gradient implies that the macroscopic diffusion overpotential in an inorganic solid electrolyte is negligible.[7] The migration of mobile cations by hopping between lattice sites is the principal conduction mechanism governing the ionic mobility in an inorganic solid electrolyte.[7] Therefore, the ionic conductivity can be measured directly from the impedance measurement, thus implicitly including the effects of correlations between the mobile cations.[22,60,63]

As material discovery is increasingly aided by computer simulations, there may be materials of interest in which the ionic diffusion coefficient is relevant. In such cases, modelling work should

focus on the nature of governing forces affecting the ionic mobility through quantum mechanical calculations and force-fields simulations.

For a ceramic-based solid electrolyte, the properties of a ceramic and how its atoms are arranged in its structure are determined predominantly by the nature and the directionality of the bonds holding the atoms together.[411] In general, two types of bonds are governing the behaviours of ceramics: ionic and covalent bonds.[411,412] Ionic bonding is an electrostatic force of attraction that results from the electrons transfer between a metal and a non-metal.[411,412] Ionic compounds are typically brittle and have poor electrical and thermal conductivity.[411,412] On the other hand, covalent bonding occurs due to sharing of outer shell electrons between two non-metals that have similar electronegativity.[411,412] Although both types of bonds are present in ceramics, ionic bonding is more dominant, and the fundamental force governing the atomic structure in ceramics is the electrostatic Coulombic force.[411,412] By using appropriate boundary conditions, Schrödinger's equation can be solved considering the dynamic equilibrium between various governing forces such as electrostatic Coulombic force and the forward electric force.[411] The outcome of such investigations could determine whether Nernst-Einstein's relation can be applied for inorganic solid electrolytes or a new relation is required to describe the interatomic forces acting in these electrolytes.

Depending on the structure and the chemical composition of the host lattice, the atomic diffusion in a solid can be described by a range of diffusion mechanisms, which include interstitial mechanisms, collective mechanisms, vacancy mechanisms, divacancy mechanisms or interstitial-substitutional exchange mechanisms.[401] For glassy solid electrolytes, atomistic simulation can be implemented to evaluate which diffusion mechanisms best describe the hopping behaviour observed experimentally in the solid electrolyte. By studying the relationship between mean displacement and time for colloidal particles, Jean Perrin and his students had performed a series of experiments in 1908 to evaluate Einstein's and Einstein-Smoluchowski's relation.[381] Instead of assuming the general applicability of Nernst-Einstein's relation for all electrolytes, the Jean Perrin's experiments can be extended to evaluate whether the Einstein's diffusion model can describe the hopping mechanisms for different types of inorganic solid electrolytes.

5.4 Conclusions

In solid-state battery research, Nernst-Einstein's model has often been used to relate the diffusion coefficient of mobile cations to the electrolyte conductivity. However, a near-zero concentration gradient across the inorganic solid electrolyte indicates that the diffusion overpotential is insignificant, and the migration of mobile cations is the primary conduction mechanism. In this case, ionic conductivity can be measured from the impedance

measurement of inorganic solid electrolytes, where the ion-ion correlations are also considered implicitly through a direct experimental measurement.

It is shown in this Chapter that the popular Nernst-Einstein's relation is not valid for all materials. Instead of using by default Nernst-Einstein's relation originally developed for fluids and strictly valid for viscoelastic materials, future studies should calculate the ionic mobility from quantum mechanical or force-field simulations. Such approach could determine how the nature of governing forces affect the ionic mobility in an inorganic solid electrolyte. Then, the calculated ionic mobility can be used in cell- and system-level solid-state battery modelling to predict battery performance.

It is also highlighted that the measurement of loss tangent is necessary to characterise the viscoelastic behaviour of inorganic solid electrolytes. If the loss tangent of inorganic solid electrolytes is less than unity in the range of batteries operating temperatures, the impacts of using Nernst-Einstein's relation in modelling the ionic mobility in inorganic solid electrolytes must be investigated before further use. A new relation describing the governing forces is required. However, if the measured loss tangent is comparable to that of polymers and Li metal, the viscoelastic behaviour of inorganic solid electrolytes should be quantified.

Chapter 6

Conclusions and future works

> Do the best you can until you know better. Then when you know better, do better.
>
> *Maya Angelou*

Based on the research questions outlined in Chapter 1, these final sections present a summary and conclusions of the thesis and propose possible directions for future works.

6.1 Thesis summary and conclusions

Multi-physics of solid-state batteries. This work has presented an in-depth multi-physics review of inorganic solid-state batteries, linking the interactions between electrochemical, thermal, chemical and mechanical behaviours to the performance and degradation of solid-state batteries. While replacing liquid electrolytes with inorganic solid electrolytes enables the use of Li-metal as the negative electrodes, the mechanical strength of inorganic solid electrolytes does not necessarily prevent the growth and propagation of Li filaments. Both LiPON and c-LLZO have a shear modulus $7-14$ times larger than the shear modulus of Li, indicating a stable deposition of Li according to Monroe-Newman's criterion. Nevertheless, despite the high shear modulus of c-LLZO, the growth of Li filaments are still observable in c-LLZO. This observation implies that Li filaments' formation depends on the critical plating and stripping current densities, grain morphologies of the solid electrolytes, surface flaws, operating temperature and applied stack pressures. A combined understanding including solid-state electrochemistry, microstructure, mechanics, operating conditions, and their interactions is required to mitigate the effects of degradation due to excessive plating and stripping.

Cell models for solid-state lithium-metal batteries. A simplified set of governing equations, rather than the conventional Poisson-Nernst-Planck (PNP) equations, are used to model the ionic transport across the solid electrolytes. Unlike conventional liquid electrolytes that consist of both moving cations and anions, only the cations are mobile in an inorganic solid electrolyte. This transport behaviour indicates a near-zero concentration gradient and a negligible diffusion overpotential across the solid electrolyte. As a result, the ionic conductivity can be measured directly from the PEIS measurements, in which the ionic interactions in the solid electrolyte can also be considered implicitly.

Performance limiting factors and model-based cell design. By using the simplified electrochemical model, various performance-limiting mechanisms were quantified under pulse operating conditions for low current densities. Based on the overpotential analysis, solid-state diffusion in the non-porous LCO is shown as the rate-limiting mechanism followed by the ohmic drop at high SOCs. As for the low SOCs, the electrode solid diffusion and charge transfer overpotential at the PE-SE interface are the two dominant mechanisms causing the voltage losses. The diffusion overpotential in the non-porous positive electrode is caused by the development of different phases and the formation of local concentration gradients in the solid electrode during the interruption of external currents. This virtual model proposes a plausible explanation to the experimental measurements by Matsuda *et al.*[27] They showed that a more severe capacity drop is observed in the cell with a thicker non-porous positive electrode, when comparing the voltage discharge profiles of 0.32 μm and 6.7 μm LCO in solid-state Li-metal cells. Nevertheless, it should be highlighted that the performance-limiting mechanisms in solid-state batteries are highly dynamic depending on the operating conditions, degradation effects and cell architectures. Future research in this field should consider how the interplay of various mechanisms limits the performance of solid-state batteries, as discussed in Chapter 2 of this thesis.

Thermally coupled large-format solid-state battery models. The desired energy and power output for large-format solid-state Li-metal batteries can be achieved by scaling and stacking unit cells. Two stack configurations, a bipolar and a parallel stack, are modelled and compared. With 63 cells stacked in series, a bipolar stack could reach a stack voltage up to 265 V. In contrast, a parallel stack with 32 double-coated cells could achieve 4 Ah. This research demonstrates that the choice of current collectors is critical in determining the gravimetric power and energy density of both stack configurations. The model-based stack design includes a polyurethane spacer between the pouch and the cell stack to reduce voids formation and volume change due to Li metal. Based on the simulated Ragone profiles of bipolar and parallel stacks, the model prediction shows that the bipolar aluminium stack has a higher volumetric energy and power density than the parallel lithium stack. In a parallel stack, if the copper foils substitute the lithium foils as the negative current collectors to minimise the volume change of Li current collectors, the gravimetric energy and power

densities were predicted to decrease by a factor of 1.77. On the other hand, due to the lower densities of carbon composite and aluminium, the model predicts that the bipolar stack with carbon composite and aluminium for bipolar plates has higher gravimetric energy and power density than the titanium and stainless steel bipolar stack.

By coupling the electrochemical stack model thermally, the Joule heating effects are shown to be negligible for bipolar stacks but become dominant for parallel stacks. This thesis concludes that bipolar stacks are better in terms of their higher energy densities and lower heat generation, but a lower Coulombic stack capacity limits their performance. In contrast, parallel stacks generate more heat and require more advanced thermal management. These thermally-coupled stack models can be used as prototypes to aid the future development of large-format solid-state batteries.

Mechanical behaviour of inorganic solid electrolytes. Due to the lower ionic conductivity of most inorganic solid electrolytes compared to liquid electrolytes, various research efforts have been devoted to improving the ionic transport *via* an array of synthesis, characterisation and modelling approaches. The ionic mobility in inorganic solid electrolytes has often been modelled with the Nernst-Einstein's relation, in which the ionic diffusion coefficient is linearly proportional to the electrolyte conductivity. Despite the widespread use of this relation for different electrolyte systems, including liquid and solid polymer electrolytes, this thesis shows that Nernst-Einstein's relation is not directly transferable to describe the ionic mobility in an inorganic solid electrolyte. By revisiting the original derivations and assumptions implicit in the Nernst-Einstein's relation, it is shown that the relationship between the diffusion coefficient and electrolyte conductivity is only applicable in a viscous or a gaseous medium. This postulation contradicts state-of-the-art experimental studies measuring the mechanical behaviour of inorganic solid electrolytes, which usually show that inorganic solid electrolytes are brittle rather than viscoelastic at ambient room temperature. Characterising the viscoelastic behaviour of inorganic solid electrolytes requires the measurement of loss tangent. If the loss tangent of inorganic solid electrolytes is less than unity in the range of batteries operating temperatures, the impacts of using the Nernst-Einstein's relation in modelling the ionic mobility should be quantified. However, if the measured loss tangent is comparable to that of solid polymers and Li metal, the viscoelasticity of inorganic solid electrolytes should be evaluated and quantified.

6.2 Future works

Throughout this research, several potential future works to further advance the breakthrough of inorganic solid-state batteries have been identified:

Next-generation positive electrodes for solid-state batteries. The prototype of commercial solid-state Li-metal cells used a non-porous positive electrode. As shown by the modelling studies presented in Chapter 3, it is impossible to increase the thickness of the non-porous positive electrode due to the diffusion limitations. As a result, the active materials account for less than 55% in the mass ratios and less than 35% in the volume ratios of the large-format bipolar and parallel stacks. The diffusion limitation in the electrode can be mitigated by replacing the non-porous positive electrode with a composite positive electrode. In this way, the diffusion overpotentials and local concentration gradients are confined within each electrode particle rather than across the bulk of the positive electrode. As a result, increasing the electrode thickness does not aggravate the build-up of concentration gradients, further reducing the number of unit cells to achieve the desired stack capacity and power output. Subsequently, the gravimetric energy and power densities of large-format solid-state batteries could be improved.

Modelling the multiphysical degradations of solid-state batteries. While this study has presented the foundations in modelling the behaviour of inorganic solid-state Li-metal batteries, the effects due to degradations caused by cycling or calendar ageing were not considered. In reality, different degradation mechanisms such as electrode-electrolyte interfacial decompositions, instability of carbon additives, surface voids, Li creep, and current collectors fracture could shorten the lifespan of solid-state batteries. A comprehensive degradation model that incorporates the different interactions limiting solid-state batteries' lifetime performance is critical to provide diagnostics and manufacture better next-generation solid-state batteries. Such analysis is especially relevant for modelling the lifetime performance of the bipolar stacks, where one unit cell's failure would cause the failure of the entire stack.

Non-linear model parametrisation. Most of the electrochemical parameters in this work were estimated based on EIS measurements, which assumes a linear relationship between the current and the voltage. While the current response to an applied potential can be approximated as linear for a small perturbation amplitude ($\leq$ 20 mV), the relationship between the current and voltage is highly non-linear in reality. This non-linearity can be attributed to interfacial reactions, current-strength dependent solid-state diffusion losses and strong concentration gradients in the electrode under load. For an operating condition near equilibrium, the kinetic parameters estimated from the linear EIS is sufficient to describe the cell behaviour. If the operating conditions deviate significantly from the equilibrium (*i.e.*, under high current densities or when the reaction rate is higher than the equilibration rate), the non-linear losses may induce additional mechanisms in solid-state batteries. Therefore, this research proposes non-linear EIS measurements in future model parametrisation works, which allows the estimated kinetic parameters and relations to be valid for both low and high current densities. Different physics-based kinetic models, such as Butler-Volmer's relation, Tafel kinetics, linear Butler-Volmer's relation, and Marcus-Hush-Chidsey kinetics, have been

proposed in the literature for electrochemical models. By comparing non-linear EIS model predictions to measurements, the most appropriate kinetic models can be distinguished and chosen for solid-state batteries.

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Appendices

A Definition of general performance metrics

Table A-1 gives a summary of the general performance metrics along with their definitions used in the literature review of this work.

Table A-1 The definition of key metrics in this work

Metrics	Definitions	Equation
Ionic conductivity, σ_{elec} [S cm^{-1}]	The electrolyte resistance to the transport of Li-ions in the SE. d_{elec} is the electrolyte thickness, A_{elec} is the active surface area and R_{elec} is the electrolyte resistance.	$\sigma_{\text{elec}} = \frac{d_{\text{elec}}}{A_{\text{elec}} R_{\text{elec}}}$
Electronic conductivity, σ_{e^-} [S cm^{-1}]	The electrolyte resistance to the transport of electrons in the SE. I_{res} is the residual current density and ΔE is the applied voltage.	$\sigma_{\text{e}^-} = \frac{d_{\text{elec}} I_{\text{res}}}{A_{\text{elec}} \Delta E}$
Relative permittivity, ϵ_{r} [-]	The ratio of the absolute permittivity of the medium, ϵ, to the absolute permittivity of the vacuum, ϵ_0.	$\epsilon_{\text{r}} = \frac{\epsilon}{\epsilon_0}$
Specific heat capacity, C_{p} [J kg^{-1} K^{-1}]	The amount of heat energy required to raise one unit of temperature of a material per unit of mass.	Effective specific heat capacity of a cell: $C_{\text{p,eff}} = \frac{\sum_i (C_{\text{p,i}} V_{\text{i}})}{V_{\text{cell}}}$
Thermal conductivity, k [W m^{-1} K^{-1}]	The ability of a material to conduct heat.	Effective cross-plane thermal conductivity, where l_{i} and k_{i} are the thickness and thermal conductivity of each cell component:[94,95] $k_{\text{eff},\perp} = \frac{l_{\text{cell}}}{\sum_i (l_{\text{i}}/k_{\text{i}})}$ Effective in-plane thermal conductivity:[95] $k_{\text{eff},\parallel} = \frac{\sum_i (l_{\text{i}} k_{\text{i}})}{l_{\text{cell}}}$
Young's modulus, E [GPa]	For a uniaxial deformation (*i.e.*, the applied stresses are normal the cross-sectional areas), the coefficient of linear proportionality is known as the Young's modulus. σ_{st} denote the applied stress and ϵ is the strain.	$E = \frac{\sigma_{\text{st}}}{\epsilon}$

Metrics	Definitions	Formula
Poisson's ratio, ν [-]	The tensile stresses cause an axial extension but a transverse contraction, whereas the compressive stress causes an axial contraction but a transverse extension. The ratio of transverse to axial strain can be described by the Poisson's ratio, in which Δx, Δy and Δz are the change of length in the corresponding xyz-coordinate; x_0, y_0 and z_0 are the original lengths.	$\nu = \frac{\Delta y/y_0}{\Delta x/x_0} = \frac{\Delta z/z_0}{\Delta x/x_0}$
Shear modulus, G [GPa]	If the applied stresses are tangential to the cross-sectional areas, the elastic modulus can be described by the shear modulus and the resulting deformation will be a tangent strain ($\gamma = \Delta x/y_0$).	$G = \frac{E}{2(1+\nu)}$
Bulk modulus, K [GPa]	If a uniform pressure is applied on all of the surfaces of the solid material, the coefficient that relates the stress and strain in the linear elastic regime is known. as the bulk modulus and the deformation is given by the volume strain ($\theta_v = \Delta V/V_0$)	$K = \frac{E}{3(1-2\nu)}$
Hardness, H_v [GPa]	The resistance of the material to the plastic deformation, which can be measured with the Vickers indentation. P_v is the indentation force and $2a_v$ is the indentation diagonal size.[105]	$H_v = \frac{1.854P_v}{(2a_v)^2}$
Fracture toughness, K_c [MPa m$^{1/2}$]	Critical stress threshold, above which cracks initiate. Fracture toughness can be measured using the indentation technique.[107] k_v is the Vickers-probe geometry constant ($k_v = 0.016$) and c_v is the crack length.	Mode I (opening mode) fracture toughness: $K_{Ic} = k_v \left(\frac{E}{H_v}\right)^{1/2} \left(\frac{P_v}{c_v^{3/2}}\right)$

B Temperature-dependent dimensional governing equations

This section summarises the governing equations of the temperature-dependent single-layer cell model. The details of the derivations can be found in Ref. 7.

Governing equations in the solid electrolyte. Temperature-dependent current distribution in the solid electrolyte domain is given by

$$i = -\sigma_{\text{elec}}(\overline{T})\frac{\partial \phi_{\text{elec}}}{\partial z}, \tag{B-1}$$

where $\sigma_{\text{elec}}(\overline{T})$ is the temperature-dependent electrolyte conductivity and ϕ_{elec} is the electrolyte potential. Current conservation across the solid electrolyte is defined by

$$\frac{\partial i}{\partial z} = 0. \tag{B-2}$$

Boundary conditions in the solid electrolyte domain are

$$\phi_{\text{s}}\Big|_{z\,=\,0} = 0, \tag{B-3}$$

$$\sigma_{\text{elec}}(\overline{T})\frac{\partial \phi_{\text{elec}}}{\partial z}\Big|_{z\,=\,d_{\text{elec}}} = i_{\text{app}}, \tag{B-4}$$

where ϕ_{s} denotes the reference potential of metallic lithium, d_{elec} is the thickness of the solid electrolyte and i_{app} is the externally applied current density.

Governing equations in the positive electrode. Molar conservation in the positive electrode domain are

$$\frac{\partial c_{\text{Li}}}{\partial t} = \frac{\partial}{\partial z}\left(D_{\text{Li}}(x_{\text{Li}},\overline{T})\frac{\partial c_{\text{Li}}}{\partial z}\right), \tag{B-5}$$

$$D_{\text{Li}}(x_{\text{Li}},\overline{T})\frac{\partial c_{\text{Li}}}{\partial z}\Big|_{z\,=\,d_{\text{elec}}} = -\frac{i}{F}, \tag{B-6}$$

$$D_{\text{Li}}(x_{\text{Li}},\overline{T})\frac{\partial c_{\text{Li}}}{\partial z}\Big|_{z\,=\,d_{\text{elec}}+d_{\text{pos}}} = 0, \tag{B-7}$$

in which c_{Li} is the lithium concentration in the positive electrode, $D_{\text{Li}}(x_{\text{Li}},\overline{T})$ represents the concentration and temperature-dependent diffusion coefficient in the non-porous positive electrode and d_{pos} denotes the thickness of the positive electrode.

Redox reactions at the solid electrolyte-electrode interfaces. Linearised Butler-Volmer expression at the negative electrode-solid electrolyte interface is

$$i = i_{0,\mathrm{neg}}(\overline{T})\frac{(\alpha_\mathrm{a}+\alpha_\mathrm{c})F}{R_\mathrm{gas}\overline{T}}\eta_\mathrm{neg}. \tag{B-8}$$

The cathodic Tafel's equation at the solid electrolyte-positive electrode interface is represented by

$$i = -i_{0,\mathrm{pos}}(\overline{T})\left(\frac{c_\mathrm{Li,surf}}{c_\mathrm{bulk}}\right)\exp\left(\frac{-\alpha_\mathrm{c}F\eta_\mathrm{pos}}{R_\mathrm{gas}\overline{T}}\right). \tag{B-9}$$

Alternatively, the cathodic Tafel's equation can be rewritten as follows:

$$i = -i_{0,\mathrm{pos}}(\overline{T})\left(\frac{c_\mathrm{Li,surf}}{c_\mathrm{bulk}}\right)\times 10^{\frac{\eta_\mathrm{pos}}{A_\mathrm{c}}}, \tag{B-10}$$

where A_c is the cathodic Tafel's slope:

$$A_\mathrm{c} = -\frac{2.303R_\mathrm{gas}\overline{T}}{\alpha_\mathrm{c}F}. \tag{B-11}$$

Calculation of overpotentials. The expressions used to calculate the charge-transfer overpotentials at both interfaces, the ohmic overpotential across the solid electrolyte and the diffusion overpotential in the positive electrode, are given by

$$\eta_\mathrm{neg/pos}|_{z\,=\,0,\,z\,=\,d_\mathrm{elec}} = \phi_\mathrm{s} - \phi_\mathrm{elec} - U, \tag{B-12}$$

$$\eta_\mathrm{ohm} = \phi_\mathrm{s}|_{z\,=\,d_\mathrm{elec}} - \phi_\mathrm{s}|_{z\,=0},^{\ddagger} \tag{B-13}$$

$$\eta_\mathrm{diff} = U_\mathrm{LCO}(c_\mathrm{Li}) - U_\mathrm{LCO}(\overline{c}_\mathrm{Li}). \tag{B-14}$$

[‡]For this specific electrochemical system in consideration, the pointwise and integral evaluations (see Equation 3.25) of ohmic overpotential yield the same results. Without modelling degradation effects, the difference between the local current density across the SE and the total current density is negligible, which allows the simplification of the integral ohmic expression (see Figure B-1).

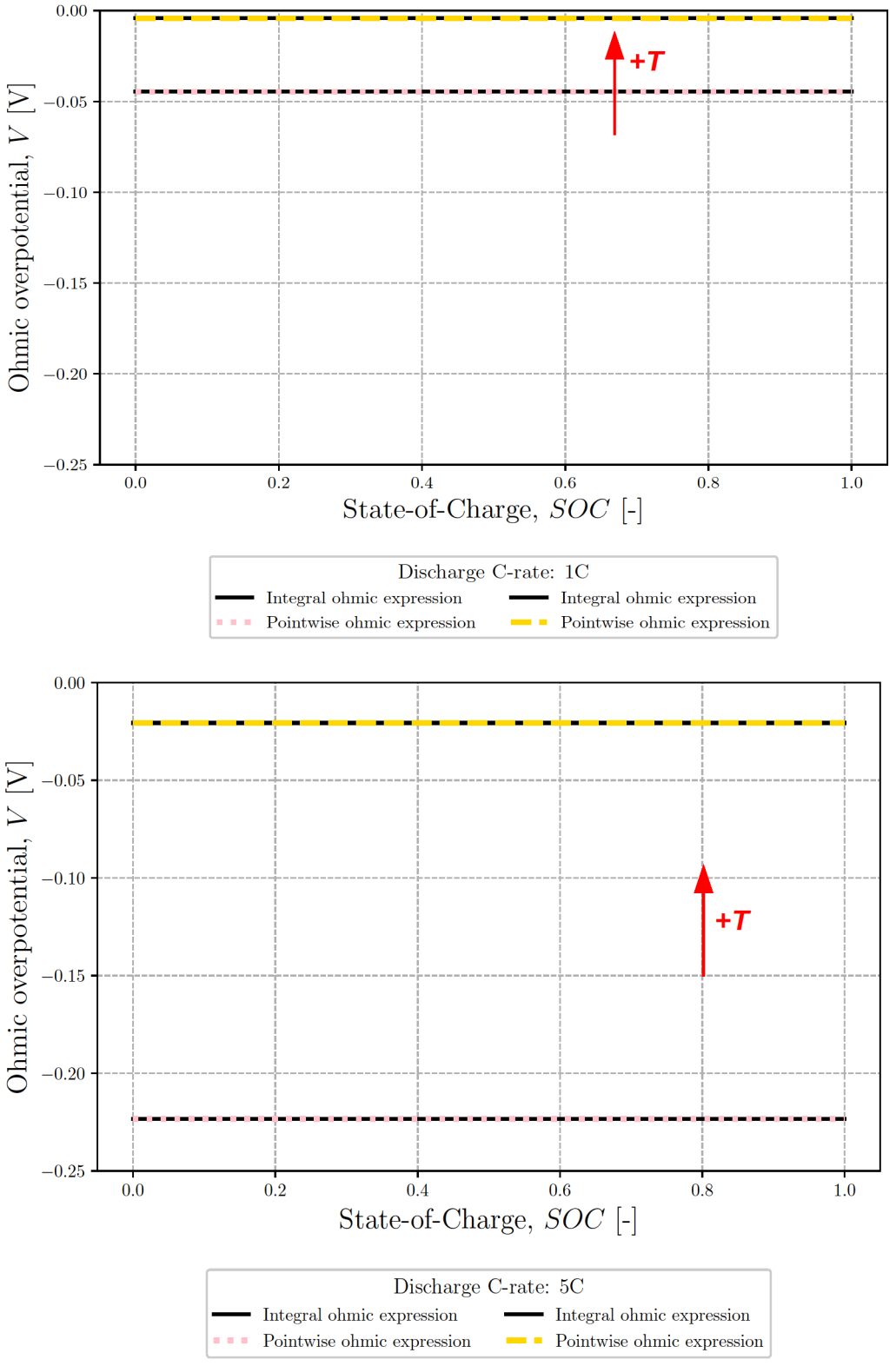


Figure B-1 Comparison of pointwise and integral evaluations of the ohmic overpotential across the SE for 1C and 5C discharge at the temperatures of 25 °C and 55 °C, respectively. For ease in comparing, the y-axis of both plots were scaled for [0V,-0.25V].

C Non-dimensional governing equations

In this section, dimensionless variables and parameters are introduced, followed by a summary of non-dimensional governing equations. Six dimensionless variables are introduced to redefine a dimensionless system of governing equations for the model. The temperature dependence is considered implicitly through the model parameters in these non-dimensional governing equations.

$$\text{length}: z_{\mathrm{n}}'' = \frac{z_{\mathrm{n}}}{L_{\mathrm{z}}}, \tag{C-15}$$

$$\text{time}: t'' = \frac{t}{\tau_{\mathrm{d}}}, \tag{C-16}$$

$$\text{potential}: \phi_{\mathrm{k}}'' = \frac{F\phi_{\mathrm{k}}}{R_{\mathrm{gas}}\overline{T}}, \quad \mathrm{k} = [\mathrm{elec,s}], \tag{C-17}$$

$$\text{lithium concentration}: c_{\mathrm{Li}}'' = \frac{c_{\mathrm{Li}}}{c_{\mathrm{LCO,max}}}, \tag{C-18}$$

$$\text{diffusion coefficient}:$$

$$D_{\mathrm{Li}}'' = \frac{\log_{10}(D_{\mathrm{Li}}(x_{\mathrm{Li}}))}{\log_{10}(\max D_{\mathrm{Li}}(x_{\mathrm{Li}}))}, \tag{C-19}$$

$$\text{current}: i'' = \frac{i}{i_{\mathrm{cell,ref}}}. \tag{C-20}$$

L_{z} denotes the total thickness of the electrode and the electrolyte, τ_{d} is the discharge timescale and $i_{\mathrm{cell,ref}}$ is the current density of the experimental cell ($i_{\mathrm{cell,ref}} = 0.6154\,\mathrm{mA\,cm^{-2}}$).

A dimensionless current distribution in the solid electrolyte domain can be obtained by substituting Equations C-15, C-17 and C-20 into Equation B-1, where σ_{elec}'' is the dimensionless electrolyte conductivity:

$$i'' = -\sigma_{\mathrm{elec}}'' \frac{\partial \phi_{\mathrm{elec}}''}{\partial z_{\mathrm{elec}}''}. \tag{C-21}$$

Similarly, by replacing the dimensional variables in Equation B-5 with Equations C-15, C-16, C-18 and C-19, a dimensionless concentration distribution can be obtained in the positive electrode:

$$\frac{\partial c_{\mathrm{Li}}''}{\partial t''} = \frac{\partial}{\partial z_{\mathrm{pos}}''}\left(D_{\mathrm{Li}}'' \frac{\partial c_{\mathrm{Li}}''}{\partial z_{\mathrm{pos}}''}\right). \tag{C-22}$$

$$\left.\frac{\partial c_{\mathrm{Li}}''}{\partial z''}\right|_{z''=z_{\mathrm{elec}}''} = -\frac{i''}{D_{\mathrm{Li}}''}, \tag{C-23}$$

$$\left.\frac{\partial c_{\mathrm{Li}}''}{\partial z''}\right|_{z''=z''_{\mathrm{elec}}+z''_{\mathrm{pos}}} = 0. \tag{C-24}$$

Assuming $\alpha_{\mathrm{neg}} = \alpha_{\mathrm{pos}} = 0.5$, the dimensionless linearised Butler-Volmer and cathodic's Tafel's expressions can be obtained by substituting Equations C-17 and C-20 into Equation B-8 and B-9 as

$$i'' = \frac{i_{0,\mathrm{neg}}}{i_{\mathrm{cell,ref}}}\eta_{\mathrm{neg}}^{"}, \tag{C-25}$$

$$i'' = -\frac{i_{0,\mathrm{pos}}}{i_{\mathrm{cell,ref}}}\left(\frac{c_{\mathrm{Li,surf}}}{c_{\mathrm{bulk}}}\right)\exp\left(-\frac{\eta_{\mathrm{pos}}^{"}}{2}\right). \tag{C-26}$$

D Stack mass and volume balance

Table D-1 Electrical and thermal properties of different current collectors and bipolar plates

Materials	Electronic conductivity ($S\,m^{-1}$)	Density ($kg\,m^{-3}$)	Specific heat capacity ($J\,kg^{-1}\,K^{-1}$)	Thermal conductivity ($W\,m^{-1}\,K^{-1}$)	Ref.
Parallel stack					
Lithium foil	1.1×10^7	534	3582	81.8	[95, 357]
Copper foil	5.96×10^7	8960	385	398	[95, 341]
Bipolar stack					
Carbon fibers	$1000 - 10^5$	1820	598	6	[339, 348, 350]
Aluminium foil	3.78×10^7	2700	897	238	[95, 341]
Titanium foil	1.79×10^6	4540	523	18.85	[413–416]
Stainless steel	1.37×10^6	7930	502	14.64	[417]

Table D-2 Mass and volume balance of the bipolar aluminium and parallel lithium stacks

		Parallel stack		
Component	Thickness	Volume	Density	Mass
Lithium current collector	10 μm	0.2438 cm^3	0.534 g cm^{-3}	0.130 g
Lithium negative electrode	10 μm	0.2438 cm^3	0.534 g cm^{-3}	0.130 g
LiPON solid electrolyte	2 μm	0.0488 cm^3	2.680 g cm^{-3}	0.131 g
LCO positive electrode	6 μm	0.1463 cm^3	3.121 g cm^{-3}	0.456 g
Aluminium current collector	10 μm	0.2438 cm^3	2.700 g cm^{-3}	0.658 g
Double-coated unit cell	56 μm	1.3650 cm^3		2.223 g
Copper tab	10 μm	0.0070 cm^3	8.960 g cm^{-3}	0.063 g
Aluminium tab	10 μm	0.0070 cm^3	2.700 g cm^{-3}	0.019 g
Double-coated unit cell with tabs	56 μm*	1.3790 cm^3		2.304 g
Polyurethane spacer	2.231 mm	54.3806 cm^3	0.035 g cm^{-3}	1.903 g
Aluminate pouch	0.162 mm	3.9488 cm^3	2.700 g cm^{-3}	10.662 g
Parallel stack (32 units)	4.195 mm	102.7081 cm^3		86.499 g
		Bipolar stack		
Lithium negative electrode	10 μm	0.2438 cm^3	0.534 g cm^{-3}	0.130 g
LiPON solid electrolyte	2 μm	0.0488 cm^3	2.680 g cm^{-3}	0.131 g
LCO positive electrode	6 μm	0.1463 cm^3	3.121 g cm^{-3}	0.457 g
Aluminium bipolar plate	10 μm	0.2438 cm^3	2.700 g cm^{-3}	0.658 g
Single unit cell	28 μm	0.6827 cm^3		1.376 g
Copper tab	10 μm	0.007 cm^3	8.960 g cm^{-3}	0.063 g
Aluminium tab	10 μm	0.007 cm^3	2.700 g cm^{-3}	0.019 g
First unit cell with copper tab	28 μm*	0.6897 cm^3		0.911 g
Last unit cell with aluminium tab	28 μm*	0.6897 cm^3		1.395 g
Fluoroelastomer seal	3.332 mm**	2.3324 cm^3	1.825 g cm^{-3}	4.257 g
Polyurethane spacer	1.426 mm	34.7588 cm^3	0.035 g cm^{-3}	1.217 g
Aluminate pouch	0.162 mm	3.9488 cm^3	2.700 g cm^{-3}	10.662 g
Bipolar stack (61 units + first unit + last unit)	3.352 mm	84.0641 cm^3		102.3780 g

* The overall thickness of the stack does not include the thickness of the tabs.
** The seal spans between the tabs and does not contribute the overall stack thickness.

E Effective ohmic resistance of the parallel stacks current collectors

Figure E-1 illustrates the side view of the current flow in the current collectors of a parallel stack. As the current moves in perpendicular and in-plane along the current collector, a two-dimensional electrical model obeying Ohm's law is used to calculate the effective resistance due to electronic conductivity in the current collectors. The calculated effective resistances from the 2D model are given in Table E-1 and compared to the analytical 1D in-plane resistance, $R_{\mathrm{CC,Par}}$ calculated by

$$R_{\mathrm{CC,Par}} = \frac{L_{\mathrm{y}}}{\sigma_{\mathrm{CC}} A_{\mathrm{cross,CC}}}, \tag{E-1}$$

where L_{y} is the height of the pouch, σ_{CC} is the electronic conductivity of the current collectors and $A_{\mathrm{cross,CC}}$ is the cross-sectional area of the the current collector ($A_{\mathrm{cross,CC}} = d_{\mathrm{CC}} L_{\mathrm{x}}$).

Table E-1 Comparison of 2D effective resistance with 1D in-plane resistance

Materials	2D effective resistance (Ω)	1D in-plane resistance (Ω)
Copper current collector		
Two-sided current flow	3.49×10^{-3}	2.62×10^{-3}
One-sided current flow	8.72×10^{-4}	
Li current collector		
Two-sided current flow	1.89×10^{-2}	1.42×10^{-2}
One-sided current flow	4.73×10^{-3}	
Aluminium current collector		
Two-sided current flow	5.50×10^{-3}	4.13×10^{-3}

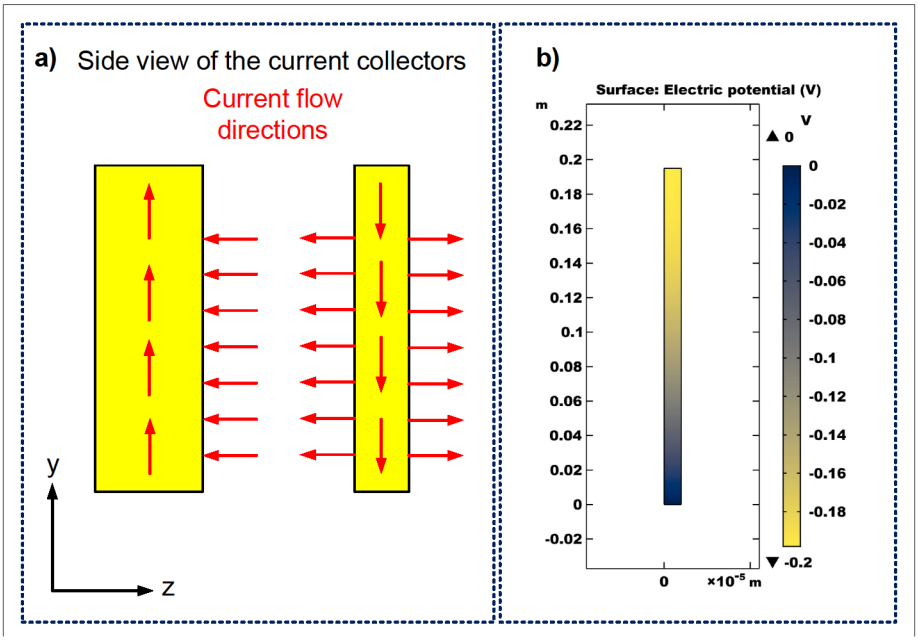


Figure E-1 (a) Side view of the current flow in the current collectors of a parallel stack. The thickness of each current collector in the middle is halved to account for the double-coated configuration. The electrical current first flows perpendicular to the surface area of the current collector and then in-plane along the current collector to the external tab. (b) A two-dimensional electrical model, where the effective resistance due to the electronic transport is calculated from the applied current density and the computed average voltage drop in the current collector.

F Electrochemical impedance spectroscopy

F.1 The theory of electrochemical impedance spectroscopy

Electrochemical Impedance Spectroscopy (EIS) is a non-destructive characterisation technique to analyse the electrochemical dynamics of a cell *in-operando* with a small-signal perturbation.[418] Although both resistance and impedance quantify the ability of a circuit element to resist the flow of electrical current, resistance does not vary with a given frequency range, whereas impedance includes a frequency-dependent measure of the opposition to the current flow. Electrochemical impedance can be measured by either applying a small amplitude of AC potential or AC current to the cell and measure the corresponding output response. If the input perturbation signal is an AC potential, and AC current is measured as the output response, the impedance technique is known as Potentiostatic Electrochemical Impedance Spectroscopy (PEIS).[1] In contrast, if AC current is used to perturbate the cell and AC potential is measured at the output, the impedance technique is denoted as Galvanostatic Electrochemical Impedance Spectroscopy (GEIS) (see Figure F-1).[1] In this work, the PEIS measurement method was chosen. Because of the significant internal resistance of the solid-state Li-metal cells,[7] unstable impedance drifts were observed with the GEIS method.

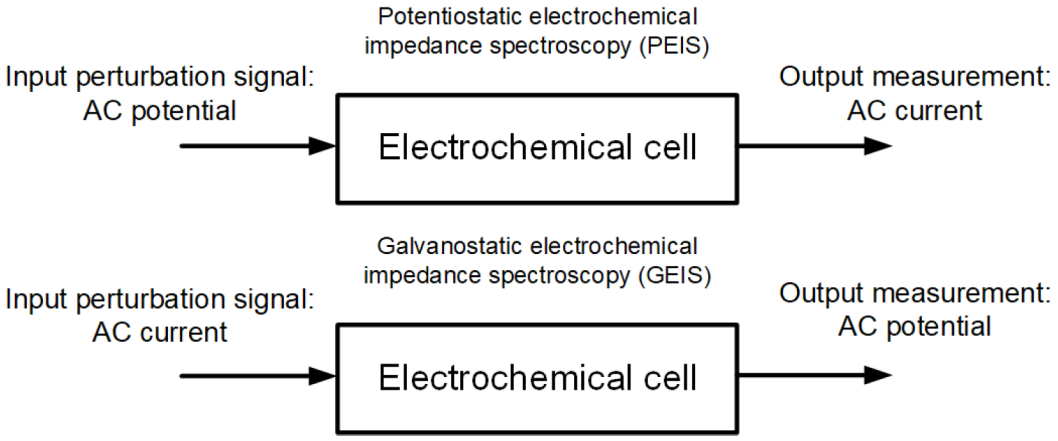


Figure F-1 Illustration of the difference between the Potentiostatic Electrochemical Impedance Spectroscopy (PEIS) and the Galvanostatic Electrochemical Impedance Spectroscopy (GEIS). In PEIS, the input perturbation signal is AC potential whereas in GEIS, AC current is the input signal.[1]

F.2 Impedance of electrochemical circuit elements

An electrochemical system's impedance usually consists of a series or a parallel combination of different circuit elements such as resistors, capacitors or inductors. For instance, for the circuit elements shown in Figure F-2, the impedance is given by

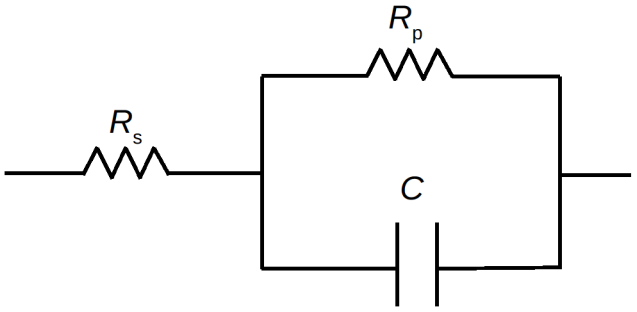


Figure F-2 The circuit of a resistor, R_s, arranged in series to a parallel circuit of resistor-capacitor elements $R_\mathrm{p} - C$.

$$\begin{aligned} Z &= R_\mathrm{s} + \frac{1}{\frac{1}{R_\mathrm{p}} + j\omega C}, \\ &= R_\mathrm{s} + \frac{R_\mathrm{p}}{1 + j\omega R_\mathrm{p} C}, \\ &= R_\mathrm{s} + \underbrace{\frac{R_\mathrm{p}}{1 + j\omega\tau}}_{=Z_\parallel}, \end{aligned} \tag{F-1}$$

where τ is the time constant ($\tau = R_\mathrm{p}C$).

The following derivations[419] focus on understanding and simplifying the impedance of the RC-circuit, $Z_\parallel$. To determine the real, Re{Z} and imaginary parts, Im{Z}, both the numerator and denominator of the fraction term must be multiplied by the complex conjugate:[419]

$$\begin{aligned} Z_\parallel &= \left[\frac{R_\mathrm{p}}{1 + j\omega\tau}\right]\left[\frac{1 - j\omega\tau}{1 - j\omega\tau}\right], \\ &= \frac{R_\mathrm{p} - j\omega\tau R_\mathrm{p}}{1 + \omega^2\tau^2}, \\ &= \underbrace{\frac{R_\mathrm{p}}{1 + \omega^2\tau^2}}_{\mathrm{Re\{Z\}}} \underbrace{- \frac{\omega\tau R_\mathrm{p}}{1 + \omega^2\tau^2}}_{\mathrm{Im\{Z\}}} j. \end{aligned} \tag{F-2}$$

Equation F-2 is also known as the impedance expression in a rectangular coordinate system. To transform an impedance expression from rectangular coordinates to polar coordinates, the magnitude and phase angle of Equation F-2 must be determined.[419] The magnitude of the impedance in a phasor diagram is r, which can be given by[419]

$$r = \sqrt{\left(\frac{R_\mathrm{p}}{1+\omega^2\tau^2}\right)^2 + \left(\frac{\omega\tau R_\mathrm{p}}{1+\omega^2\tau^2}\right)^2}, \\ = \sqrt{\frac{{R_\mathrm{p}}^2}{1+\omega^2\tau^2}}. \tag{F-3}$$

The phase angle θ for $Z_\parallel$ can be calculated by[419]

$$\theta = \tan^{-1}\left[\left(\frac{-\omega\tau R_\mathrm{p}}{1+\omega^2\tau^2}\right)\left(\frac{1+\omega^2\tau^2}{R_\mathrm{p}}\right)\right], \\ = \tan^{-1}(-\omega\tau). \tag{F-4}$$

Therefore, for a $Z_\parallel$ circuit, the magnitude, r is a function of the resistance R_p, frequency ω and time constant τ, whereas the phase angle θ depends on the frequency ω and time constant τ.[419]

An RC circuit has a perfect semi-circular arc, representing the effects of a faradaic charge-transfer resistance and a non-faradaic double-layer capacitance at the electrode-electrolyte interface. However, the real-world impedance is usually non-homogeneous due to a rough interface or a non-uniform charge storage mechanism.[418] In this case, Equation F-1 can be modified to[418]

$$Z = R_\mathrm{s} + \underbrace{\frac{R_\mathrm{p}}{1+(j\omega\tau)^n}}_{=Z_\parallel}, \tag{F-5}$$

where n denotes the non-ideality. Such circuit element is known as a RQ-element or a Constant Phase Element (CPE). An ideal CPE represents a perfect double-layer capacitance, which has a non-depressed semicircular arc ($n \approx 1$).[418] Figure F-3 shows the simulated impedance of a synthetic RC and a RQ circuit using Equation F-1 and Equation F-5, where R_s is zero. From this figure, it can be deduced that the non-ideality of an impedance increases with smaller n values.

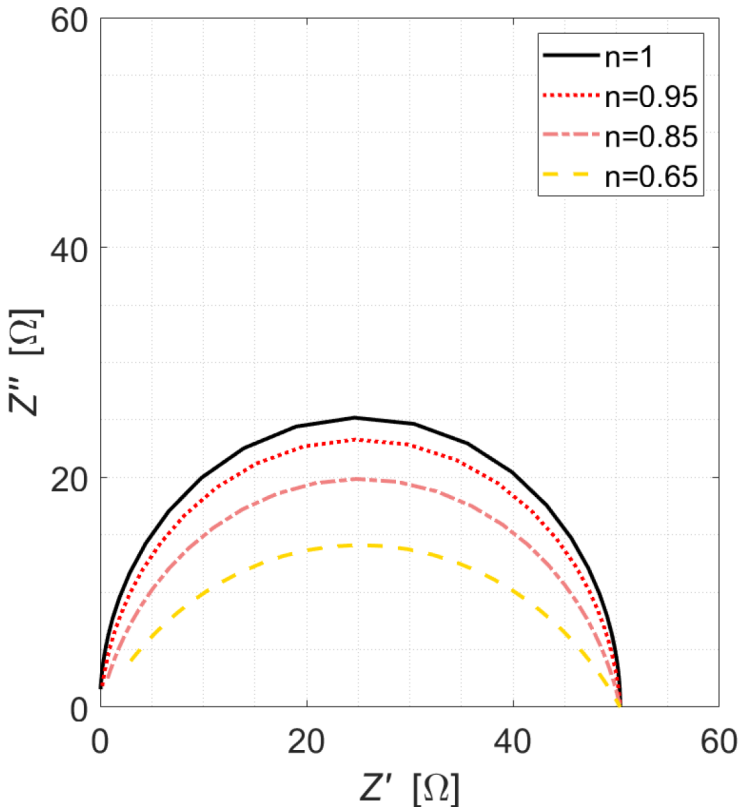


Figure F-3 A synthetic impedance of a RC and RQ circuit with different n-values.

Figure F-4 shows different Nyquist plots from the literature for solid-state Li-metal cells (Li|LiPON|LCO). By using different cell configurations such as Pt|LiPON|Pt, Li|LiPON|Li and Li|LiPON|LCO, Iriyama *et al.*[211] showed in Figure F-4(a) that up to three semicircular arcs can be observed in a pristine solid-state Li-metal cell, where the second semi-circle (A) corresponding to the Li-LiPON interface has a smaller impedance contribution. The first semi-circle was attributed to the electrolyte resistance in LiPON, whereas the third semi-circle was assigned to the LiPON-LCO interface.[211] Figure F-4(b)[7] compares the impedance of a pristine cell to a degraded cell due to overdischarged. Under an overdischarge condition, Li is stripped excessively from the NE into the PE. As a result, the different contributions of convoluted semi-circles can be better distinguished.[7] The observations of three semicircular arcs in Figure F-4(a) and Figure F-4(b) are consistent with those observed by Fabre *et al.*[60] They proposed an equivalent circuit consists of three CPE pairs, where each circuit pair corresponds to one electrochemical process.[60] Nevertheless, Larfaillou *et al.*[63] showed later that four electrochemical processes could also be observed, where the third and fourth semi-circles were attributed to the LCO behaviour.

While equivalent circuits models illustrated in the insets of Figure F-4(a) and Figure F-4(c) are helpful in extracting resistance and capacitance values from a given impedance dataset, different circuit elements can be arranged to fit the same impedance curve.[7,313] Moreover,

different electrochemical processes often appear convoluted in a Nyquist plot.[7,314] For instance, Figure F-4(c) displays two distinct semi-circles. However, the impedance curve consists of three semi-circles in reality, where the second semi-circle is convoluted with the first semi-circle. Each semi-circle usually represents an electrochemical process. To aid the separation of different polarisation processes and the deconvolution of semi-circles, the Distribution Function of Relaxation Times (DRT) analysis was used in this thesis.

Because the DRT model is sensitive to measurement errors,[418] the linearity, causality and stability of the measured impedance should be checked with the Kramers-Kronig (KK) Relation before analysing a measured impedance with a DRT model.

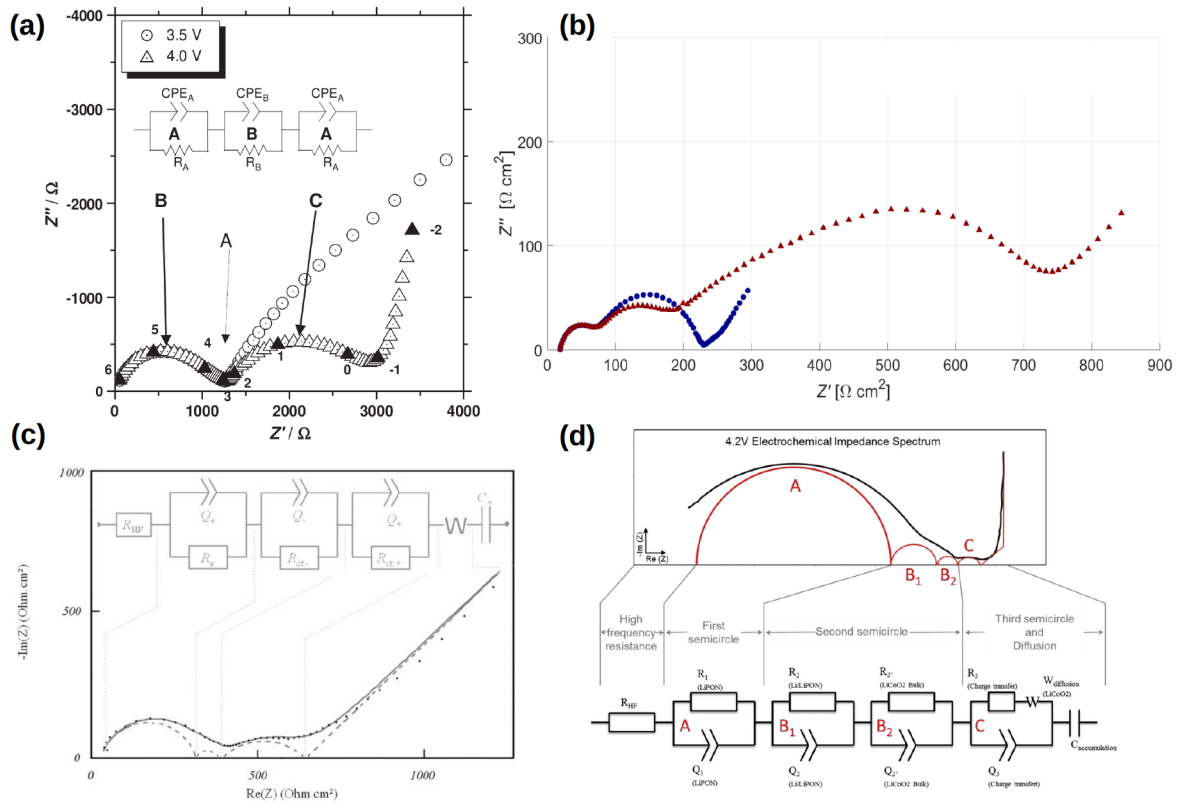


Figure F-4 A literature survey of Nyquist plots for Li|LiPON|LCO cell chemistry: While three semicircular arcs are usually observed for this type of cell chemistry, four semi-circles were also observed in the literature. Reproduced with permissions from Ref. 7,60,63,211.

F.3 Kramers-Kronig Relations

The Kramers-Kronig (KK) Relation can be described as "integral equations that constrain the real and imaginary components of complex quantities for systems that satisfy the conditions of linearity, causality and stability."[419] There are four fundamental theorems underpin the theory of KK relations, which include[419]

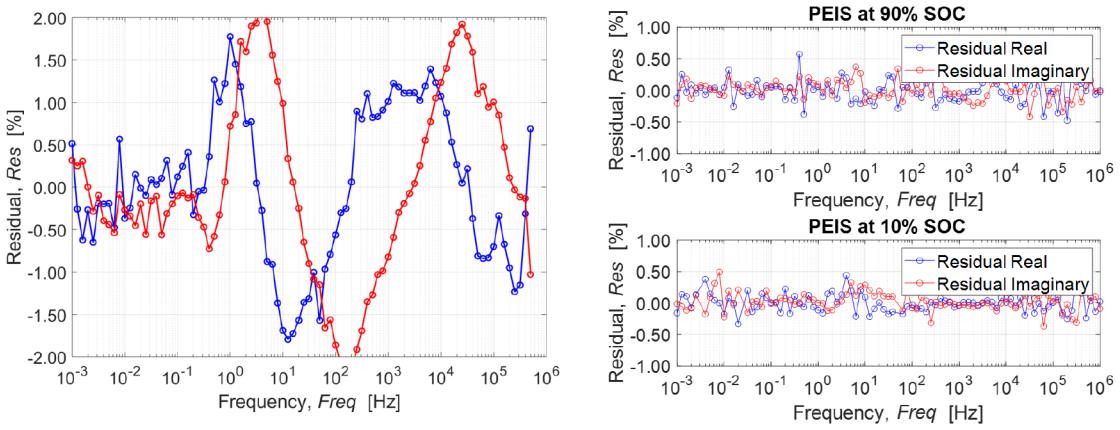


Figure F-5 The compliance of impedance measurements to the Kramers-Kronig (KK) relations: (Left panel) The real and imaginary residuals of the particular impedance measurement fluctuate significantly with time, indicating a violation of the KK criteria. (Right panel) The residuals of both real and imaginary components fall within the range $\pm\,0.50-1.00\%$.

(i) **Linearity:** The output is linearly dependent on the input;

(ii) **Time-translation Independence:** The output depends only on the input. If the input signal is advanced or delayed by a time increment, then the output response will be changed by the same time increment;

(iii) **Causality:** The input signal is the only cause of the output response;

(iv) **Stability:** The output response to an input impulse cannot increase with time.[419]

Impedance measurement can be considered as linear when the perturbation signal is small such that the output response will be a sinusoid at the same frequency but shifted in phase compared to the input signal.[1,418] The KK relations are useful to check whether the real part of an impedance (Z') is internally consistent with the corresponding imaginary part (Z'') or vice versa, as shown by[311,312,419]

$$Z' = \frac{2}{\pi}\int_0^{\infty} \frac{\omega' \cdot Z''(\omega')}{\omega^2 - \omega'^2} d\omega', \tag{F-6}$$

$$Z'' = \frac{-2}{\pi}\int_0^{\infty} \frac{\omega \cdot Z'(\omega')}{\omega^2 - \omega'^2} d\omega'. \tag{F-7}$$

Failure to comply with the KK relations can be caused by instrumental errors such as a loose connection, the presence of external noises or evolution of time-dependent phenomena during measurements.[312,419] Figure F-5 (left panel) shows fluctuating real and imaginary residuals, which imply that the particular impedance responses were not stable and were significantly

influenced by external errors. Therefore, if the application of the KK relations to an experimental impedance measurement reveals significant variations with large residuals, the measurement conditions should be checked, and the affected measurements should be repeated. In contrast to the large fluctuations of the real and imaginary residuals shown, Figure F-5 (right panel) illustrates a stable and linearly dependent impedance measurement, where the residuals have a range between $\pm\,0.50-1.00\%$.

F.4 Distribution Function of Relaxation Times (DRT) analysis

The fundamentals on the DRT analysis are summarised from the works of Wan *et al.*,[315] who have also published an open-source DRT-tool that forms the basis of the DRT analysis in this thesis. The readers are directed to their works to understand the DRT basics.

As shown by[313,315,316]

$$\begin{aligned} Z(\omega) &= R_{\text{ohmic}} + Z_{\text{pol}}(\omega), \\ &= R_{\text{ohmic}} + \sum_{k=1}^{N} \frac{R_{\text{pol},k}}{1 + j\omega\tau_k}, \end{aligned} \tag{F-8}$$

a DRT model consists of an ohmic resistance (R_{ohmic}) and the sum of infinite series of parallel resistors and capacitors. Dynamic processes are represented by peaks in the distribution of a DRT model. For an ideal RC process, each electrochemical process can be represented by Dirac impulse functions at the corresponding relaxation time, whereas real processes often exhibit peaks around the main relaxation time (see Figure F-6).[313,315]

In principle, the distribution functions in the DRT model can be estimated with either Piece-Wise Linear (PWL) or Radial Basis Function (RBF) approximation methods. Figure F-7 compares the DRT results computed with RBF and PWL methods. While RBF-based DRT illustrates complete peaks across the time range, the first and last peaks of the PWL-based DRT are truncated.[315] This truncation occurs because the functions decrease linearly to zero outside the frequency range.[315] There are two main types of RBFs: (1) Gaussian-RBF and differentiable Matérn-RBF up to orders six.[315] Wan *et al.*[315] had developed a general DRT-tool to distinguish different electrochemical processes and showed that the DRT result obtained by the Gaussian-RBF closely matches the exact DRT. Based on their analysis, the Gaussian-RBF is chosen for all impedance deconvolution in this thesis. The Gaussian discretisation function can be given by[315]

$$\phi_\mu(x) = \exp\Big(-(\mu x)^2\Big), \tag{F-9}$$

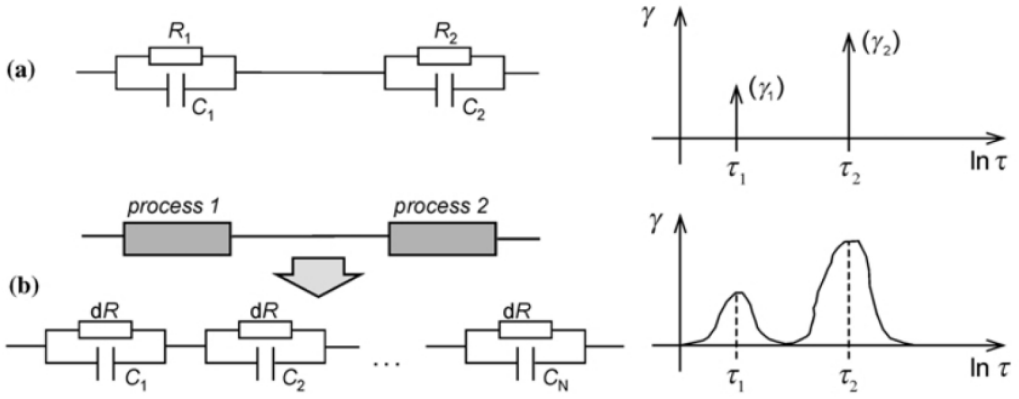


Figure F-6 Representation of dynamic processes in a Distribution Function of Relaxation Times (DRT) model: An ideal electrochemical process is represented by Dirac impulse functions at the corresponding relaxation time, whereas real processes are represented by peaks distributed around the main relaxation time. Reproduced with permission from Ref. 313, Copyright (2002), Journal of Applied Electrochemistry.

where μ is the coefficient to Full Width at Half Maximum (FWHM), $x = |\ln\tau - \ln\tau_k|$ and $\tau_k = 1/(2\pi f_k)$.[315] By overlaying the DRT spectrum with the imaginary part of an impedance, as exemplified by Figure 3.7 in Chapter 3, the choice of optimum μ-coefficient can be estimated.

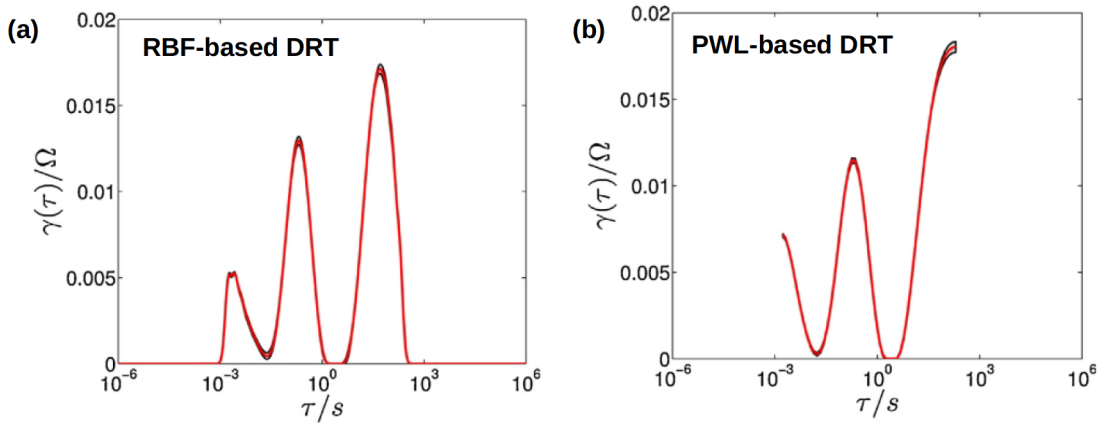


Figure F-7 Radial Basis Function (RBF)-based and Piece-Wise Linear (PWL)-based Distribution Function of Relaxation Times (DRT) analysis: The DRT results computed with the RBF method illustrates three complete peaks, whereas parts of the first and last peaks discretised with the PWL method were truncated. Reproduced with permission from Ref. 315, Copyright (2015), Elsevier.

Fitting experimental impedance (Z_{exp}) to DRT model (Z_{DRT}) requires the minimisation of the following sum of squares, S:[315]

$$S = \sum_{n=1}^{N} \left[w'_n (Z'_{\text{DRT}}(f_n) - Z'_{\text{exp}}(f_n))^2 + w''_n (Z''_{\text{DRT}}(f_n) - Z''_{\text{exp}}(f_n))^2 \right], \tag{F-10}$$

where Z'_{DRT} and Z''_{DRT} represent the real and imaginary components of the DRT model, whereas Z'_{exp} and Z''_{exp} are the real and imaginary parts of the experimental impedance. The Tikhonov regularisation method is needed to minimise Equation F-10 and the oscillations of DRT peaks can be controlled with the regularisation parameter, λ_{DRT}.[315] Figure F-8[418] illustrates the impacts of choosing different λ_{DRT} on the DRT oscillations. λ_{DRT} has a range of values between 10^{-2} and 10^{-8}: the larger the λ_{DRT}, the lesser are the DRT oscillations.[418] By comparing the minimum residuals and the optimal λ_{DRT} to the values obtained from cross validation tests, Wan *et al.*[315] demonstrates that the optimal λ_{DRT} is between 10^{-2} and 10^{-3} for the Gaussian-RBF of most electrochemical systems. Therefore, based on their analysis, 10^{-3} is chosen as the optimal regularisation parameter.

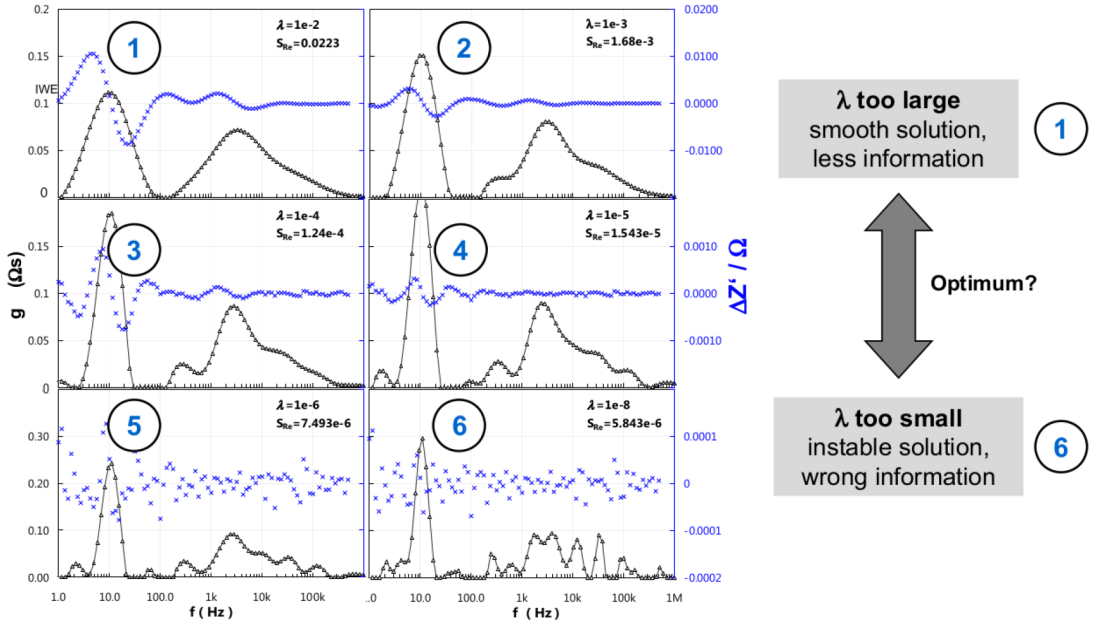


Figure F-8 The impacts of different regularisation parameters, λ_{DRT} on the Distribution Function of Relaxation Times (DRT) peaks: A too large λ_{DRT} will cause a loss of features whereas a too small λ_{DRT} will result in instable and wrong information.[418] For most electrochemical systems, the optimum is between 10^{-2} and 10^{-3}.[315] Reproduced from Ref. 418.

In addition to the regularisation parameter, two types of regularisation derivative can be used as penalties to the distribution functions:[315]

$$\begin{aligned} \text{First-order derivative}: & \left|\left|\frac{d\gamma(\tau)}{d\ln\tau}\right|\right|^2, \\ \text{Second-order derivative}: & \left|\left|\frac{d^2\gamma(\tau)}{d\ln\tau^2}\right|\right|^2. \end{aligned} \tag{F-11}$$

Figure F-9 illustrates the influence of regularisation derivatives on the local DRT peaks computed in this thesis. While both derivatives indicate the same number of peaks, the local peaks can be better resolved with the second-order derivative.

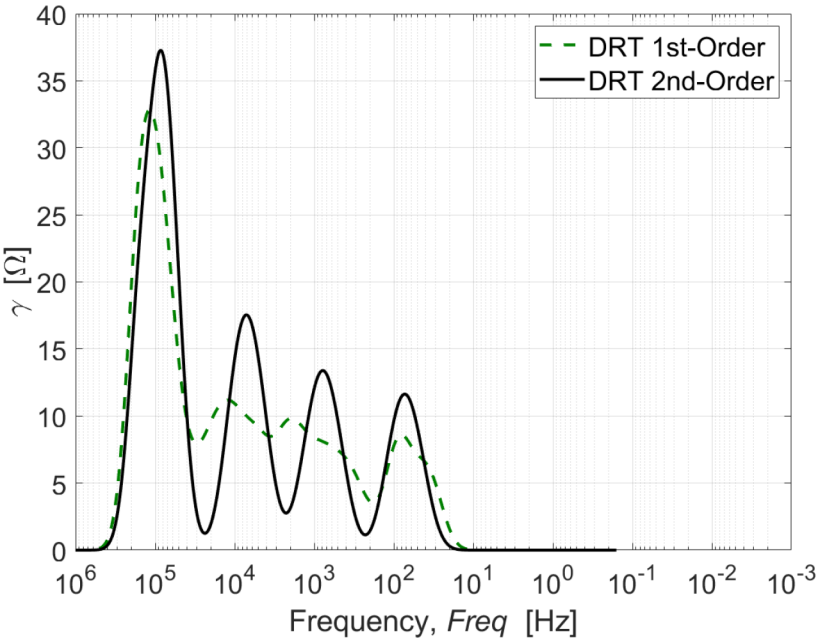


Figure F-9 The influence of different regularisation derivatives in the Distribution Function of Relaxation Times (DRT) model, where the second order derivative has a higher resolution compared to the first-order derivative in this analysis.

The DRT spectra can then be used with the equivalent circuit model to fit the measured impedance, where the size of each semi-circle corresponds approximately to the DRT peaks. In this work, the DRT tool is only used as a qualitative analysis to distinguish the electrochemical peaks of an impedance spectrum, where the resistance (R_k) and capacitance (C_k) values were extracted from the equivalent circuit model. These values were subsequently simulated based on

$$Z(\omega) = R_{\text{ohmic}} + \sum_{k=1}^{N} \frac{R_k}{1 + (j\omega R_k C_k)^n} \tag{F-12}$$

to ensure that the semi-circles do not intersect. Although the equivalent circuit model has been commonly used to fit impedance spectra in the literature, not all resistance and capacitance values given by an equivalent circuit model are always sensible. Figure F-10 illustrates an example of an incorrect fit, where the first and second semi-circles intersect. An intersected semi-circle indicates an overlapping resistance, which is not physical and plausible in reality. Secondly, the simulated semi-circles based on the fitted values from the equivalent circuit model also indicate an unaccounted impedance contribution towards the end of the spectrum. Thirdly, by comparing the fitted semi-circles to those proposed in the literature (see Figure F-4), Figure

F-10 indicates that the size of the first and second semi-circles are not proportional. Therefore, it is essential to simulate the fitted semi-circles before estimating the model parameters with the resistance or capacitance values, as shown by the bottom panel of Figure F-10.

Although four semi-circles could be observed compared to those impedance spectra proposed in the literature, the fourth semi-circle's physical origin is unclear. Unlike Larfaillou *et al.*,[63] who had assigned the third semi-circle to LCO bulk behaviour and the fourth semi-circle to LiPON-LCO charge transfer, the third semi-circle was attributed to the interfacial rather than electrode bulk behaviour in this thesis. This attribution was made based on different cell configurations proposed by Iriyama *et al.*[211] By comparing the impedance contributions from symmetrical and non-symmetrical solid-state cells, the third semi-circle was attributed unambiguously to the interfacial charge-transfer behaviour.[211] Although no additional experiments such as TEM and EELS could be undertaken to identify the chemical compositions of the fourth peak, this impedance contribution could originate from an additional film resistance, as observed by Wang *et al.*[86] Therefore, future works are required to investigate the origins of this impedance contribution.

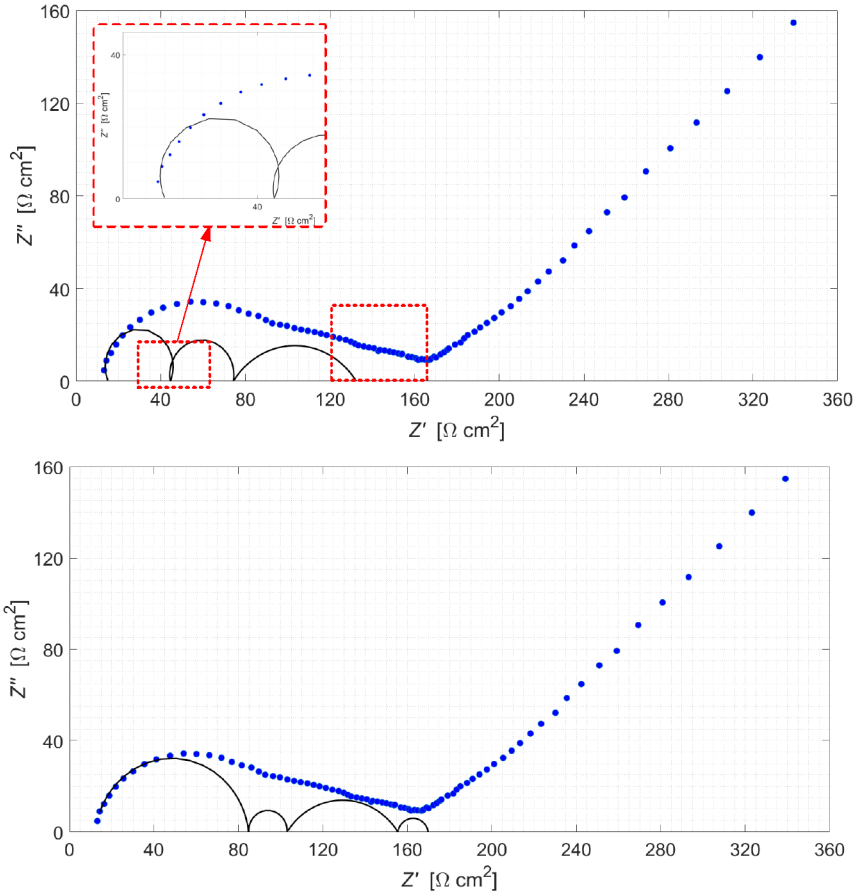


Figure F-10 (Top) Incorrectly fitted semi-circles with (i) the intersection of the first and second semi-circles; (ii) an unaccounted impedance contribution towards the end of the semicircular spectrum; and (iii) non-proportional size of the first and second semi-circles. (Bottom) Simulated semi-circles based on Equation F-12 to ensure that the semi-circles do not intersect and the size of each semi-circle is plausible compared to the Nyquist plots from the literature shown in Figure F-4.

F.5 Space-charge effects in the time domain

Due to the accumulation or depletion of the charged species at the electrode-electrolyte interface, the surface concentration of Li^+ ions usually deviate from the bulk ionic concentration to form a space-charge region (see Figure 2.15). While the bulk SE is electroneutral, the space-charge effects cause the interface to be non-electroneutral.[83,84] An in-depth discussion on the space-charge formation can be found in Chapter 2 of this thesis.

Space-charge cell model. As discussed in Section 2.3.1.3, the space-charge effects are most obvious for a very short time constant. Nevertheless, no conclusive studies have been undertaken in the literature to show how the space-charge formation affects the constant-current discharge performance of solid-state Li-metal batteries. To account for the non-faradaic current due to the capacitive effects at the interface, the electrochemical cell model presented in Chapter 3 of this thesis is modified to include both faradaic current due to charge-transfer and non-faradaic

current due to space-charge effects at the interface. Therefore, the sum of interfacial current becomes[40,251,252]

$$i_{\text{int}} = i_{\text{ct}} + \underbrace{c\frac{\partial(\phi_{\text{s}} - \phi_{\text{e}})}{\partial t}}_{i_{\text{DL}}}, \tag{F-13}$$

,

where i_{ct} is the charge-transfer current at the interface and i_{DL} represents the capacitive or double-layer current density. c is the specific capacitance estimated from the EIS measurements. Figure F-11 plots the specific capacitance for both LCO-LiPON and Li-LiPON interfaces. Because the capacitive contributions have decreased significantly at 328.15 K, as shown by the PEIS and DRT in Figure 4.5, the specific capacitance was estimated for the temperature range between 298.15 K and 318.15 K in this thesis. From Figure F-11, it can be deduced that the specific capacitance of the LiPON-LCO interface is dominating, especially at the low-temperature regime. While the specific capacitance at LiPON-Li interface shows no significant changes over the range of temperatures, the specific capacitance at LiPON-LCO interface decreases with increasing temperatures. This trend can be correlated to the decreasing size of the semi-circles at higher temperatures, which could be attributed to a more homegenous interfacial charge distribution at higher temperatures. It should be noted that the values for specific capacitance was estimated from the PEIS spectra, in which the semi-circles do not intersect, as shown by Figure F-10. The exact specific capacitance will be slightly larger due to a larger n-factor (see Figure F-3).

Initial conditions. For both cell models with and without the space-charge contributions, a temperature-dependent OCV was used as the initial conditions:

$$U_{\text{cell}}(T) = U_{\text{cell,ref}} + (T - T_{\text{ref}})\frac{\partial U(x_{\text{Li}})}{\partial T}, \tag{F-14}$$

where $U_{\text{cell,ref}}$ is the OCP at 25 °C and $\partial U(x_{\text{Li}})/\partial T$ is the measured entropic heat coefficient between 95% SOC and 25% SOC. By defining the OCV following Equation F-14, an initial condition for different intermediate temperatures between 25 °C and 45 °C can be estimated.

F.5.1 Single-layer space-charge cell model

By using the temperature-dependent specific capacitances estimated from the experimental measurements, the space-charge effects are first evaluated for a single-layer cell model.

Figure F-12 shows the predicted constant-current discharge performance for a cell model with and without the space-charge effects at the temperature of 25 °C for 0.1 C, indicating that the space-charge effects can be considered negligible for very low current densities. By comparing

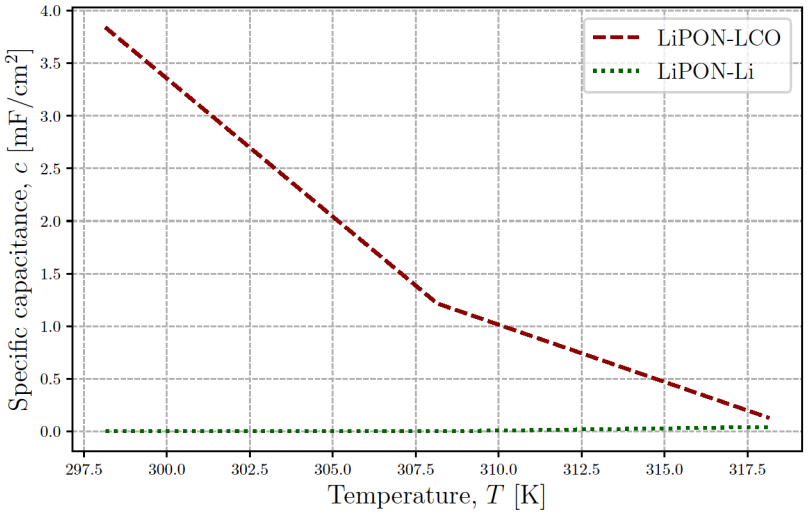


Figure F-11 Specific capacitance of LCO-LiPON and Li-LiPON interfaces for the temperature range between 298.15 K and 318.15 K.

the total internal resistance and cell impedance at different SOCs, Figure 3.6 in Chapter 3 shows that the instantaneous voltage drops at low C-rates are caused predominantly by the faradaic charge-transfer kinetics, ionic transport across the SEs and the slow diffusion across the PEs.

However, as the current densities increase, as shown by Figure F-13, the space-charge effects become apparent. In a time-domain cell model simulation, the space-charge effects cause an instantaneous voltage drop at the beginning of cell discharge. While the discharge at 0.5C has an initial voltage drop between 0.08 V-0.1 V, the magnitude of voltage drop approaches 0.18 V at a 5C discharge. This observation implies that the distribution of surface concentration and local electric potential at the interface depends strongly on the discharge current densities.

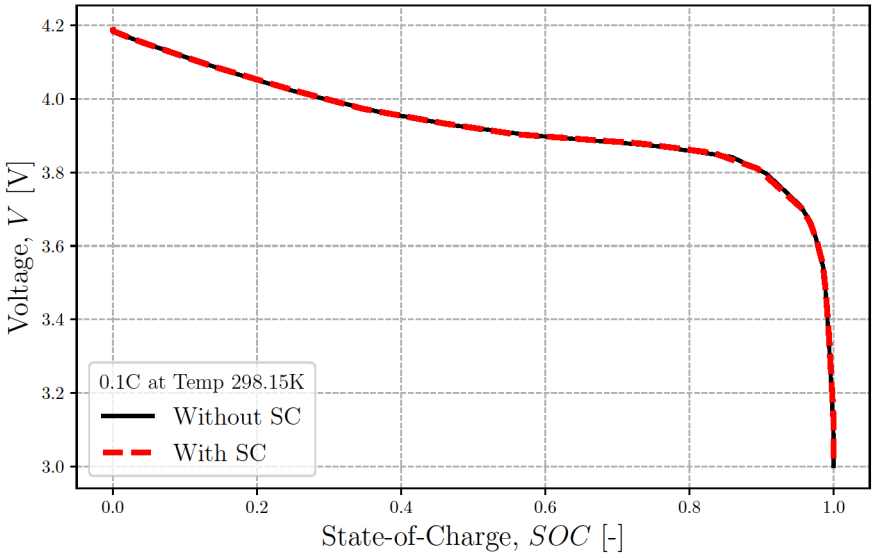


Figure F-12 The discharge cell performance with and without the space-charge contributions at the temperature $25\,^{\circ}\mathrm{C}$ for the discharge C-rate of $0.1\,\mathrm{C}$. The black solid line represents the discharge curve without the space-charge model, whereas the red dotted line denotes the discharge curve including the space-charge effects.

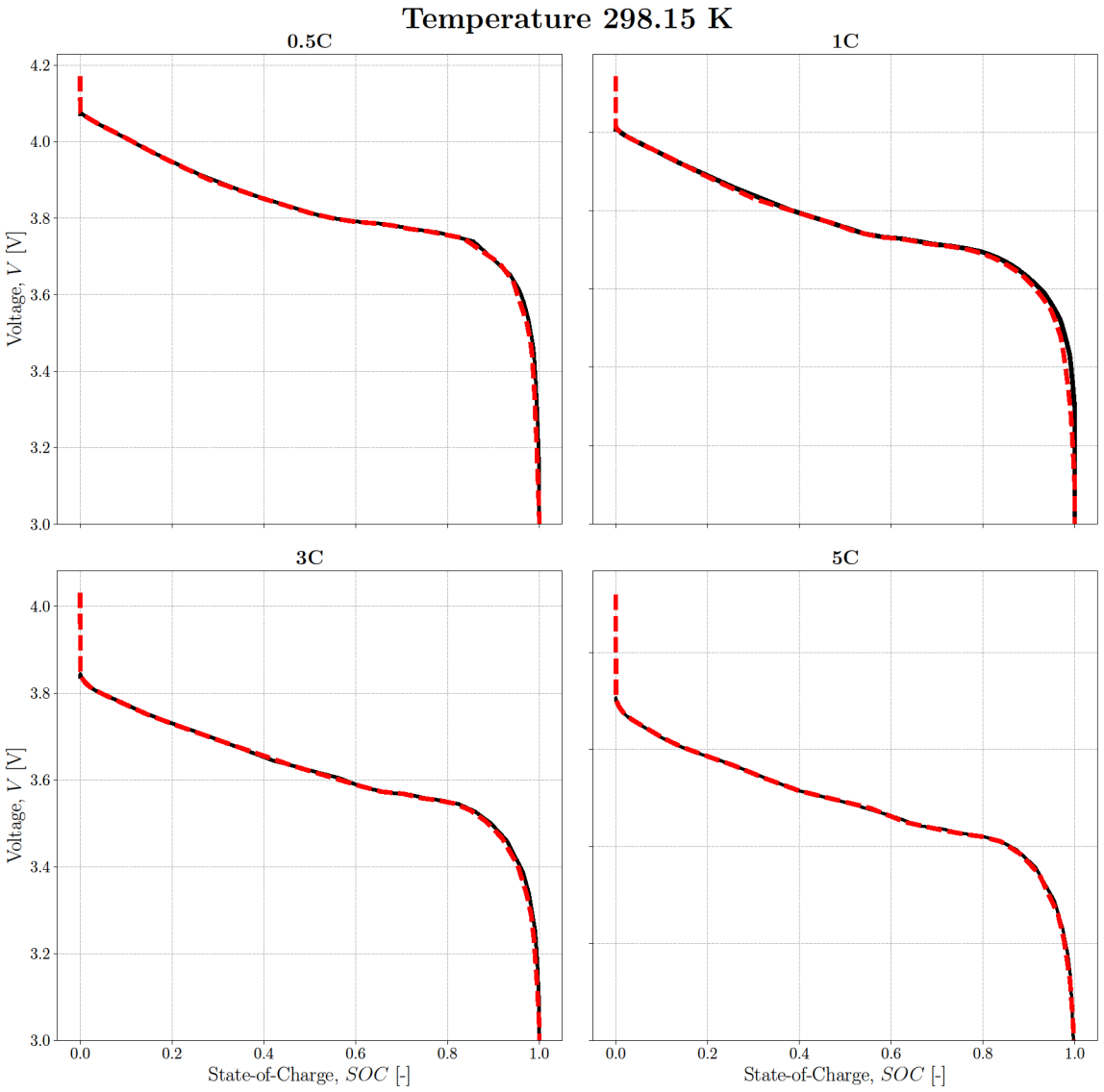


Figure F-13 Constant-current model predictions with and without the space-charge model for different C-rates at 298.15 K. Compared to low C-rates, the initial voltage drop due to the space-charge effects become more significant at high C-rates.

As the operating temperature increases from 25 °C to 45 °C, the initial voltage drop corresponding to the space-charge effects decreases. Figure F-14 illustrates the space-charge impacts for different C-rates at 45 °C. Compared to the magnitude of voltage drops at 25 °C, the initial voltage drops at 45 °C have a range of values of approximately $\approx$ 0.1V at a 5C discharge. This comparison suggests that the space-charge effects are more significant at the low-temperature regime. The interfacial kinetics increase at higher operating temperatures, causing the charge and local potential distribution to be more homogeneous and subsequently a lower magnitude of voltage drop at the interface.

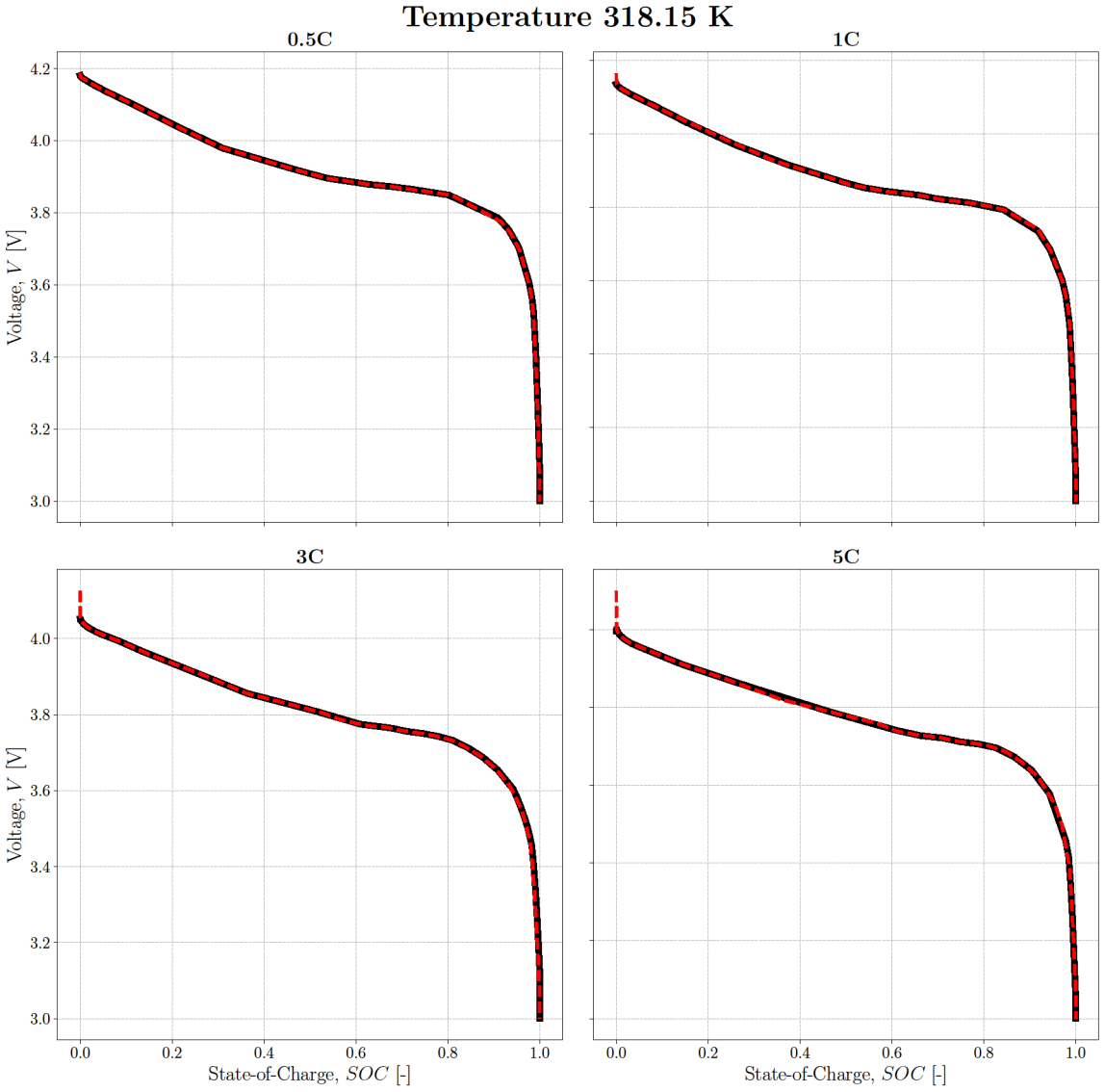


Figure F-14 Constant-current model predictions with and without the space-charge model for different C-rates at 318.15 K: the green dotted curve in all subplots represents the cell model with the space-charge effects, whereas the black solid curves denote the model predictions without considering the space-charge formation.

While the formation of space-charge causes an instantaneous voltage drop for most operating

conditions, a positive space-charge effect was predicted for very low current densities such as 0.1 C-0.2 C at high temperature. Figure F-15 illustrates the positive space-charge effect, where a small magnitude of an initial voltage spike rather than a voltage drop could be observed. At very low C-rates and high temperatures, this positive space-charge effect may indicate that the actual OCV behaviour, $U_{\text{cell}}(T = 45\,^{\circ}\text{C})$, is slightly higher than the estimated OCV behaviour given by Equation F-14 due to minimal interfacial losses.

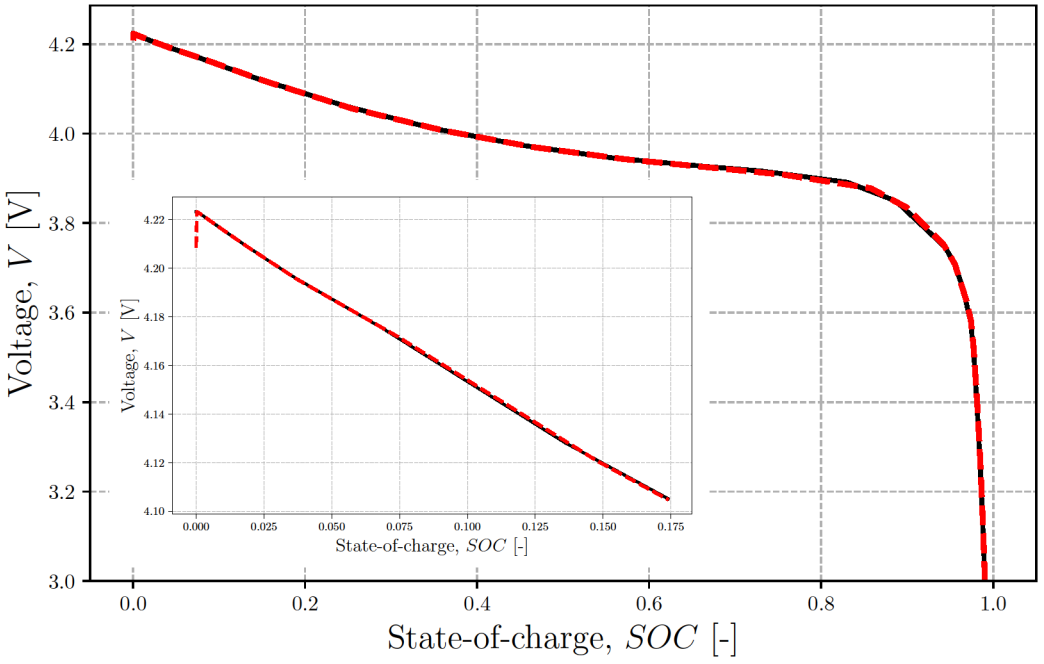


Figure F-15 Positive space-charge effects at a very low current density (0.2C) and high temperature (318.15 K).

Figure F-16 maps the contour of initial voltage drops caused by the space-charge effects at different C-rates and temperatures. While the blue and dark purple regions indicate that the space-charge impacts are negligible, the orange to light yellow region shows that the initial voltage drops due to space-charge effects approaching 0.18 V for high C-rates discharge at 25 °C. Nevertheless, the model predictions show that the voltage drop only occurs for a very short time constant at the beginning of discharge. For all current densities (*i.e.* 0.1C to 5C) and operating temperatures (*i.e.* 25 °C to 45 °C) evaluated in this thesis, the space-charge effects do not affect the cell performance above this short time constant, corroborating the conclusions obtained in Chapter 3 of this thesis.

Due to this very short time constant, the space-charge effect can be easily overlooked in an experimental measurement. This is because the space-charge region is limited to an immediate voltage change corresponding to only two data points in space (P1-P2), as indicated by Figure F-17. For most constant-current discharge experiments, P2 is usually regarded as the first data

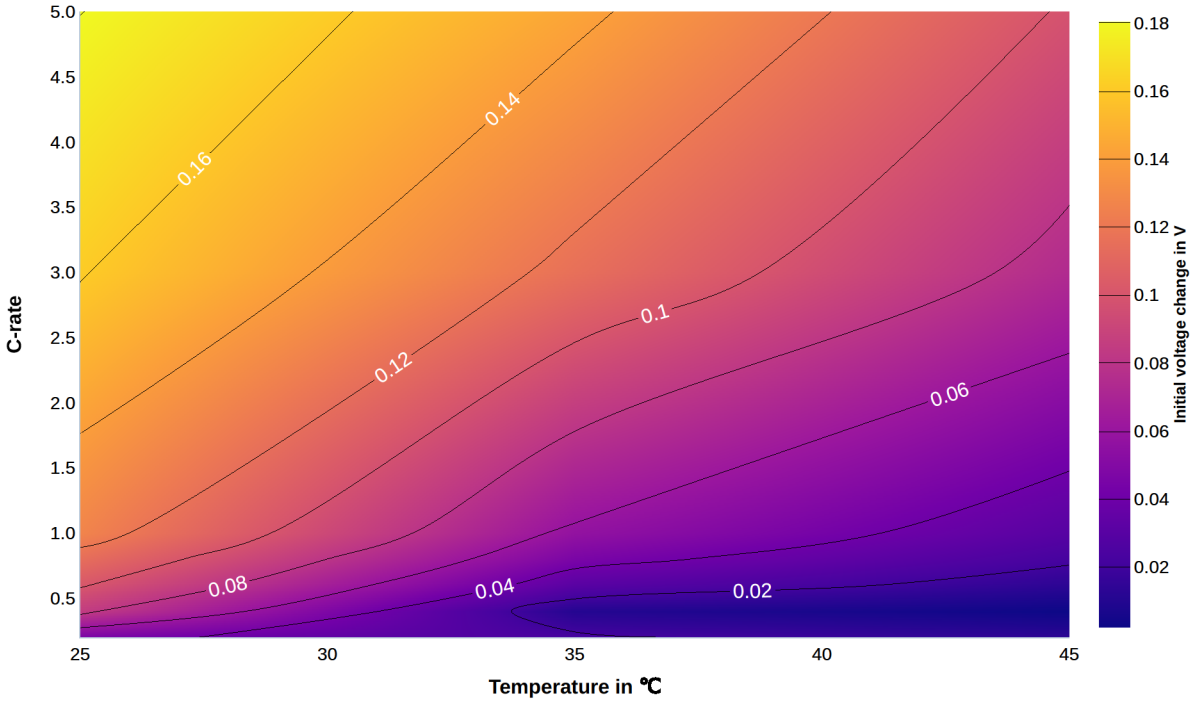


Figure F-16 A contour map to illustrate the initial voltage changes due to the space-charge effects at different C-rates and temperatures.

point from the constant-current discharge dataset. The instantaneous voltage change from P1 to P2 will only be visible when a constant-current discharge experiment is evaluated including a rest period, whereas P1 is the last data point of the rest period (see Figure F-18).

To account for the space-charge effect in experimental measurements, this comparative analysis shows that a constant-current experimental sequence should always be analysed along the rest period before the discharge or charge experiments. However, it should be noted that the instantaneous voltage change is not necessarily caused by the non-faradaic space-charge effect alone. Other mechanisms such as faradaic charge-transfer, ionic transport across the SE and diffusion kinetics in the electrode could also cause this voltage drop. Hence, it is essential to distinguish and separate the contributions of these different mechanisms to the instantaneous voltage change in future works.

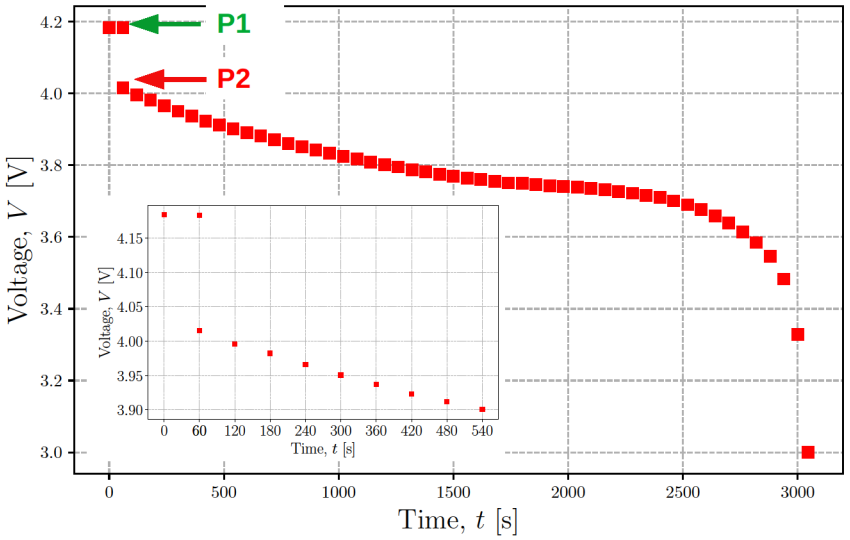


Figure F-17 Experimental indication of a space-charge effect in solid-state lithium-metal cells. The inset shows that the instantaneous voltage drop occurs in less than one second. The timestep taken to record each data point is 60 s.

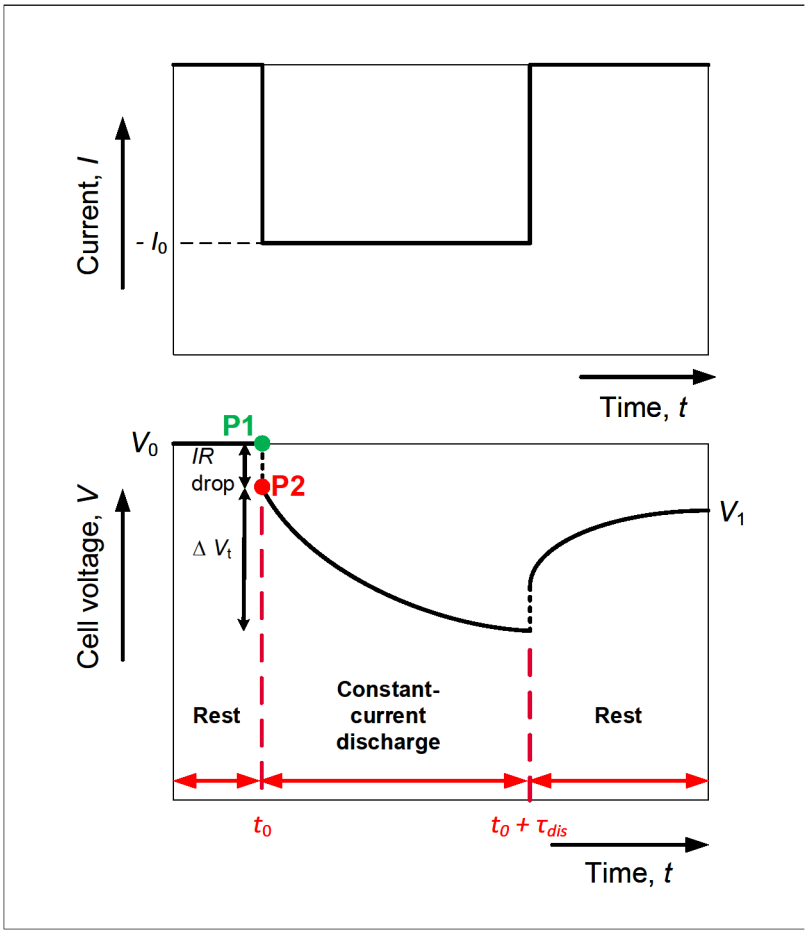


Figure F-18 Experimental measurement including the rest and constant-current discharge period, where P1 is the last data point of the rest period and P2 is the first point of the constant-current discharge sequence.

F.5.2 Space-charge stack model

The stack models proposed in Chapter 4 of this thesis are extended to evaluate the effects of space-charge. Assuming that the materials, electrode composition and the manufacturing process remain the same for the small-scale and large-scale cells,[338] scaling the electrode active area, A_{ref}, will cause the capacitance, C, to increase linearly, as defined by the following relation:

$$C = \epsilon \frac{A_{\text{ref}}}{d}, \tag{F-15}$$

where ϵ is the permittivity, and d is the length of the space-charge region. If ϵ and d do not change assuming an ideal scaling process, the specific capacitance (C/A_{ref}) will be the same for both small-scale and large-scale cells.

For a parallel stack model, the total specific capacitance can be calculated by summing the individual specific capacitance of each double-coated unit cell, as given by

$$c_{\text{tot}} = \sum_{i}^{N_{\text{Par}}} 2c_i, \tag{F-16}$$

where N_{Par} is the number of unit cells stacked in parallel, and factor 2 represents the double-coated configuration. Figure F-19 illustrates the impacts of space-charge in a parallel stack model. Under the most critical operating conditions relevant for the space-charge observations (*i.e.* 5C from an initial temperature of 25 °C), the space-charge effects are found to cause a maximum voltage drop between 0.16 V - 0.18 V. For a fully coupled electrochemical-thermal model, the heat generations cause the stack temperature to increase and the specific capacitance to decrease. As a result, the instantaneous voltage drop due to the space-charge contributions correspond to only 0.16 V - 0.18 V despite the number of unit cells stacked in parallel. Nevertheless, it should be noted that different cooling strategies may affect the heat generations and, therefore, the temperature-dependent space-charge behaviour in a different manner.

For a bipolar stack model, the total specific capacitance is defined by

$$\frac{1}{c_{\text{tot}}} = \sum_{i}^{N_{\text{BP}}} \frac{1}{c_i}, \tag{F-17}$$

in which N_{BP} is the number of unit cells stacked in series. Figure F-20 shows the implications of space-charge for a bipolar stack model. Under a constant-current discharge at 5C from an

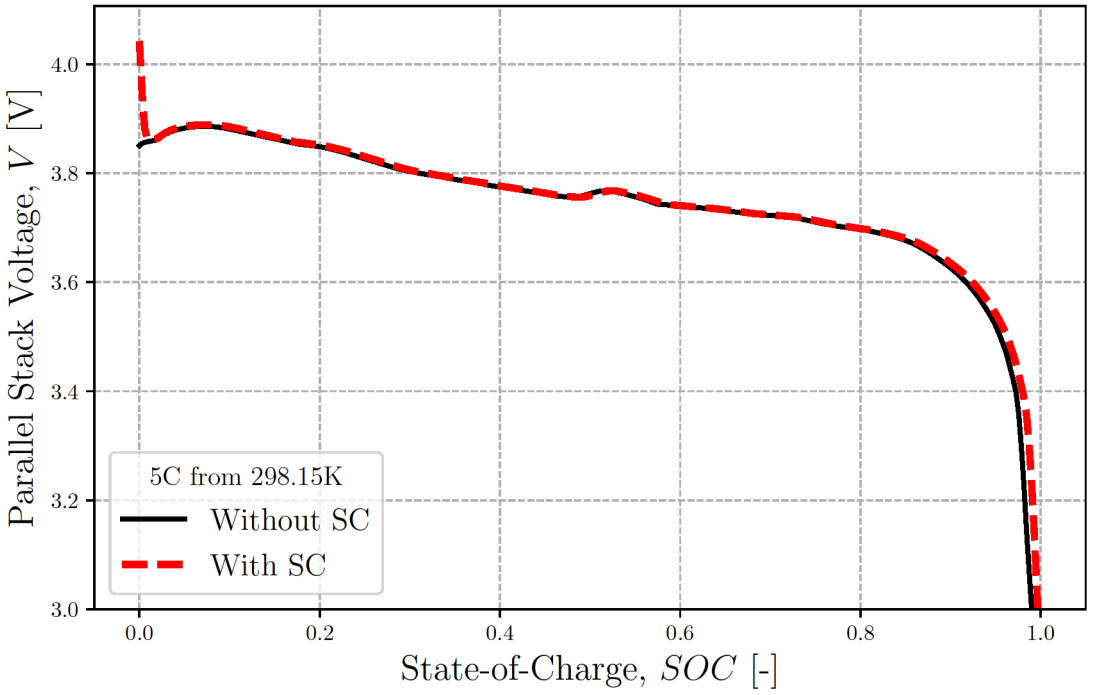


Figure F-19 A parallel stack model with and without the space-charge effects: the black solid line denotes the stack model without the non-faradaic space-charge contributions, whereas the red dotted line represents the stack model including the space-charge impacts.

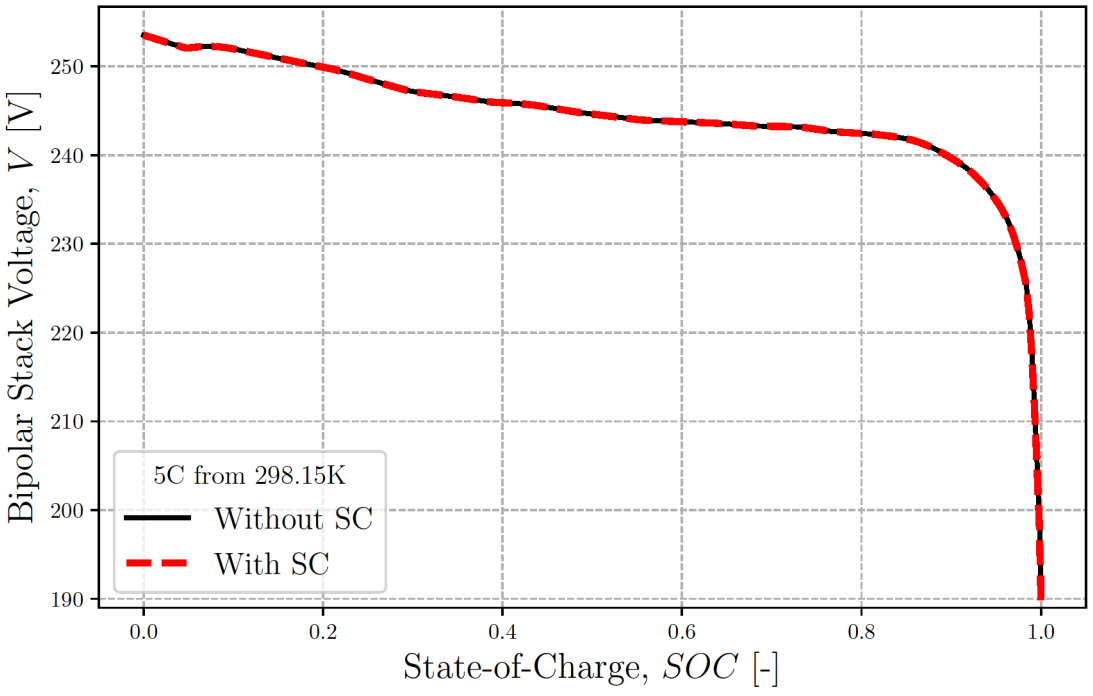


Figure F-20 A bipolar stack model with and without the space-charge effects.

initial temperature of 298.15 K, the immediate voltage drop due to the space-charge effects are found to be negligible for a bipolar stack model. Due to the serial stacking of unit cells, the

total specific capacitance becomes smaller than each unit cell's specific capacitance.

Based on the evaluations in Section F.5.1 and Section F.5.2, it can be concluded that the instantaneous voltage drops due to the space-charge formations are most apparent for

(I) high C-rate discharge;

(II) low-temperature operating conditions;

(III) very short time constant ($< 1\,\mathrm{s}$);

(IV) a parallel stack.

Nonetheless, as shown by Figure F-19 and Figure F-20, the stack voltage with and without the space-charge contributions remain the same after the very short time constant. Even for the most critical operating conditions relevant for the space-charge observations, the space-charge formations are found to cause negligible impacts to the stack performance in terms of their energy and power densities.

Acknowledgements and author contributions

M.-C. Pang acknowledges the discussion with P. Vadhva in the early-stage development of the space-charge models.

G Derivations

This section describes the derivations for understanding the fundamental assumptions of relevant equations in this thesis. Part of the derivations of the Butler-Volmer (BV) Equation in Section G.1 and Nernst's Equation in Section G.2 were adapted and reproduced with permissions from Plett and Xue.[420] The derivations of the Nernst-Einstein's equation in Section G.5 were minimally adapted and reproduced with permission from Brett.[377]

G.1 Derivations of the Butler-Volmer's equation

According to the transition state theory, for a given chemical reaction, the reactants (A and B) have to overcome the activation energy, E_a, forming activated complex ($AB^{\ddagger}$) before reaching the final products (C and D) (see Figure G-1a).

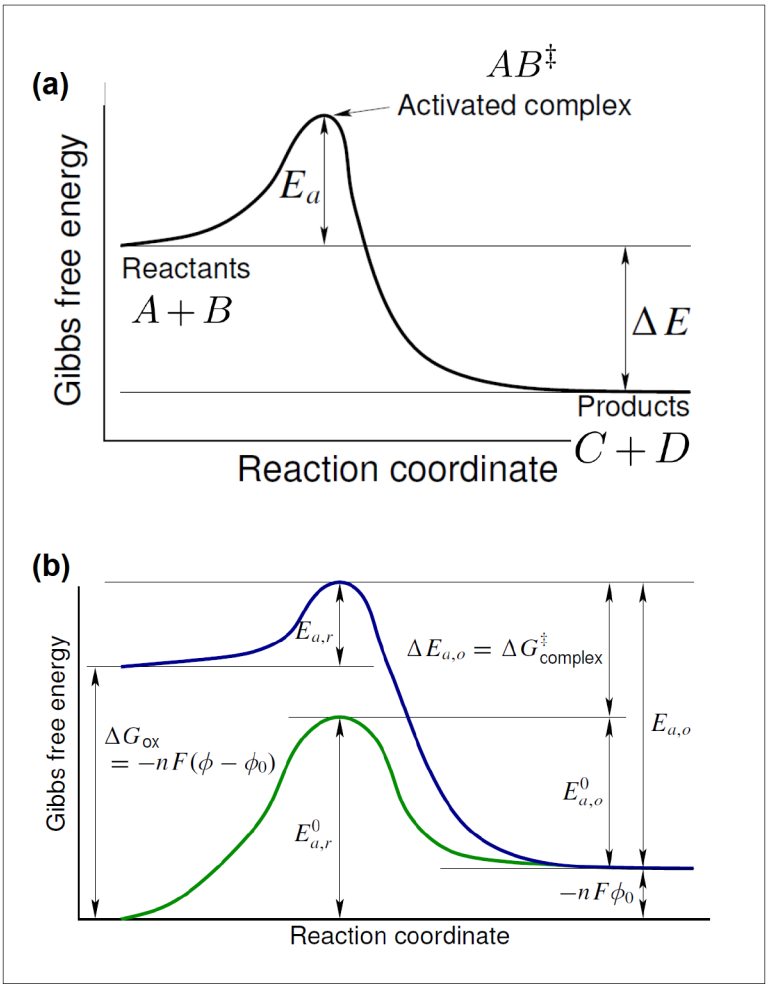


Figure G-1 (a) The formation of activated complex, $AB^{\ddagger}$, in a chemical reaction: A and B have to overcome the activation energy, E_a, to reach C and D. (b) The changes in the Gibbs free energy in the electrochemical oxidation and reduction reaction as a function of electrode potentials. Reproduced with permissions from Ref. 420.

$$A + B \underset{E_{a,2}}{\overset{E_{a,1}}{\rightleftharpoons}} AB^{\ddagger} \underset{E_{a,4}}{\overset{E_{a,3}}{\rightleftharpoons}} C + D \tag{G-1}$$

An electrochemical reaction occurs at the electrode-electrolyte interface, and electrons are produced or consumed:

$$\text{oxidant} + ne^{-} \underset{E_{a,o}}{\overset{E_{a,r}}{\rightleftharpoons}} \text{reductant}, \tag{G-2}$$

where $E_{a,r}$ represents the reduction activation energy and $E_{a,o}$ denotes the oxidation activation energy. Unlike other types of chemical reactions, the activation energies of an electrochemical reaction depend on the electrode potential (Figure G-1b).

The Butler-Volmer (BV) equation can be derived considering an electrochemical reduction, where the initial electrode potential is ϕ_0 and the activation energy for reduction is $E^0_{a,r}$. When an electric field is applied, the initial electrode potential, ϕ_0 is changed to ϕ, thereby altering the initial state of Gibb's free energy, ΔG_{ox}:

$$\Delta G_{ox} = -nF(\phi - \phi_0). \tag{G-3}$$

From Figure G-1b, one can deduce that

$$E_{a,r} - nF(\phi - \phi_0) = \Delta E_{a,o} + E^0_{a,r}. \tag{G-4}$$

Equation G-4 can be rearranged by grouping the reduction activation energy together:

$$\begin{aligned} \Delta E_{a,o} &= E_{a,r} - E^0_{a,r} - nF(\phi - \phi_0), \\ &= \Delta E_{a,r} - nF(\phi - \phi_0), \end{aligned} \tag{G-5}$$

where

$$\Delta E_{a,r} \equiv E_{a,r} - E^0_{a,r}. \tag{G-6}$$

The charge transfer coefficient, α denotes the fraction of the applied potential that promotes the reduction, whereas $1-\alpha$ is the fraction of the applied potential that favours the oxidation. These coefficients can be defined as follows:

$$\alpha = \left| \frac{\Delta E_{\mathrm{a,r}}}{\Delta G_{\mathrm{ox}}} \right|, \tag{G-7}$$

$$1 - \alpha = \left| \frac{\Delta E_{\mathrm{a,o}}}{\Delta G_{\mathrm{ox}}} \right|. \tag{G-8}$$

Therefore, the reduction activation energy, $\Delta E_{\mathrm{a,r}}$, and the oxidation activation energy, $\Delta E_{\mathrm{a,o}}$, can be given by

$$\begin{aligned} \Delta E_{\mathrm{a,r}} &= \alpha n F(\phi - \phi_0), \\ \Delta E_{\mathrm{a,o}} &= -(1-\alpha) n F(\phi - \phi_0). \end{aligned} \tag{G-9}$$

The rate of reaction, r_{red}, can be expressed as a function of concentration species, electrode potentials and temperature:

$$\begin{aligned} r_{\mathrm{red}} &= k^0_{\mathrm{ox}} c_{\mathrm{ox}} \exp\left(-\frac{E_{\mathrm{a,r}}}{R_{\mathrm{gas}} T} \right), \\ &= k^0_{\mathrm{ox}} c_{\mathrm{ox}} \exp\left(-\frac{E^0_{\mathrm{a,r}} + \alpha n F(\phi - \phi_0)}{R_{\mathrm{gas}} T} \right), \end{aligned} \tag{G-10}$$

where $E_{\mathrm{a,r}}$ is given by Equation G-6 and Equation G-9. Similarly, r_{ox} is defined by

$$\begin{aligned} r_{\mathrm{ox}} &= k^0_{\mathrm{red}} c_{\mathrm{red}} \exp\left(-\frac{E_{\mathrm{a,o}}}{R_{\mathrm{gas}} T} \right), \\ &= k^0_{\mathrm{red}} c_{\mathrm{red}} \exp\left(-\frac{E^0_{\mathrm{a,o}} - (1-\alpha) n F(\phi - \phi_0)}{R_{\mathrm{gas}} T} \right). \end{aligned} \tag{G-11}$$

According to the Faraday's law, the rate of reaction is equal to the current ($i_{\mathrm{n}} = nF r_{\mathrm{n}}$). Therefore, the reduction and oxidation current densities (i_{red} and i_{ox}) become

$$\begin{aligned} i_{\mathrm{red}} &= -nF r_{\mathrm{red}}, \\ &= -nF k^0_{\mathrm{ox}} c_{\mathrm{ox}} \exp\left(-\frac{E^0_{\mathrm{a,r}} + \alpha n F(\phi - \phi_0)}{R_{\mathrm{gas}} T} \right). \end{aligned} \tag{G-12}$$

$$
\begin{aligned}
i_{\mathrm{ox}} &= nFr_{\mathrm{ox}}, \\
&= nFk^0_{\mathrm{red}}c_{\mathrm{red}}\exp\left(-\frac{E^0_{\mathrm{a,o}}-(1-\alpha)nF(\phi-\phi_0)}{R_{\mathrm{gas}}T}\right).
\end{aligned} \tag{G-13}
$$

By defining the initial potential, ϕ_0 as zero, Equation G-12 and Equation G-13 become

$$
\begin{aligned}
i_{\mathrm{red}} &= -nFk^0_{\mathrm{ox}}c_{\mathrm{ox}}\exp\left(-\frac{E^0_{\mathrm{a,r}}+\alpha nF\phi}{R_{\mathrm{gas}}T}\right), \\
i_{\mathrm{ox}} &= nFk^0_{\mathrm{red}}c_{\mathrm{red}}\exp\left(-\frac{E^0_{\mathrm{a,o}}-(1-\alpha)nF\phi}{R_{\mathrm{gas}}T}\right).
\end{aligned} \tag{G-14}
$$

The cell potential at equilibrium is equal to the rest potential ($\phi=\phi_{\mathrm{rest}}$), whereas the potential under load can be defined in terms of overpotential ($\eta=\phi-\phi_{\mathrm{rest}}$). Hence, i_{red} and i_{ox} under load can be reformulated to be

$$
\begin{aligned}
i_{\mathrm{red}} &= -nFk^0_{\mathrm{ox}}c_{\mathrm{ox}}\exp\left(-\frac{E^0_{\mathrm{a,r}}+\alpha nF(\phi_{\mathrm{rest}}+\eta)}{R_{\mathrm{gas}}T}\right), \\
&= -nFk^0_{\mathrm{ox}}c_{\mathrm{ox}}\exp\left(-\frac{E^0_{\mathrm{a,r}}+\alpha nF\phi_{\mathrm{rest}}+\alpha nF\eta}{R_{\mathrm{gas}}T}\right), \\
i_{\mathrm{ox}} &= nFk^0_{\mathrm{red}}c_{\mathrm{red}}\exp\left(-\frac{E^0_{\mathrm{a,o}}-(1-\alpha)nF(\phi_{\mathrm{rest}}+\eta)}{R_{\mathrm{gas}}T}\right), \\
&= nFk^0_{\mathrm{red}}c_{\mathrm{red}}\exp\left(-\frac{E^0_{\mathrm{a,o}}-(1-\alpha)nF\phi_{\mathrm{rest}}-(1-\alpha)nF\eta}{R_{\mathrm{gas}}T}\right).
\end{aligned} \tag{G-15}
$$

At equilibrium, there is no overpotential and current densities such that $\eta=0$ and $i=i_{\mathrm{ox}}+i_{\mathrm{red}}=0$. As a result, i_{red} and i_{ox} become

$$
\begin{aligned}
i_{\mathrm{red}} &= -nFk^0_{\mathrm{ox}}c_{\mathrm{ox}}\exp\left(-\frac{E^0_{\mathrm{a,r}}}{R_{\mathrm{gas}}T}\right)\exp\left(-\frac{\alpha nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}\right), \\
i_{\mathrm{ox}} &= nFk^0_{\mathrm{red}}c_{\mathrm{red}}\exp\left(-\frac{E^0_{\mathrm{a,o}}}{R_{\mathrm{gas}}T}\right)\exp\left(\frac{(1-\alpha)nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}\right).
\end{aligned} \tag{G-16}
$$

Under this condition, the exchange current densities, i_0, can be defined as the current density, at which the rate of reduction is equal to the rate of oxidation ($i_0=i_{\mathrm{ox}}=-i_{\mathrm{red}}$):

$$
\begin{aligned}
i_0 &= nFk^0_{\mathrm{ox}}c_{\mathrm{ox}}\exp\left(-\frac{E^0_{\mathrm{a,r}}}{R_{\mathrm{gas}}T}\right)\exp\left(-\frac{\alpha nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}\right),\\
&= nFk^0_{\mathrm{red}}c_{\mathrm{red}}\exp\left(-\frac{E^0_{\mathrm{a,o}}}{R_{\mathrm{gas}}T}\right)\exp\left(\frac{(1-\alpha)nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}\right).
\end{aligned}
\tag{G-17}
$$

By substituting Equation G-17 into Equation G-15, i_{red} and i_{ox} can be simplified into

$$
\begin{aligned}
i_{\mathrm{red}} &= -i_0\exp\left(-\frac{\alpha nF\eta}{R_{\mathrm{gas}}T}\right),\\
i_{\mathrm{ox}} &= i_0\exp\left(\frac{(1-\alpha)nF\eta}{R_{\mathrm{gas}}T}\right).
\end{aligned}
\tag{G-18}
$$

Then, the total electrode current density becomes

$$
\begin{aligned}
i &= i_{\mathrm{ox}} + i_{\mathrm{red}},\\
&= i_0\left[\exp\left(\frac{(1-\alpha)nF\eta}{R_{\mathrm{gas}}T}\right) - \exp\left(\frac{-\alpha nF\eta}{R_{\mathrm{gas}}T}\right)\right].
\end{aligned}
\tag{G-19}
$$

Equation G-19 is the Butler-Volmer's equation, which describes the dependence of the total current densities as a function of concentration species, temperature and electrode potential. An oxidation reaction is also an anodic electrochemical reaction such that $(1-\alpha)$ can be rewritten as α_{a}, whereas α in the cathodic reduction can be represented by α_{c}. For a monovalent electrochemical cell such as Li-ion, $n = 1$. Therefore, the BV-Equation can be finally expressed by[†]

$$
i = i_0\left[\exp\left(\frac{\alpha_{\mathrm{a}}F\eta}{R_{\mathrm{gas}}T}\right) - \exp\left(\frac{-\alpha_{\mathrm{c}}F\eta}{R_{\mathrm{gas}}T}\right)\right].
\tag{G-20}
$$

[†]Part of these derivations were adapted and reproduced with permissions from Plett and Xue.[420]

G.2 Derivations of the Nernst's equation

By defining $\xi^0_{\mathrm{a,r}}$ and $\xi^0_{\mathrm{a,o}}$ as

$$\begin{aligned}\xi^0_{\mathrm{a,r}} &= \exp\left(-\frac{E^0_{\mathrm{a,r}}}{R_{\mathrm{gas}}T}\right),\\ \xi^0_{\mathrm{a,o}} &= \exp\left(-\frac{E^0_{\mathrm{a,o}}}{R_{\mathrm{gas}}T}\right),\end{aligned} \tag{G-21}$$

the exchange current densities at equilibrium, i_0, given by Equation G-17 can be reformulated to

$$nFk^0_{\mathrm{red}}c_{\mathrm{red}}\xi^0_{\mathrm{a,o}}\exp\left(\frac{(1-\alpha)nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}\right) = nFk^0_{\mathrm{ox}}c_{\mathrm{ox}}\xi^0_{\mathrm{a,r}}\exp\left(-\frac{\alpha nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}\right). \tag{G-22}$$

By grouping the exponential terms, Equation G-22 can be written as

$$\frac{\exp\left(\frac{(1-\alpha)nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}\right)}{\exp\left(-\frac{\alpha nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}\right)} = \frac{k^0_{\mathrm{ox}}c_{\mathrm{ox}}\xi^0_{\mathrm{a,r}}}{k^0_{\mathrm{red}}c_{\mathrm{red}}\xi^0_{\mathrm{a,o}}}, \tag{G-23}$$

Equation G-23 can be further simplified to

$$\begin{aligned}\frac{(1-\alpha)nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T} + \frac{\alpha nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T} &= \ln\left(\frac{k^0_{\mathrm{ox}}c_{\mathrm{ox}}\xi^0_{\mathrm{a,r}}}{k^0_{\mathrm{red}}c_{\mathrm{red}}\xi^0_{\mathrm{a,o}}}\right),\\ \frac{nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T} - \cancel{\frac{\alpha nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}} + \cancel{\frac{\alpha nF\phi_{\mathrm{rest}}}{R_{\mathrm{gas}}T}} &= \ln\left(\frac{k^0_{\mathrm{ox}}\xi^0_{\mathrm{a,r}}}{k^0_{\mathrm{red}}\xi^0_{\mathrm{a,o}}}\right) + \ln\left(\frac{c_{\mathrm{ox}}}{c_{\mathrm{red}}}\right).\end{aligned} \tag{G-24}$$

Therefore, ϕ_{rest} can be given by[†]

$$\phi_{\mathrm{rest}} = \underbrace{\frac{R_{\mathrm{gas}}T}{nF}\ln\left(\frac{k^0_{\mathrm{ox}}\xi^0_{\mathrm{a,r}}}{k^0_{\mathrm{red}}\xi^0_{\mathrm{a,o}}}\right)}_{\phi^0_{\mathrm{ref}}} + \frac{R_{\mathrm{gas}}T}{nF}\ln\left(\frac{c_{\mathrm{ox}}}{c_{\mathrm{red}}}\right). \tag{G-25}$$

Equation G-25 is the Nernst's equation derived from the exchange current densities under equilibrium, which describes the concentration dependence of the rest potential.

[†]Part of these derivations were adapted and reproduced with permissions from Plett and Xue.[420]

G.3 Derivations of the linear Butler-Volmer's equation

When the overpotential is small such that η is smaller than $R_{\text{gas}}T/F$, the BV expression given by Equation G-20 can be linearised. In general, the Taylor series of an exponential term is

$$\exp x = \sum_{k=0}^{\infty} \frac{x^k}{k!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \cdots + \frac{x^n}{n!}. \tag{G-26}$$

For small overpotentials, higher orders in the exponential series can be neglected such that the exponential terms in Equation G-20 can be rewritten as

$$\begin{aligned} \exp\underbrace{\left(\frac{\alpha_{\text{a}} F\eta}{R_{\text{gas}}T}\right)}_{x} &= 1 + \frac{\alpha_{\text{a}} F\eta}{R_{\text{gas}}T}, \\ \exp\underbrace{\left(-\frac{\alpha_{\text{c}} F\eta}{R_{\text{gas}}T}\right)}_{x} &= 1 - \frac{\alpha_{\text{c}} F\eta}{R_{\text{gas}}T}. \end{aligned} \tag{G-27}$$

By substituting Equation G-27 into Equation G-20, the total current densities become

$$\begin{aligned} i &= i_{\text{ox}} + i_{\text{red}}, \\ &= i_0 \left[\left(1 + \frac{\alpha_{\text{a}} F\eta}{R_{\text{gas}}T}\right) - \left(1 - \frac{\alpha_{\text{c}} F\eta}{R_{\text{gas}}T}\right) \right], \\ &= i_0 \left[\frac{(\alpha_{\text{a}} + \alpha_{\text{c}}) F\eta}{R_{\text{gas}}T} \right]. \end{aligned} \tag{G-28}$$

Equation G-28 is the linearised BV-Equation, which is used in Chapter 4 of this thesis to represent the electrode kinetics at the NE-SE interface.

G.4 Derivations of the cathodic Tafel's equation

For a large charge-transfer overpotential, the forward reaction can be considered irreversible. The oxidative contribution to the reversible kinetics given by Equation G-20 can be neglected. Under such condition, the BV-Equation can be reformulated to

$$
\begin{aligned}
i &= i_0 \left[\cancel{\exp\left(\frac{\alpha_a F \eta}{R_{gas} T}\right)} - \exp\left(\frac{-\alpha_c F \eta}{R_{gas} T}\right) \right], \\
&= -i_0 \exp\left(\frac{-\alpha_c F \eta}{R_{gas} T}\right).
\end{aligned} \tag{G-29}
$$

Equation G-29 is the cathodic Tafel's equation, which is used in this thesis to represent the charge-transfer kinetics at the PE-SE interface. From a theoretical point of view, the charge-transfer at the PE-SE interface can also be considered a function of the surface diffusion. This consideration implies that the available sites for a charge-transfer's occurrence depend on how fast the intercalated atoms diffuse into the bulk PE. Therefore, a concentration-dependent term is added into Equation G-29 to give

$$
i = -i_{0,pos} \left(\frac{c_{Li,surf}}{c_{bulk}}\right) \exp\left(\frac{-\alpha_c F \eta}{R_{gas} T}\right), \tag{G-30}
$$

where $c_{Li,surf}$ is the surface Li concentration and c_{bulk} represents the bulk Li concentration within the PE.

G.5 Derivations of Nernst-Einstein's equation

As shown by the top-left panel of Figure 5.1, the electrolyte conductivity is caused by the mobility of all ions under the influence of an applied electric field. The movement of the ion is caused by the forward electric force and counterbalanced by a backward viscous force:

$$\underbrace{6\pi\eta_{\mathrm{v}} r v}_{\text{Viscous force}} = \underbrace{zeE_{\mathrm{F}}}_{\text{Electric force}}, \tag{G-31}$$

in which ze is the charge of each ion; E_{F} is the applied electric field between two electrodes; r is the radius of the particle, η_{v} is the dynamic viscosity of the fluid, and v is the velocity vector of the single-particle. The dynamic viscosity given in the viscous force is a measure of the fluid resistance to flow. Under dynamic equilibrium, the drift velocity of the ion becomes

$$v = \underbrace{\frac{ze}{6\pi\eta_{\mathrm{v}} r}}_{u} E_{\mathrm{F}}, \tag{G-32}$$

where the fraction before E_{F} is known as the proportionality coefficient between the velocity and electric field strength, u. The flux of the ion can be described by

$$j = zevcN_{\mathrm{A}}, \tag{G-33}$$

in which cN_{A} is the numerical ion density. For one mole of electrons, $F_{\acute{e}} = eN_{\mathrm{A}}$.* Therefore, Equation G-33 can be reformulated to

$$\begin{aligned} j &= zvcF_{\acute{e}}, \\ &= zcF_{\acute{e}} u E_{\mathrm{F}}, \end{aligned} \tag{G-34}$$

where $v = uE_{\mathrm{F}}$ is given by Equation G-32.

As shown by Figure **??**, the current, I that passes between two parallel electrodes of area A is related to the flux of charge, j, and to the potential difference between them, $\Delta\phi$:

Part of this section has been accepted for publication in M.-C. Pang, M. Marinescu, H. Wang and G. J. Offer. Physical Chemistry Chemical Physics: PCCP (2021).

*$F_{\acute{e}}$ in this subsection represents the Faraday's constant to distinguish from the force, $\overrightarrow{F}$.

$$I = jA = \sigma_{\text{elec}} \underbrace{\frac{\Delta\phi}{d}}_{\equiv E_{\text{F}}} A = \sigma_{\text{elec}} E_{\text{F}} A, \tag{G-35}$$

where σ_{elec} is the electrolyte conductivity, $\Delta\phi$ is the potential difference, d is the distance between two parallel electrodes and A is the electrode surface area.

By evaluating Equation G-34 and Equation G-35 together

$$j = \sigma_{\text{elec}} \cancel{E_{\text{F}}} = zcF_{\acute{e}} u \cancel{E_{\text{F}}}, \tag{G-36}$$

the electrolyte conductivity of each ion i can be expressed as

$$\sigma_{\text{elec},i} = z_i c_i u_i F_{\acute{e}}. \tag{G-37}$$

Therefore, the molar conductivity of the ion, λ_i, becomes

$$\lambda_i = \frac{\sigma_{\text{elec},i}}{c_i} = z_i u_i F_{\acute{e}}. \tag{G-38}$$

For a sufficiently dilute solute, i, the chemical potential gradient, $\mu_{\text{chem},i}$, due to concentration gradient can be described by

$$\mu_{\text{chem},i} = \mu^0_{i,\text{chem,ref}} + R_{\text{gas}} T \ln c_i. \tag{G-39}$$

When Equation G-39 is differentiated with respect to distance, one would obtain

$$\left(\frac{\partial \mu_{\text{chem},i}}{\partial x}\right)_{\text{P,T}} = \frac{R_{\text{gas}} T}{c_i} \left(\frac{\partial c_i}{\partial x}\right)_{\text{P,T}}. \tag{G-40}$$

Therefore, the diffusive force experienced by particle i becomes

$$\overrightarrow{F} = -\left(\frac{\partial \mu_{\text{chem},i}}{\partial x}\right)_{\text{P,T}} = -\frac{R_{\text{gas}} T}{c_i} \left(\frac{\partial c_i}{\partial x}\right)_{\text{P,T}}. \tag{G-41}$$

For one mole of electrons, the flux of ions i, J_i, is

$$\begin{aligned} J_i &= \frac{j_i}{z_i e}, \\ &= c_i u_i E_{\mathrm{F}}. \end{aligned} \tag{G-42}$$

Given that $E_{\mathrm{F}} = \overrightarrow{F}/z_i e$ from Figure **??**, Equation G-42 can also be rewritten as

$$J_i = \frac{c_i u_i \overrightarrow{F}}{z_i e}. \tag{G-43}$$

After substituting Equation G-41 into Equation G-43, J_i becomes

$$\begin{aligned} J_i &= \frac{\cancel{c_i} u_i}{z_i e}\left[-\frac{R_{\mathrm{gas}} T}{\cancel{c_i}}\left(\frac{\partial c_i}{\partial x}\right)\right], \\ &= -\frac{u_i R_{\mathrm{gas}} T}{z_i F_{\acute{e}}}\left(\frac{\partial c_i}{\partial x}\right), \end{aligned} \tag{G-44}$$

By comparing Equation G-44 with Fick's first law of diffusion:

$$J_i = -D_i\left(\frac{\partial c_i}{\partial x}\right), \tag{G-45}$$

the diffusion coefficient, D_i can be written as

$$D_i = \frac{R_{\mathrm{gas}} T}{z_i F_{\acute{e}}} u_i. \tag{G-46}$$

This is Einstein's equation, which relates the diffusion coefficient of species i to its proportionality coefficient, u_i. From Equation G-32, one can see that u_i depends on the dynamic viscosity of the fluid, η_{v} and radius of the particle, r. Einstein[376] first developed the theory of Brownian movement to describe the movement of a single suspended particle in a liquid with a viscosity coefficient of η_{v}.

By rearranging Equation G-46 to be

$$u_i = \frac{D_i z_i F_{\acute{e}}}{R_{\mathrm{gas}} T}, \tag{G-47}$$

and substituting into Equation G-38, the relationship between equivalent electrolyte molar conductivity, λ_i and diffusion coefficient, D_i can be obtained:

$$\begin{aligned} \lambda_i &= z_i F_{\acute{e}} \left[\frac{D_i z_i F_{\acute{e}}}{R_{\text{gas}} T} \right], \\ &= \frac{z_i^2 F_{\acute{e}}^2 D_i}{R_{\text{gas}} T}. \end{aligned} \tag{G-48}$$

This is the Nernst-Einstein's relation, which is frequently used to correlate the relationship between electrolyte conductivity and ionic diffusion coefficient for a wide range of electrolytes. In the literature, λ_i is sometimes written as σ_i to represent the electrolyte conductivity.

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Figure 1.4	National Transportation Safety Board (NTSB) [12]	NTSB	Yes
Figure 1.5 and Figure 1.8	Li, Ma, Chi, Liang, and Dudney [11]	John Wiley and Sons	Yes
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Figure 2.1 and Figure 2.7c,d	Lewis, Cortes, Boebinger, Tippens, Marchese, Kondekar, Liu, Chi, and McDowell [33]	American Chemical Society	Yes
Figure 2.1	Yu, Bates, Jellison Jr., and Hart [34]	The Electrochemical Society	Yes
Figure 2.1 and Figure 2.5	Yu, Taha, Thompson, Taylor, Drews, Sakamoto, and Thornton [36]	Elsevier	Yes
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Figure 2.11d, e	Zhang, Leichtweiß, Culver, Koerver, Das, Weber, Zeier, and Janek[119]	American Chemical Society	Yes
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Figure F-4d	Larfaillou, Guy-Bouyssou, Le Cras, and Franger[63]	Elsevier	Yes
Figure F-6	Schichlein, Müller, Voigts, Krügel, and Ivers-Tiffée[313]	Journal of Applied Electrochemistry	Yes
Figure F-7	Wan, Saccoccio, Chen, and Ciucci[315]	Elsevier	Yes
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Author: Anja Bielefeld, Dominik A. Weber, Jürgen Janek
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Author: Wenbo Zhang, Thomas Leichtweiß, Sean P. Culver, et al

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Author: Marm B. Dixit, Ankit Verma, Wahid Zaman, et al
Publication: ACS Applied Energy Materials
Publisher: American Chemical Society
Date: Oct 1, 2020

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Effect of Surface Microstructure on Electrochemical Performance of Garnet Solid Electrolytes

Author: Lei Cheng, Wei Chen, Martin Kunz, et al

Publication: Applied Materials

Publisher: American Chemical Society

Date: Jan 1, 2015

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Author: Abhik Banerjee, Xuefeng Wang, Chengcheng Fang, et al

Publication: Chemical Reviews

Publisher: American Chemical Society

Date: Jul 1, 2020

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Fabrication, Testing, and Simulation of All-Solid-State Three-Dimensional Li-Ion Batteries

Author: A. Alec Talin, Dmitry Ruzmetov, Andrei Kolmakov, et al

Publication: Applied Materials

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Publication: ACS Energy Letters

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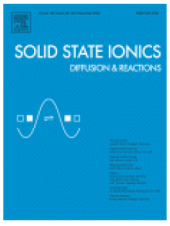
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In situ Raman spectroscopy of Li x CoO2 cathode in Li/Li3PO4/LiCoO2 all-solid-state thin-film lithium battery

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Author: Kikuko Hayamizu, Yuichi Aihara, Shigemasa Arai, et al

Publication: The Journal of Physical Chemistry B

Publisher: American Chemical Society

Date: Jan 1, 1999

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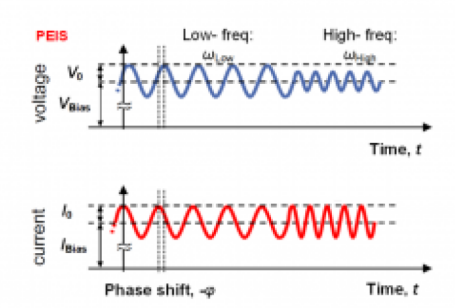
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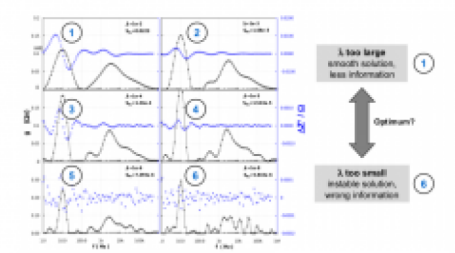
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