

# Contents

<i>Preface</i>	xiii
<i>About the Editor</i>	xv
<i>About the Authors</i>	xvii
<b>1. Fundamental Aspects of Achievable Energy Densities in Electrochemical Cells</b>	<b>1</b>
<i>Kai Peter Birke and Desirée Nadine Schweitzer</i>	
Annex . . . . .	19
A. Specific capacity of each element . . . . .	19
B. Series voltage of each element . . . . .	22
C. Specific energy of each element . . . . .	24
D. Volumetric energy density of each element . . . . .	27
Bibliography . . . . .	30
<b>2. Lithium-ion Cells: Discussion of Different Cell Housings</b>	<b>31</b>
<i>Kai Peter Birke and Shkendije Demolli</i>	
2.1 Cell Housings . . . . .	31
2.2 Cylindrical Cells . . . . .	32
2.3 Prismatic Cells . . . . .	32
2.4 Stabilization of Electrode and Separator Layers . . . . .	35
2.5 Gas Evolution . . . . .	37
2.6 Flexibility with Respect to Cell Size . . . . .	38

2.7	Producing Pouch Cells . . . . .	38
2.8	Status Quo of Cell Concepts . . . . .	39
2.9	Outlook . . . . .	40
	Bibliography . . . . .	41

### **3. Integral Battery Architecture with Cylindrical Cells as Structural Elements 43**

*Christoph Bolsinger, Marcel Berner and Kai Peter Birke*

3.1	State of the Art Battery Systems . . . . .	45
	3.1.1 Block architecture . . . . .	45
	3.1.2 Modular architecture . . . . .	46
	3.1.3 Cell circuitry . . . . .	46
3.2	The Battery Cell as a Structural Element . . . . .	47
	3.2.1 Cylindrical cells . . . . .	48
	3.2.2 Prismatic cells . . . . .	49
	3.2.3 Battery cells as structural elements . . . . .	49
3.3	Construction of the Battery Module . . . . .	51
	3.3.1 Cell connection . . . . .	51
	3.3.2 Moisture proof . . . . .	52
	3.3.3 Lifetime . . . . .	52
	3.3.4 Automotive standards . . . . .	52
	3.3.5 No further load bearing elements . . . . .	53
	3.3.6 Thermal management . . . . .	54
	3.3.7 Safety aspects . . . . .	54
	3.3.8 Scalability . . . . .	55
	3.3.9 Exchangeable single battery cells . . . . .	55
	3.3.10 Gas channels . . . . .	56
3.4	Integrated Cell Supervision Circuit . . . . .	56
	3.4.1 Balancing . . . . .	57
	3.4.2 Mechanical integration . . . . .	58
	3.4.3 Communication . . . . .	58
	3.4.4 Energy saving . . . . .	59
3.5	Cell Connectors . . . . .	60
	3.5.1 State of the art . . . . .	60
	3.5.2 Electrical contact resistance . . . . .	61
	3.5.3 Clamped cell connectors . . . . .	63
	3.5.4 Conclusion . . . . .	65
3.6	Battery Thermal Management . . . . .	66

3.6.1	State of the art . . . . .	67
3.6.1.1	Air cooling for BTM . . . . .	67
3.6.1.2	Liquid cooling for BTM . . . . .	69
3.6.1.3	Phase change materials for BTM . . . . .	70
3.6.1.4	Heat pipe . . . . .	71
3.6.1.5	Thermoelectric cooler (TEC) . . . . .	72
3.6.2	BTM for integral single cell . . . . .	74
3.6.2.1	Non-uniform temperature distribution inside battery cells . . . . .	74
3.6.2.2	Terminal cooling . . . . .	75
	Acknowledgment . . . . .	77
	Bibliography . . . . .	77
<b>4.</b>	<b>Parallel Connection of Lithium-ion Cells — Purpose, Tasks and Challenges</b>	<b>81</b>
	<i>Alexander Fill</i>	
4.1	Introduction . . . . .	81
4.2	Main Issues and Challenges . . . . .	82
4.3	Influences on the Current Distribution . . . . .	83
4.3.1	Simplified model — Analytical solution . . . . .	84
4.3.2	Effects of cell resistance and capacity variations . . . . .	90
4.3.3	Influence of the open circuit voltage bending . . . . .	94
4.4	Thermal Effects . . . . .	97
4.5	Aging . . . . .	98
	Bibliography . . . . .	100
<b>5.</b>	<b>Fundamental Aspects of Reconfigurable Batteries: Efficiency Enhancement and Lifetime Extension</b>	<b>101</b>
	<i>Nejmeddine Bouchhima, Matthias Gossen and Kai Peter Birke</i>	
5.1	Introduction . . . . .	101
5.2	Modeling . . . . .	103
5.2.1	Energy efficiency . . . . .	103
5.2.1.1	Energy loss . . . . .	104
5.2.1.2	Rest energy versus equalization energy . . . . .	104
5.3	Dynamic Optimization Problem . . . . .	105

5.4	Optimal Control . . . . .	107
5.4.1	Vector-based dynamic programming . . . . .	107
5.4.2	Complexity of the control strategy . . . . .	108
5.4.3	Optimal control policy . . . . .	110
5.5	Efficiency Enhancement . . . . .	110
5.5.1	Simulation setup . . . . .	111
5.5.2	Results . . . . .	112
5.6	Lifetime Enhancement . . . . .	114
5.6.1	Aging model . . . . .	115
5.6.2	Results . . . . .	115
5.7	Summary . . . . .	117
	Bibliography . . . . .	118
<b>6.</b>	<b>Volume Strain in Lithium Batteries</b>	<b>121</b>
	<i>Jan Patrick Singer and Kai Peter Birke</i>	
6.1	Introduction . . . . .	121
6.2	Fundamentals of Volume Strain . . . . .	121
6.2.1	Intercalation . . . . .	123
6.2.2	Alloying . . . . .	124
6.2.3	Conversion . . . . .	125
6.3	Volume Strain on Cells Level . . . . .	125
6.4	Volume Strain on Systems Level . . . . .	126
6.5	Measurement Techniques . . . . .	128
6.5.1	Unpressurized . . . . .	130
6.5.2	Pressurized . . . . .	133
6.6	State Diagnostics . . . . .	135
6.6.1	SoH diagnostics . . . . .	135
6.6.2	SoC diagnostics . . . . .	136
	Bibliography . . . . .	138
<b>7.</b>	<b>Every Day a New Battery: Aging Dependence of Internal States in Lithium-ion Cells</b>	<b>141</b>
	<i>Severin Hahn and Kai Peter Birke</i>	
7.1	Operation and Degradation Processes in the Electrode State Diagram . . . . .	141
7.1.1	Introduction . . . . .	141
7.1.2	Absolute potentials and the electrode state diagram . . . . .	142

7.1.3	Charge and discharge . . . . .	144
7.1.4	Charge and discharge limits . . . . .	145
7.1.5	Combined electrode reactions . . . . .	146
7.1.6	Anodic side reactions — Growth of solid electrolyte interface (SEI) . . . . .	148
7.1.7	Cathodic side reactions — Possible formation of solid permeable interface (SPI) . . . . .	151
7.1.8	Transition metal dissolution . . . . .	152
7.1.9	Loss of active material . . . . .	154
7.2	Experimental Verification and Analysis Techniques . . . . .	155
7.2.1	Loss of anode active material . . . . .	156
7.2.2	Loss of active lithium . . . . .	157
7.2.3	Loss of cathode active lithium . . . . .	158
7.2.4	The principle of limitation . . . . .	158
7.2.5	Example of an aged cell . . . . .	159
7.2.6	Inhomogeneities and limitations in real cells . . . . .	160
7.3	Conclusion . . . . .	161
	Bibliography . . . . .	163

## 8. Thermal Propagation 167

*Sascha Koch*

8.1	Introduction . . . . .	167
8.2	Process of Thermal Propagation . . . . .	167
8.2.1	Thermal runaway . . . . .	167
8.2.2	Propagation . . . . .	169
8.2.3	Resulting effects . . . . .	171
8.3	Testing . . . . .	172
8.3.1	Relevance . . . . .	172
8.3.2	Trigger methods . . . . .	172
8.3.3	Measurement equipment and methods . . . . .	174
8.3.4	Experiment setup and conditions . . . . .	177
8.3.5	Analyzing the results . . . . .	178
8.4	Influencing Variables . . . . .	181
8.4.1	Cell format . . . . .	181
8.4.2	Energy density . . . . .	182
8.4.3	System design . . . . .	183
	Bibliography . . . . .	184

<b>9.</b>	<b>Potential of Capacitive Effects in Lithium-ion Cells</b>	<b>187</b>
	<i>Alexander Uwe Schmid and Kai Peter Birke</i>	
9.1	Brief Introduction to the Principles of Electrostatic and Electrochemical Storage . . . . .	187
9.1.1	Double-layer capacitance . . . . .	188
9.1.2	Intercalation . . . . .	190
9.1.3	Pseudocapacitance . . . . .	190
9.2	Similarities and Differences between Capacitors and Lithium-ion Cells . . . . .	191
9.2.1	Carbons as electrode material . . . . .	192
9.2.2	The solid electrolyte interface . . . . .	193
9.2.3	Summary . . . . .	194
9.3	Methods of Measurement of Capacitive Effects . . . . .	195
9.3.1	Electrochemical impedance spectroscopy . . . . .	195
9.3.1.1	Modeling approaches based on equivalent circuit elements . . . . .	196
9.3.2	Cyclic voltammetry . . . . .	203
9.3.3	Current pulse method . . . . .	204
9.3.4	Summary . . . . .	205
9.4	Utilization of Capacitive Effects in Li-ion Cells . . . . .	205
9.4.1	Li-ion cell development . . . . .	205
9.4.2	Li-ion capacitor . . . . .	206
9.4.3	Estimation of DL capacitance on cell level . . . . .	207
9.4.4	Potential on the system level . . . . .	211
9.5	Conclusion and Outlook . . . . .	216
	Nomenclature . . . . .	217
	Bibliography . . . . .	220
<b>10.</b>	<b>Battery Recycling: Focus on Li-ion Batteries</b>	<b>223</b>
	<i>Daniel Horn, Jörg Zimmermann, Andrea Gassmann, Rudolf Stauber and Oliver Gutfleisch</i>	
10.1	Battery Materials and their Supply . . . . .	223
10.2	Motivation for Battery Recycling and Legal Framework in Europe . . . . .	227
10.3	Available Recycling Technologies . . . . .	228
10.3.1	Pre-processing treatments . . . . .	229
10.3.2	Pyro- and hydrometallurgy for extraction . . . . .	231

10.4	Electrohydraulic Fragmentation, an Innovative Recycling Process for Battery Recycling . . . . .	234
10.5	Outlook . . . . .	236
	Bibliography . . . . .	236
<b>11.</b>	<b>Power-to-X Conversion Technologies</b>	<b>239</b>
	<i>Friedrich-Wilhelm Speckmann and Kai Peter Birke</i>	
11.1	Definition of Power-to-X . . . . .	239
11.2	Potential of Cross-Sectoral Applications . . . . .	239
11.3	Power-to-X as a Primary Battery . . . . .	244
11.4	Power-to-Gas . . . . .	244
	11.4.1 Hydrogen generation . . . . .	245
	11.4.2 Electrolytic hydrogen generation . . . . .	245
	11.4.2.1 Thermochemical hydrogen generation . . . . .	248
	11.4.2.2 Photochemical hydrogen generation . . . . .	249
	11.4.3 Methanation . . . . .	250
	11.4.3.1 Catalytic/chemical methanation . . . . .	250
	11.4.3.2 Biological methanation . . . . .	251
	11.4.3.3 Plasma-based methanation . . . . .	251
11.5	Power-to-Liquid . . . . .	252
	11.5.1 Technological overview . . . . .	252
	11.5.2 Carbon sources . . . . .	255
11.6	Power-to-Solid . . . . .	256
11.7	Basic Gas Management Systems . . . . .	258
11.8	Sustainable Energy Chains — Closing Remarks . . . . .	259
	Bibliography . . . . .	260
	<i>Epilogue</i>	263
	<i>Acknowledgments</i>	275
	<i>Index</i>	277