Contents

	Page
Preface	i
Using Quantum Chemistry to Determine Electrochemical Potential Dependencies of Adsorbate Properties and Redox Activation Energies A. Anderson	1
Molecular Simulation Techniques K.-Y. Chan	8
The Potential Distribution at the Semiconductor/Solution Interface P. Searson	24
A Semi-Analytical Method for Predicting Current and Potential Distributions V. Subramanian & R. White	36
Mathematical Modeling of Localized Corrosion Processes K. Hebert	54
Tutorial: Application of Mathematical Models for Interpretation of Impedance Spectra M. Orazem	68
Separation of Variables for Diffusion in Composite Electrodes with Flux Boundary Conditions V. Subramanian & R. White	100
Mathematical Modeling of Electrodeposition Processes for ULSI Copper-Interconnect Technology A. West, A. Shehata & V. Modi	114
Computational Aspects of the Terminal Effect on Wafer-Scale Uniformity H. Deligianni, J. Dukovic & S. Mehdizadeh	124
Progress in the Modeling of Cylindrical Alkaline Cells H. Cheh & Y. Zhang	141
Mathematical Modeling of the Electrochemical Impedance Response of Batteries M. Doyle & J. Newman	144
Use of a Fundamentally Based Lead-Acid Battery Model in Hybrid Vehicle Simulations J. Harb	163
Mathematical Analysis of Transport in Ion-Exchange Membranes P. Pintauro & Y. Yang	178
Electrolyte Migration in Fuel Cell Modeling H. Kunz	191
Applications of AC Impedance to Fuel Cell Modeling T. Springer	208
Modeling Two-Phase Flow in the Porous Electrodes of Proton Exchange Membrane T. Nguyen	222
NL3BO, A Framework for Electrochemical Systems R. Spotnitz	242

Page

Development of Multi-Disciplinary Simulation Tools for Electrochemical Systems
A. Krishnan & M. Giridharan..... 250

Parameter Estimation and Electrochemical Reactor Optimization Using Fundamental Electrochemical Engineering Models
R. Venkataraman, L. Achenie & J. Fenton..... 261

Effect of Operating Conditions on Water Transport in PEM Anhydrous HCl Electrolyzers
S. Motupally, A. Becker & J. Weidner..... 280

Multiscale Modeling in Plasma Engineering and Parallels to Electrochemical Engineering
D. Economou..... 296

Subject Index..... 303