MODERN ASPECTS OF ELECTROCHEMISTRY

No. 43

Modern Aspects of Electrochemistry

Topics in Number 42 include:

- The electrochemistry and electrocatalysis of Ruthenium in regards to the development of electrodes for Polymer Electrolyte Membrane (PEM) fuel cells
- Breakthroughs in Solid Oxide Fuel Cell (SOFC) anodes and cathodes leading to improved electrocatalysis
- Electrocatalysis of the electrochemical reduction of CO_2 on numerous metals
- The interfacial phenomena of electrodeposition and codeposition, and the need for new theoretical analyses of the electrode-electrolyte interface
- Advantages of scanning tunneling microscopy (STM) in understanding the basics of catalysis, electrocatalysis and electrodeposition
- The role of electrochemistry in emerging technologies including electrodeposition and electroforming at the micro and nano levels, semiconductor and information storage, including magnetic storage devices, and modern medicine

Topics in Number 41 include:

- Solid State Electrochemistry, including the major electrochemical parameters needed for the treatment of electrochemical cells as well as the discussion of electrochemical energy storage and conversion devices such as fuel cells
- Nanoporous carbon and its electrochemical application to electrode materials for super capacitors in relationship to the key role nanoporous carbons have played in the purification of liquids and the storage of energy
- The analysis of variance and covariance in electrochemical science and engineering
- The use of graphs in electrochemical reaction networks, specifically: (1) reaction species graphs, (2) reaction mechanism graphs, and (3) reaction route graphs

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Modeling and Numerical Simulations

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Preface

The present volume is devoted to modeling and numerical simulations in electrochemistry. Such a volume cannot be expected to limit itself to the treatment of topics and systems that narrowly defined the field of electrochemistry in the past. On the contrary, the clear demarcation lines between disciplines have become increasingly less pronounced. This positive development, which is considered by many to be the hallmark of the new century, means that related or neighboring fields are in position to cross-fertilize each other as never before, which will benefit everyone. It is in this light that readers of the present volume should view the eight chapters presented here.

Chapter 1 introduces a discussion of the two tools widely considered to be the most important for modeling. These are the finite element and finite difference methods. Chapter 2, by G. Drake, is an in-depth presentation of modeling in atomic physics. It becomes evident that even for as few as three bodies an analytical treatment is not possible and one must resort to a type of modeling. Chapter 3, by Lasia, treats the modeling of impedance of porous electrodes. Chapter 4 is authored by Kottke, Fedorov and Gole. They treat multi-scale mass transport in porous silicon gas sensors.

The next three chapters deal with modeling in the area of fuel cells. In Chapter 5, Eikerling and Malek take up the issue of electrochemical materials for PEM fuel cells, while in Chapter 6, Meyers models catalyst structure degradation in PEM fuel cells. Chapter 7, which concludes this group of three chapters, presents a thorough discussion by Weber, Balliet, Gunterman, and Newman of modeling water management in PEM fuel cells. Chapter 8, by Verbrugge, deals with modeling of electrochemical energy storage devices for hybrid electric vehicle applications.

Each chapter is self contained and independent of the other chapters, which means that the chapters do not have to be read in consecutive order or as a continuum. Readers who are familiar with the material in certain chapters may skip those chapters and still derive maximum benefit from the chapters they read.

Finally, thanks are due to each of the fifteen authors who helped make the volume possible.

Windsor, Ontario, Canada *Mordechay Schlesinger*

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