Combinatorial Methods for Chemical and Biological Sensors

Integrated Analytical Systems

Series Editor:
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GE Global Research Center
Niskayuna, NY

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Springer

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Series Preface

In my career I've found that "thinking outside the box" works better if I know what's "inside the box."
Dave Grusin, composer and jazz musician

Different people think in different time frames: scientists think in decades, engineers think in years, and investors think in quarters.
Stan Williams, Director of Quantum Science Research, Hewlett Packard Laboratories

Everything can be made smaller, never mind physics;
Everything can be made more efficient, never mind thermodynamics;
Everything will be more expensive, never mind common sense.
Tomas Hirschfeld, pioneer of industrial spectroscopy

Integrated Analytical Systems

Series Editor: Dr. Radislav A. Potyrailo, GE Global Research, Niskayuna, NY

The book series *Integrated Analytical Systems* offers the most recent advances in all key aspects of development and applications of modern instrumentation for chemical and biological analysis. The key development aspects include: (i) innovations in sample introduction through micro- and nano-fluidic designs, (ii) new types and methods of fabrication of physical transducers and ion detectors, (iii) materials for sensors that became available due to the breakthroughs in biology, combinatorial materials science and nanotechnology, and (iv) innovative data processing and mining methodologies that provide dramatically reduced rates of false alarms.

A multidisciplinary effort is required to design and build instruments with previously unavailable capabilities for demanding new applications. Instruments with more sensitivity are required today to analyze ultra-trace levels of environmental pollutants, pathogens in water, and low vapor pressure energetic materials in air. Sensor systems with faster response times are desired to monitor transient in-vivo events and bedside patients. More selective instruments are sought to analyze

specific proteins in vitro and analyze ambient urban or battlefield air. For these and many other applications, new analytical instrumentation is urgently needed. This book series is intended to be a primary source on both fundamental and practical information of where analytical instrumentation technologies are now and where they are headed in the future.

Looking back over peer-reviewed technical articles from several decades ago, one notices that the overwhelming majority of publications on chemical and biological analysis has been related to chemical and biological sensors and has originated from Departments of Chemistry in universities and Divisions of Life Sciences of governmental laboratories. Since then, the number of disciplines involved in this research field has dramatically increased because of the ever-expanding needs for miniaturization (e.g. for in-vivo cell analysis, embedding into soldier uniforms), lower power consumption (e.g. harvested power), and the ability to operate in complex environments (e.g. whole blood, industrial water, or battlefield air) for more selective, sensitive, and rapid determination of chemical and biological species. Compact analytical systems that have a sensor as one of the system components are becoming more important than individual sensors. Thus, in addition to traditional sensor approaches, a variety of new themes have been introduced to achieve an attractive goal of analyzing chemical and biological species on the micro- and nano-scale.

Foreword

Combinatorial Development of Sensing Materials: Where We Are and Where We Are Going

A significant portion of sensor research involves design of new sensing materials. Early sensing schemes were often based on accidental discoveries and labor-intensive rational optimization of materials. In recent years, strategies have changed greatly because rational design often has been complemented by combinatorial approaches. Combinatorial chemistry, initially developed to synthesize large libraries of organic compounds, has experienced a tremendous growth in many respects. In the pharmaceutical industry, thousands or tens of thousands of new compounds are being synthesized and tested daily. It was only a question of time until this technology was transferred to materials research, in particular to the chemistry of organic and inorganic materials for use in sensors. Now, large numbers of different types of such sensing materials can be produced. Once such libraries are available, methods for high-throughput screening of the respective materials have to be found. In fact, development of combinatorial screening tools appears to require a sizable time commitment and effort because each material is likely to be tested for its response to more than just a single analyte. However, as has already been shown by many research groups worldwide, these investments do have significant and fast pay-offs.

This book reflects the exciting developments that have been made in the areas of combinatorial chemistry and high-throughput screening of sensing materials. I have to congratulate the editors for having compiled this book on this extremely timely subject, and the authors for having contributed state-of-the-art chapters to the various sections. This volume will be an invaluable source of information to all scientists and practitioners working in this field.

Regensburg, Germany — Otto S. Wolfbeis

Preface

Sensing materials play a key role in the successful implementation of chemical and biological sensors. The multidimensional nature of the interactions between function and composition, preparation method, and end-use conditions of sensing materials often makes their rational design for real-world applications very challenging. These practical challenges in rational design of sensing materials provide tremendous potential for combinatorial and high-throughput research, which is the applied use of technologies and automation for the rapid synthesis and performance screening of relatively large number of compounds. Ideally, from these experiments, relevant descriptors are determined to understand the details of materials design and to establish quantitative structure–function relationships. This attractive goal has been reached only for a few sensing materials systems. In other cases, empirical screening and simple data mining are being used.

This book is the compilation and critical analysis of work recently performed in research laboratories around the world on the implementation of combinatorial and high-throughput research methodologies for the discovery and optimization of new sensing materials. The book will be of interest to the reader because of its several innovative aspects. First, it provides a detailed description and analysis of strategies for setting up successful processes for screening of sensing materials for both chemical and biological sensors. Second, it summarizes the advances, remaining challenges and suggests the opportunities in combinatorial research in the areas chemical and biosensors based on polymeric, inorganic, biological, and formulated sensing materials. Third, it provides an insight into how to improve the efficiency of the combinatorial screening of sensing materials and generation of new knowledge by combining combinatorial experimentation and advanced data mining techniques.

This book is intended to be a primary source on both fundamental and practical information of where high-throughput analysis technologies are now and where they are headed in the future. It is addressed to the rapidly growing number of active practitioners and those who are interested in starting research in the field of sensing materials for chemical sensors and biosensors, directors of industrial and government research centers, laboratory supervisors and managers, students and lecturers. Combinatorial and high-throughput materials screening approaches

analyzed in this book will be also of interest to researchers from many other fields of experimental science working on materials design. The structure of this book offers a basis for a high-throughput instrumentation course at advanced undergraduate or graduate level.

We thank Ken Howell at Springer for his patience during the implementation of this book project and for encouraging us during the various stages of this project. We express our gratitude to the authors for their efforts in preparing their chapters on time and to the referees for reviewing them. R.A.P. thanks the leadership team at GE Global Research for supporting the whole GE Combinatorial Chemistry effort. V.M.M. is grateful to Prof. O.S. Wolfbeis for initiating the development of combinatorial approaches on discovery and optimization of sensing materials in the University of Regensburg. Last, but not least, we thank our families for their patience and enthusiastic support of this project.

Niskayuna, NY — Radislav A. Potyrailo
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