

传感材料与传感技术丛书

Sensing Material and Sensing Technology Series

# CHEMICAL SENSORS SIMULATION AND MODELING

## Volume 3 Solid-State Devices

EDITED BY GHENADII KOROTCENKOV

影印版

### 化学传感器：仿真与建模

### 第3卷 固态设备

上册



哈尔滨工业大学出版社  
HARBIN INSTITUTE OF TECHNOLOGY PRESS

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# 黑版贸审字08-2014-080号

Ghenadii Korotcenkov

Chemical Sensors : Simulation and Modeling Volume 3 : Solid-State Devices

9781606503157

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Originally published by Momentum Press, LLC

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## 图书在版编目 ( CIP ) 数据

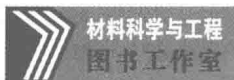
化学传感器: 仿真与建模. 第3卷, 固态设备 = Chemical Sensors : Simulation and Modeling. Volume 3 : Solid-State Devices. 上册: 英文 / ( 摩尔 ) 科瑞特森科韦 ( Korotcenkov, G. ) 主编. —影印本. —哈尔滨: 哈尔滨工业大学出版社, 2015.1

( 传感材料与传感技术丛书 )

ISBN 978-7-5603-4904-6

I. ①化… II. ①科… III. ①化学传感器-研究-英文 ②固态化学-化学传感器-研究-英文  
IV. ①TP212.2

中国版本图书馆CIP数据核字 ( 2014 ) 第242678号



责任编辑 许雅莹 杨 桦 张秀华

出版发行 哈尔滨工业大学出版社

社 址 哈尔滨市南岗区复华四道街10号 邮编 150006

传 真 0451-86414749

网 址 <http://hitpress.hit.edu.cn>

印 刷 哈尔滨市石桥印务有限公司

开 本 787mm × 960mm 1/16 印张 16.75

版 次 2015 年 1 月 第 1 版 2015 年 1 月 第 1 次印刷

书 号 ISBN 978-7-5603-4904-6

定 价 80.00元

( 如因印刷质量问题影响阅读, 我社负责调换 )



## 影印版说明

1. 《传感材料与传感技术丛书》中第一个影印系列 MOMENTUM PRESS 的 *Chemical Sensors: Fundamentals of Sensing Materials & Comprehensive Sensor Technologies* (6 卷, 影印为 10 册) 2013 年出版后, 受到了专家学者的一致好评。为了满足广大读者进一步的教学和科研需要, 本次影印其 *Chemical Sensors: Simulation and Modeling* 系列 (5 卷, 每卷均分为上下册)。本书是第 3 卷 *Solid-State Devices* 的上册 (第 3 卷 1~5 章内容)。

2. 原书的文前介绍、索引等内容在上下册中均完整呈现。

材料科学与工程图书工作室

联系电话 0451-86412421

0451-86414559

邮 箱 yh\_bj@aliyun.com

xuyaying81823@gmail.com

zhxh6414559@aliyun.com

# PREFACE

This series, *Chemical Sensors: Simulation and Modeling*, is the perfect complement to Momentum Press's six-volume reference series, *Chemical Sensors: Fundamentals of Sensing Materials* and *Chemical Sensors: Comprehensive Sensor Technologies*, which present detailed information about materials, technologies, fabrication, and applications of various devices for chemical sensing. Chemical sensors are integral to the automation of myriad industrial processes and everyday monitoring of such activities as public safety, engine performance, medical therapeutics, and many more.

Despite the large number of chemical sensors already on the market, selection and design of a suitable sensor for a new application is a difficult task for the design engineer. Careful selection of the sensing material, sensor platform, technology of synthesis or deposition of sensitive materials, appropriate coatings and membranes, and the sampling system is very important, because those decisions can determine the specificity, sensitivity, response time, and stability of the final device. Selective functionalization of the sensor is also critical to achieving the required operating parameters. Therefore, in designing a chemical sensor, developers have to answer the enormous questions related to properties of sensing materials and their functioning in various environments. This five-volume comprehensive reference work analyzes approaches used for computer simulation and modeling in various fields of chemical sensing and discusses various phenomena important for chemical sensing, such as surface diffusion, adsorption, surface reactions, sintering, conductivity, mass transport, interphase interactions, etc. In these volumes it is shown that theoretical modeling and simulation of the processes, being a basic for chemical sensor operation, can provide considerable assistance in choosing both optimal materials and optimal configurations of sensing elements for use in chemical sensors. The theoretical simulation and modeling of sensing material behavior during interactions with gases and liquid surroundings can promote understanding of the nature of effects responsible for high effectiveness of chemical sensors operation as well. Nevertheless, we have to understand that only very a few aspects of chemistry can be computed exactly.

However, just as not all spectra are perfectly resolved, often a qualitative or approximate computation can give useful insight into the chemistry of studied phenomena. For example, the modeling of surface-molecule interactions, which can lead to changes in the basic properties of sensing materials, can show how these steps are linked with the macroscopic parameters describing the sensor response. Using quantum mechanics calculations, it is possible to determine parameters of the energetic (electronic) levels of the surface, both inherent ones and those introduced by adsorbed species, adsorption complexes, the precursor state, etc. Statistical thermodynamics and kinetics can allow one to link those calculated surface parameters with surface coverage of adsorbed species corresponding to real experimental conditions (dependent on temperature, pressure, etc.). Finally, phenomenological modeling can tie together theoretically calculated characteristics with real sensor parameters. This modeling may include modeling of hot platforms, modern approaches to the study of sensing effects, modeling of processes responsible for chemical sensing, phenomenological modeling of operating characteristics of chemical sensors, etc.. In addition, it is necessary to recognize that in many cases researchers are in urgent need of theory, since many experimental observations, particularly in such fields as optical and electron spectroscopy, can hardly be interpreted correctly without applying detailed theoretical calculations.

Each modeling and simulation volume in the present series reviews modeling principles and approaches particular to specific groups of materials and devices applied for chemical sensing. *Volume 1: Microstructural Characterization and Modeling of Metal Oxides* covers microstructural characterization using scanning electron microscopy (SEM), transmission electron spectroscopy (TEM), Raman spectroscopy, in-situ high-temperature SEM, and multiscale atomistic simulation and modeling of metal oxides, including surface state, stability, and metal oxide interactions with gas molecules, water, and metals. *Volume 2: Conductometric-Type Sensors* covers phenomenological modeling and computational design of conductometric chemical sensors based on nanostructured materials such as metal oxides, carbon nanotubes, and graphenes. This volume includes an overview of the approaches used to quantitatively evaluate characteristics of sensitive structures in which electric charge transport depends on the interaction between the surfaces of the structures and chemical compounds in the surroundings. *Volume 3: Solid-State Devices* covers phenomenological and molecular modeling of processes which control sensing characteristics and parameters of various solid-state chemical sensors, including surface acoustic wave, metal-insulator-semiconductor (MIS), microcantilever, thermoelectric-based devices, and sensor arrays intended for “electronic nose” design. Modeling of nanomaterials and nanosystems that show promise for solid-state chemical sensor design is analyzed as well. *Volume 4: Optical Sensors* covers approaches used for modeling and simulation of various types of optical sensors such as fiber optic, surface plasmon resonance, Fabry-Pérot interferometers, transmittance in the mid-infrared region,

luminescence-based devices, etc. Approaches used for design and optimization of optical systems aimed for both remote gas sensing and gas analysis chambers for the nondispersive infrared (NDIR) spectral range are discussed as well. A description of multiscale atomistic simulation of hierarchical nanostructured materials for optical chemical sensing is also included in this volume. *Volume 5: Electrochemical Sensors* covers modeling and simulation of electrochemical processes in both solid and liquid electrolytes, including charge separation and transport (gas diffusion, ion diffusion) in membranes, proton–electron transfers, electrode reactions, etc. Various models used to describe electrochemical sensors such as potentiometric, amperometric, conductometric, impedimetric, and ion-sensitive FET sensors are discussed as well.

I believe that this series will be of interest of all who work or plan to work in the field of chemical sensor design. The chapters in this series have been prepared by well-known persons with high qualification in their fields and therefore should be a significant and insightful source of valuable information for engineers and researchers who are either entering these fields for the first time, or who are already conducting research in these areas but wish to extend their knowledge in the field of chemical sensors and computational chemistry. This series will also be interesting for university students, post-docs, and professors in material science, analytical chemistry, computational chemistry, physics of semiconductor devices, chemical engineering, etc. I believe that all of them will find useful information in these volumes.

G. Korotcenkov



## ABOUT THE EDITOR

**Ghenadii Korotcenkov** received his Ph.D. in Physics and Technology of Semiconductor Materials and Devices in 1976, and his Habilitate Degree (Dr. Sci.) in Physics and Mathematics of Semiconductors and Dielectrics in 1990. For a long time he was a leader of the scientific Gas Sensor Group and manager of various national and international scientific and engineering projects carried out in the Laboratory of Micro- and Optoelectronics, Technical University of Moldova. Currently, Dr. Korotcenkov is a research professor at the Gwangju Institute of Science and Technology, Republic of Korea.

Specialists from the former Soviet Union know Dr. Korotcenkov's research results in the field of study of Schottky barriers, MOS structures, native oxides, and photoreceivers based on Group III-V compounds very well. His current research interests include materials science and surface science, focused on nanostructured metal oxides and solid-state gas sensor design. Dr. Korotcenkov is the author or editor of 11 books and special issues, 11 invited review papers, 17 book chapters, and more than 190 peer-reviewed articles. He holds 18 patents, and he has presented more than 200 reports at national and international conferences.

Dr. Korotcenkov's research activities have been honored by an Award of the Supreme Council of Science and Advanced Technology of the Republic of Moldova (2004), The Prize of the Presidents of the Ukrainian, Belarus, and Moldovan Academies of Sciences (2003), Senior Research Excellence Awards from the Technical University of Moldova (2001, 2003, 2005), a fellowship from the International Research Exchange Board (1998), and the National Youth Prize of the Republic of Moldova (1980), among others.





# CONTRIBUTORS

**Samir H. Mushrif** (Chapter 1)

Catalysis Centre for Energy Innovation and Department of  
Chemical Engineering  
University of Delaware  
Newark, Delaware 19716, USA

**Gilles H. Peslherbe** (Chapter 1)

Centre for Research in Molecular Modeling and  
Department of Chemistry and Biochemistry  
Concordia University Montréal, Québec, Canada H4B 1R6

**Alejandro D. Rey** (Chapter 1)

Department of Chemical Engineering  
McGill University, Montréal, Québec, Canada H3A 2B2

**Karin Larsson** (Chapter 2)

Department of Chemistry—Ångström Laboratory  
Uppsala University  
753 10 Uppsala, Sweden

**James L. Gole** (Chapter 3)

Schools of Physics and Mechanical Engineering  
Georgia Institute of Technology  
Atlanta, Georgia 30332, USA

**William Laminack** (Chapter 3)

Schools of Physics and Mechanical Engineering  
Georgia Institute of Technology  
Atlanta, Georgia 30332, USA

**Vinod Kumar Khanna** (Chapter 4)

MEMS & Microsensors

CSIR—Central Electronics Engineering Research Institute

Pilani-333031 (Rajasthan), India

**Linfeng Zhang** (Chapter 5)

Department of Electrical Engineering

University of Bridgeport

Bridgeport, Connecticut 06604, USA

**Gerhard Fischerauer** (Chapter 6)

Chair of Metrology and Control Engineering

Universität Bayreuth

95440 Bayreuth, Germany

**Florian Thalmayr** (Chapter 6)

Micro Electro Mechanical Systems Design

Sand 9 Inc.

Cambridge, Massachusetts 02139, USA

**Viatcheslav Barkaline** (Chapter 7)

System Dynamics & Material Mechanics Laboratory

Belarusian National Technical University

Minsk, 220013, Belarus

**Aliaksandr Chashynski** (Chapter 7)

System Dynamics & Material Mechanics Laboratory

Belarusian National Technical University

Minsk, 220013, Belarus

**Sophie Martin** (Chapter 8)

Institut des Matériaux Jean Rouxel (IMN), CNRS

Université de Nantes

44322 Nantes cedex 3, France

**Guy Louarn** (Chapter 8)

Institut des Matériaux Jean Rouxel (IMN), CNRS

Université de Nantes

44322 Nantes cedex 3, France

**Sergi Udina** (Chapter 9)

Departament d'Electrònica

Universitat de Barcelona

08028 Barcelona, Spain

*and*

Artificial Olfaction Group

Institute for Bioengineering of Catalonia (IBEC)

08028 Barcelona, Spain

**Manuel Carmona** (Chapter 9)

Electronics Department

Universitat de Barcelona

08028 Barcelona, Spain

**Carlos Calaza** (Chapter 9)

Instituto de Microelectrónica de Barcelona—Centro Nacional de Microelectrónica (IMB-CNM)

Consejo Superior de Investigaciones Científicas (CSIC)

08193 Barcelona, Spain

**R. D. S. Yadava** (Chapter 10)

Sensors & Signal Processing Laboratory

Department of Physics, Faculty of Science

Banaras Hindu University

Varanasi 221005, India



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