

传感材料与传感技术丛书

Sensing Material and Sensing Technology Series

CHEMICAL SENSORS SIMULATION AND MODELING

Volume I Microstructural Characterization and Modeling of Metal Oxides

EDITED BY GHENADII KOROTCENKOV

影印版

化学传感器：仿真与建模

第1卷 金属氧化物的显微结构表征与建模

上册



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

CHEMICAL SENSORS SIMULATION AND MODELING

Volume I

Microstructural Characterization and
Modeling of Metal Oxides

EDITED BY GHENADII KOROTCENKOV

影印版

化学传感器：仿真与建模

第1卷 金属氧化物的显微结构表征与建模

上册

黑版贸审字08-2014-082号

Ghenadii Korotcenkov

Chemical Sensors : Simulation and Modeling Volume 1 : Microstructural Characterization and Modeling of Metal Oxides

9781606503096

Copyright © 2012 by Momentum Press, LLC

All rights reserved.

Originally published by Momentum Press, LLC

English reprint rights arranged with Momentum Press, LLC through McGraw-Hill Education (Asia)

This edition is authorized for sale in the People's Republic of China only, excluding Hong Kong, Macao SAR and Taiwan.

本书封面贴有McGraw-Hill Education公司防伪标签，无标签者不得销售。
版权所有，侵权必究。

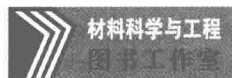
图书在版编目 (CIP) 数据

化学传感器：仿真与建模. 第1卷，金属氧化物的显微结构表征与建模 = Chemical Sensors : Simulation and Modeling. Volume 1 : Microstructural Characterization and Modeling of Metal Oxides. 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 978-7-5603-4900-8

I. ①化… II. ①科… III. ①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242682号



责任编辑 杨 桦 张秀华 许雅莹

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 15.75

版 次 2015年1月第1版 2015年1月第1次印刷

书 号 ISBN 978-7-5603-4900-8

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 1 卷 *Microstructural Characterization and Modeling of Metal Oxides* 的上册 (第 1 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 four-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.

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

Jian Wang (Chapter 1)

Shanghai Applied Radiation Institute
School of Environmental and Chemical Engineering
Shanghai University
Shanghai 200444, People's Republic of China

Zheng Jiao (Chapter 1)

Shanghai Applied Radiation Institute and
Institute of Nanochemistry and Nanobiology
School of Environmental and Chemical Engineering
Shanghai University
Shanghai 200444, People's Republic of China

Minghong Wu (Chapter 1)

Shanghai Applied Radiation Institute and
Institute of Nanochemistry and Nanobiology
School of Environmental and Chemical Engineering
Shanghai University
Shanghai 200444, People's Republic of China

Chan-Hung Shek (Chapter 1)

Department of Physics and Materials Science
City University of Hong Kong
Kowloon Tong, Hong Kong

C. M. Lawrence Wu (Chapter 1)

Department of Physics and Materials Science
City University of Hong Kong
Kowloon Tong, Hong Kong

Joseph K. L. Lai (Chapter 1)
Department of Physics and Materials Science
City University of Hong Kong
Kowloon Tong, Hong Kong

Zhiwen Chen (Chapter 1)
Shanghai Applied Radiation Institute
School of Environmental and Chemical Engineering
Shanghai University
Shanghai 200444, People's Republic of China
and
Department of Physics and Materials Science
City University of Hong Kong
Kowloon Tong, Hong Kong

Hiromi Nakano (Chapter 2)
Cooperative Research Facility Center
Toyohashi University of Technology
Tempaku, Toyohashi, Aichi 441-8580, Japan

Hidehiko Tanaka (Chapter 2)
National Institute for Materials Science
International Center for Materials Nanoarchitectonics
Tsukuba, Ibaraki 305-0044, Japan

Thierry Pagnier (Chapter 3)
Laboratoire d'Electrochimie et de Physicochimie des Matériaux et
Interfaces (LEPMI)
Grenoble Institute of Technology
38402 Saint-Martin-d'Hères, France

J. Daniel Prades (Chapter 4)
Departament d'Electrònica, MIND-IN2UB
Universitat de Barcelona
08028 Barcelona, Spain

Albert Cirera (Chapter 4)
Departament d'Electrònica, MIND-IN2UB
Universitat de Barcelona
08028 Barcelona, Spain

Ghenadii Korotcenkov (Chapter 4)

Department of Material Science and Engineering
Gwangju Institute of Science and Technology
Gwangju, 500-712, Republic of Korea
and

Technical University of Moldova
Chisinau 2004, Republic of Moldova

Beongki Cho (Chapter 4)

Department of Material Science and Engineering and
Department of Nano Bio Materials and Electronics
Gwangju Institute of Science and Technology
Gwangju 500-712, Republic of Korea

Michelle J. S. Spencer (Chapter 5)

Department of Chemistry
La Trobe Institute for Molecular Science
La Trobe University Bundoora, Victoria 3086, Australia
and

Applied Physics, School of Applied Sciences
RMIT University
Victoria 3001, Australia

Lukas Vlcek (Chapter 6)

Chemical Sciences Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831, USA

Panchapakesan Ganesh (Chapter 6)

Center for Nanophase Materials Sciences
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831, USA

Andrei Bandura (Chapter 6)

Department of Quantum Chemistry
The St. Petersburg State University
198504 Petrodvorets, Russia

Eugene Mamontov (Chapter 6)

Chemical & Engineering Materials Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831, USA

Milan Predota (Chapter 6)
Institute of Physics and Biophysics
University of South Bohemia
Ceske Budejovice, 37005 Czech Republic

P. T. Cummings (Chapter 6)
Department of Chemical and Biomolecular Engineering
Vanderbilt University
Nashville, Tennessee 37235, USA
and
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831, USA

D. J. Wesolowski (Chapter 6)
Chemical Sciences Division
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831, USA

Chenggang Zhou (Chapter 7)
Department of Chemistry
National University of Singapore
Singapore 117543
and
Faculty of Materials Science and Chemistry
China University of Geosciences Wuhan
Wuhan 430074, People's Republic of China

Hansong Cheng (Chapter 7)
Department of Chemistry
National University of Singapore
Singapore 117543

Liang Chen (Chapter 8)
Ningbo Institute of Materials Technology and Engineering
Chinese Academy of Sciences
Ningbo 315201, People's Republic of China

Ming Yang (Chapter 8)
Sustainable Energy Laboratory
China University of Geosciences
Wuhan 430074, People's Republic of China

Hansong Cheng (Chapter 8)
Department of Chemistry
National University of Singapore
Singapore 117543

Riccardo Ferrando (Chapter 9)
Dipartimento di Fisica
Università di Genova
16146 Genova, Italy

Alessandro Fortunelli (Chapter 9)
CNR-IPCF
Istituto per i Processi Chimico-Fisici del Consiglio Nazionale delle Ricerche
Pisa 56124, Italy

Shuang Li (Chapter 10)
USTC—CityU Joint Advanced Research Centre
Suzhou 215123, People's Republic of China
and
Department of Physics and Materials Science
City University of Hong Kong
Hong Kong SAR, People's Republic of China

Qing Jiang (Chapter 10)
Key Laboratory of Automobile Materials, Ministry of Education
and
School of Materials Science and Engineering
Jilin University
Changchun 130022, People's Republic of China

Robert Luis González Romero (Chapter 11)
Departamento de Física de la Materia Condensada
Universidad de Sevilla
41080 Sevilla, Spain

Juan José Meléndez Martínez (Chapter 11)
Departamento de Física
Universidad de Extremadura
06006 Badajoz, Spain

Francisco Luis Cumbreña Hernández (Chapter 11)
Departamento de Física de la Materia Condensada
Universidad de Sevilla
41080 Sevilla, Spain

Diego Gómez García (Chapter 11)

Departamento de Física de la Materia Condensada

Universidad de Sevilla

41080 Sevilla, Spain