

传感材料与传感技术丛书

Sensing Material and Sensing Technology Series

CHEMICAL SENSORS SIMULATION AND MODELING

Volume 4 Optical Sensors

EDITED BY GHENADII KOROTCENKOV

影印版

化学传感器：仿真与建模

第4卷 光学传感器

下册



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

CHEMICAL SENSORS SIMULATION AND MODELING

Volume 4

Optical Sensors

EDITED BY **GHENADII KOROTCENKOV**

影印版

化学传感器：仿真与建模

第4卷 光学传感器

下册



哈爾濱工業大學出版社
HARBIN INSTITUTE OF TECHNOLOGY PRESS

黑版贸审字08-2014-079号

Ghenadii Korotcenkov

Chemical Sensors : Simulation and Modeling Volume 4 : Optical Sensors

9781606503188

Copyright © 2013 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

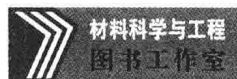
化学传感器: 仿真与建模. 第4卷, 光学传感器 = Chemical Sensors : Simulation and Modeling. Volume 4 : Optical Sensors. 下册: 英文 / (摩尔) 科瑞特森科韦 (Korotcenkov, G.) 主编. —影印本. —哈尔滨: 哈尔滨工业大学出版社, 2015.1

(传感材料与传感技术丛书)

ISBN 978-7-5603-4907-7

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

中国版本图书馆CIP数据核字 (2014) 第244958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 18.5

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

书 号 ISBN 978-7-5603-4907-7

定 价 90.00元



(如因印刷质量问题影响阅读, 我社负责调换)

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 nano-systems 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

Alexander Bagaturyants (Chapter 1)

Photochemistry Center
Russian Academy of Sciences
Moscow 119421, Russia

Michael Alfimov (Chapter 1)

Photochemistry Center
Russian Academy of Sciences
Moscow 119421, Russia

Sergey Belousov (Chapter 2)

NRC Kurchatov Institute
Moscow 123182, Russia
and

Kintech Lab
Moscow 123182, Russia

Ilya Polishchuk (Chapter 2)

NRC Kurchatov Institute
Moscow 123182, Russia

Boris Potapkin (Chapter 2)

NRC Kurchatov Institute
Moscow 123182, Russia
and

Kintech Lab
Moscow 123182, Russia

Stefano Lettieri (Chapter 3)

Institute for Superconductors, Oxides and Innovative Materials and Devices
National Research Council (SPIN-CNR) U.O.S. Napoli
Complesso Universitario di Monte S. Angelo
Napoli I-80126, Italy

Christophe Caucheteur (Chapter 4)

Faculty of Engineering
University of Mons
Mons, Belgium

Marc Debliquy (Chapter 4)

Faculty of Engineering
University of Mons
Mons, Belgium

Gautier Ravet (Chapter 4)

Faculty of Engineering
University of Mons
Mons, Belgium

Driss Lahem (Chapter 4)

Materia Nova
Mons, Belgium

Patrice Megret (Chapter 4)

Faculty of Engineering
University of Mons
Mons, Belgium

Banshi D. Gupta (Chapter 5)

Physics Department
Indian Institute of Technology Delhi
New Delhi 110016, India

Rajan Jha (Chapter 5)

School of Basic Sciences
Indian Institute of Technology Bhubaneswar
Bhubaneswar 751007, Odisha, India

Guy Louarn (Chapter 6)

Institut des Matériaux Jean Rouxel, UMR 6502
CNRS-Université de Nantes
Nantes 44322, France

Malak Kanso (Chapter 6)

Institut des Matériaux Jean Rouxel, UMR 6502
CNRS-Université de Nantes
Nantes 44322, France

Tahereh Makiabadi (Chapter 6)

Institut des Matériaux Jean Rouxel, UMR 6502
CNRS-Université de Nantes
Nantes 44322, France

Zhengtian Gu (Chapter 7)

Laboratory of Photo-electric Functional Films
College of Science, University of Shanghai for Science and Technology
Shanghai 200093, People's Republic of China

Everardo Vargas-Rodriguez (Chapter 8)

Departamento de Estudios Multidisciplinarios
División de Ingenierías, Campus Irapuato-Salamanca
Universidad de Guanajuato
Yuriria, Gto., México

Harvey N. Rutt (Chapter 8)

Optoelectronics Research Centre
University of Southampton, Highfield Campus
Southampton, United Kingdom

David Claudio-Gonzalez (Chapter 8)

Departamento de Estudios Multidisciplinarios
División de Ingenierías, Campus Irapuato-Salamanca
Universidad de Guanajuato
Yuriria, Gto., México

Roberto Rojas-Laguna (Chapter 8)

Departamento de Electrónica
División de Ingenierías, Campus Irapuato-Salamanca
Universidad de Guanajuato, Palo Blanco
Salamanca, Gto., México

Jose Amparo Andrade-Lucio (Chapter 8)

Departamento de Electrónica
División de Ingenierías, Campus Irapuato-Salamanca
Universidad de Guanajuato, Palo Blanco
Salamanca, Gto., México

Andreas Wilk (Chapters 9 and 10)

Institute of Analytical and Bioanalytical Chemistry
University of Ulm
Ulm 89081, Germany

Boris Mizaikoff (Chapters 9 and 10)

Institute of Analytical and Bioanalytical Chemistry
University of Ulm
Ulm 89081, Germany

Xiaofeng Wang (Chapter 10)

Institute of Analytical and Bioanalytical Chemistry
University of Ulm
Ulm 89081, Germany

Seong-Soo Kim (Chapter 10)

Institute of Analytical and Bioanalytical Chemistry
University of Ulm
Ulm 89081, Germany

Ingo Sieber (Chapter 11)

Karlsruhe Institute of Technology
Institute for Applied Computer Science
Eggenstein-Leopoldshafen 76344, Germany

Ulrich Gengenbach (Chapter 11)

Karlsruhe Institute of Technology
Institute for Applied Computer Science
Eggenstein-Leopoldshafen 76344, Germany

Tatsuo Shiina (Chapter 12)

Graduate School of Advanced Integration Science
Chiba University
Chiba 263-8522, Japan

CONTENTS

PREFACE	ix
ABOUT THE EDITOR	xiii
CONTRIBUTORS	xv
7 NOVEL LONG-PERIOD FIBER GRATING SENSOR BASED ON DUAL-PEAK RESONANCE AND SPR	227
<i>Zhengtian Gu</i>	
1 Introduction	227
2 Dual Peak Resonance in Coated LPFG	231
2.1 Coupled Theoretical Analysis of Coated LPFG	231
2.2 Determination of Dual Resonance Wavelengths	232
2.3 Transmission Characteristics of Dual Resonance LPFG	235
3 Model Analysis Of SPR-Based LPFG with Metal Coating	239
3.1 Establishing the Complex Characteristic Equation	241
3.2 Equation Solution Method	243
3.3 Intensity Profile of Cladding Mode	248
4 Optimization of Coated LPFG Sensor Based on DPR and SPR	249
4.1 Definition of Sensor Sensitivity	249
4.2 Optimization of Design of LPFG Sensors	250
5 Dispersion in Metal-Coated LPFG Sensors	255
5.1 Dispersion Expression	255
5.2 Material Dispersion Influence on Resonance Characteristics	257
5.3 Jump Region in Response of Resonance Wavelength	260
5.4 Optimization Based on Consideration of Dispersion	262
6 Conclusion	264
Acknowledgments	266
References	266

8	ANALYTICAL APPROACHES TO OPTIMIZATION OF GAS DETECTION USING FABRY-PÉROT INTERFEROMETERS	271
	<i>E. Vargas-Rodriguez</i>	
	<i>H. N. Rutt</i>	
	<i>D. Claudio-Gonzalez</i>	
	<i>R. Rojas Laguna</i>	
	<i>J. A. Andrade-Lucio</i>	
1	Introduction	271
1.1	Gas Sensor Design	273
2	The Narrow-Gap FPI Gas Sensor	273
2.1	Sensor Response and the Cross-Correlation Spectroscopy Principle	275
2.2	Optimal FPI Mirror Reflectivity	278
2.3	Multiple Gas Sensors Based on the Narrow-Gap Design	279
2.4	Narrow-Gap Sensor Design with a Narrow Band-Pass Filter	281
2.5	Narrow-Gap Sensor Design and MEMS	283
3	The Wide-Gap FPI Gas Sensor	284
3.1	The Convolution Method	286
4	Internal Reflection Effects	300
5	Conclusions	301
	References	302
9	SPECTROSCOPIC MODELING OF MID-INFRARED CHEMICAL SENSORS	305
	<i>A. Wilk</i>	
	<i>B. Mizaikoff</i>	
1	Introduction	305
2	Example #1: Accessing the “Active” Sensing Regions of an ATR Element via Ray Tracing	308
3	Example #2: Sensor Response Simulation—Toward Virtual Calibrations	318
3.1	Experimental Spectra Acquisition	320
3.2	Dielectric Function Modeling	321
3.3	Model Establishment and Validation	324
3.4	Sensor Response Simulation	329
3.5	Spectrum Prediction	336
4	Example #3: Extended Applications	338
4.1	Exploration of the Sources of Deviations in Beer’s Law Plots	338
4.2	Optical Tolerance Study I: Assessing the In-Coupling Ratio—Sharpness of the Focal Point	343

4.3 Optical Tolerance Study II: Mirror Misalignment	343
4.4 Shining Light on Experimentally Challenging Domains: Effects of Displacing the In-Coupling OAPM	345
4.5 Extended Sensor Design Evaluation: Simulation of Complex Objects	347
5 Conclusions and Outlook	353
6 Future Trends	354
Acknowledgments	355
References	355
10 FINITE-ELEMENT MODELING OF INFRARED SENSORS	363
<i>X. Wang</i>	
<i>S.-S. Kim</i>	
<i>A. Wilk</i>	
<i>B. Mizaikoff</i>	
1 Introduction	363
2 Introduction to FEM Modeling Theory	364
2.1 Electromagnetic Wave Equation	364
2.2 Background on FEM	366
3 Near-Infrared Evanescent Field Sensors: From Simulation to Application	375
3.1 Example 1	376
3.2 Example 2	379
4 From Near-Infrared to Mid-Infrared Sensing: Potential and Challenges	380
4.1 Quantum Cascade Lasers—A Revolution in MIR Sensor Technology	381
4.2 Trends in Miniaturization	382
5 Simulation of Mid-Infrared Evanescent Field Waveguides	384
5.1 Planar Waveguides	384
5.2 Strip/Slot Waveguides	392
6 Conclusions and Outlook	400
References	401
11 DESIGN AND OPTIMIZATION OF OPTICAL GAS SENSOR SYSTEMS	405
<i>I. Sieber</i>	
<i>U. Gengenbach</i>	
1 Introduction	405

1.1 Gas Sensing Based on the Lambert-Beer Law	405
1.2 State of the Art of Folded-Optical-Path Gas Sensor Cells	408
1.3 General Setup of Multipass Gas Sensors	412
2 Design of Optical Multipass Gas Sensor Cells	418
2.1 General Introduction to Design Methodology for Optical Multipass Gas Sensor Cells	418
2.2 Design Rules for Optical Multipass Gas Sensor Cells	421
2.3 Case Study: NDIR Gas Sensor for CO ₂ Detection: Detailed Design	427
3 Modeling and Simulation	432
3.1 Optical Simulation Techniques	432
3.2 Case Study: NDIR Gas Sensor for CO ₂ Detection: Simulation	435
4 Design Optimization	443
4.1 Optimization Strategy	443
4.2 Case Study: NDIR Gas Sensor for CO ₂ Detection: Optimization of the Analysis Cell	444
5 Conclusion	449
References	452
12 SIMULATION AND MODELING FOR OPTICAL DESIGN OF LASER REMOTE SENSING FOR GAS MEASUREMENTS	455
<i>Tatsuo Shiina</i>	
1 Introduction	455
2 Lidar Techniques	457
2.1 Lidar Structure	457
2.2 Lidar Techniques	462
3 Calculations	464
3.1 Lidar Equation	464
3.2 Simulation	467
3.3 Analysis	471
4 Applications	475
4.1 Mie Lidar	475
4.2 Raman Lidar	478
4.3 LED Mini-Lidar	481
5 Summary	486
References	486
INDEX	489

NOVEL LONG-PERIOD FIBER GRATING SENSOR BASED ON DUAL-PEAK RESONANCE AND SPR

Zhengtian Gu

1. INTRODUCTION

A long-period fiber grating (LPFG) is a kind of fiber device with photo-induced periodic modulation of the refractive index in the core, which was first reported in 1995 (Vengsarkar et al. 1996a). The periodicity of an LPFG is typically in the range of 100–1000 μm . An LPFG can couple the fundamental core mode to the co-propagating cladding modes, producing a series of discrete attenuation peaks in the transmission spectrum. By virtue of advantages such as ease of fabrication, low insertion loss, low-level back reflection, and compactness, LPFGs have been used increasingly over the last few years in communications (Vengsarkar et al. 1996a, 1996b) and sensing applications (Bhatia and Vengsarkar 1996; Patrick et al. 1998; James and Tatam 2003).

Because the field distributions and effective refractive index (ERI) of the cladding modes are easily affected by the surrounding medium, LPFGs are very suitable for refractive index sensing (Lee et al. 1997; Tong et al. 2002; Chong et al. 2004). However, this kind of LPFG sensor is sensitive only to a surrounding medium whose refractive index is less than that of the silica cladding, and in addition, it is not species-specific, which limits the extent of its applications. Recently,

an LPFG chemical sensor whose cladding is coated with a sensitive thin film has been attracting much interest and attention. N. D. Rees coated an organic-material thin film on the cladding of an LPFG using Langmuir-Blodgett technique, and studied the influence of the thickness of the overlay material on the LPFG response (Nicholas et al. 2002). Ignacio et al. (2005, 2006), Wang et al. (2005), and Cusano et al. (2006) studied the resonance shift and the mode transition in high-refractive-index-coated long-period gratings. The theoretical analysis as well as experimental data suggest that the sensitivity of LPFG-based chemical/biosensors can be improved by appropriate choice of the cladding mode order, the film thickness, and the refractive index, and there is an optimum overlay thickness for each combination of ambient and overlay refractive indices. Based on this coated LPFG structure, Pilla et al. (2005), Gu et al. (2006), and Jesus et al. (2007) designed optical chemo-, gas-, and pH sensors. The coated LPFG sensors overcome the limitation of noncoated LPFGs that the refractive index of the external medium must be less than or equal to that of the cladding, and has the advantages of specification of chemical analyte and broad response range.

In 1999, Shu et al. (1999) found that when the grating period of an LPFG was short ($\sim 100\ \mu\text{m}$), dual resonance peaks of the higher cladding mode appeared during the writing process of the LPFG. They also found that the dual resonance wavelengths shifted in opposite directions with variation of the environmental refractive index. Based on this dual peak effect, Shu and Huang (1999) fabricated a kind of high-sensitivity liquid concentration sensor, for which the sensitivity of the LP_{015} cladding mode is 20 times higher than that of the scheme with conventional grating period ($400\ \mu\text{m}$). If the dual-peak resonance effect is utilized in an LPFG coated with a sensitive thin film, the LPFG not only has high sensitivity to refractive index, due to dual peak resonance, but also enlarges the sensing application range which can be applied in monitoring the solution concentration, gas concentration, and so on. When this kind of LPFG is brought into contact with the external surroundings, the change of refractive index of the thin film leads to variation of the interval between the dual resonance peaks. This coated LPFG based on dual peak resonance is first discussed in this chapter.

Surface plasmon resonance (SPR) is one of the promising optical techniques with potential applications in various fields (Flavio et al. 2005; Chen et al. 2005; Wang and Knoll 2006; Shin et al. 2007). SPR sensors have advantages such as flexibility, low cost, and small size (Lotierzo et al. 2004; Gupta and Sharma 2005). The principle of SPR sensors is that the surface plasmon wave (SPW), which can be excited at the interface between a metal film and an absorbing medium, is extremely sensitive to tiny changes in the refractive index (RI) of the absorbing medium. SPR sensors have been developed into three types: prism-coupled, integrated optical waveguide-coupled, and optical fiber-coupled sensors (Dostalek et al. 2001; Ho et al. 2001; Cao et al. 2006). In recent years, considerable attention has focused on SPR sensors based on metal-coated LPFGs, which are extremely