传感材料与传感技术丛书

Sensing Material and Sensing Technology Series

CHEMICAL SENSORS SIMULATION AND MODELING

Volume 1 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

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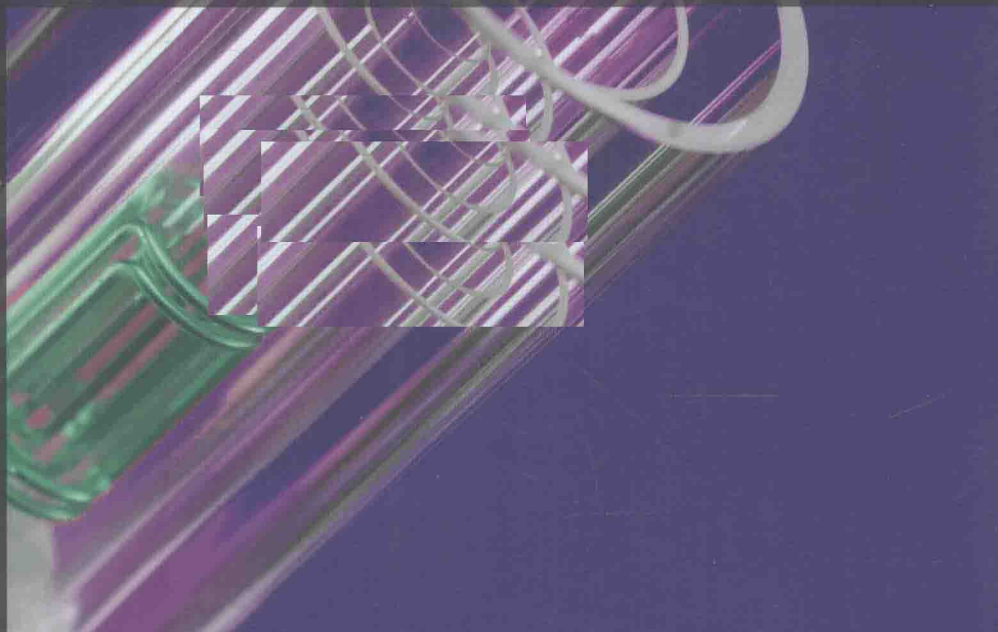

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PREFACE

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.

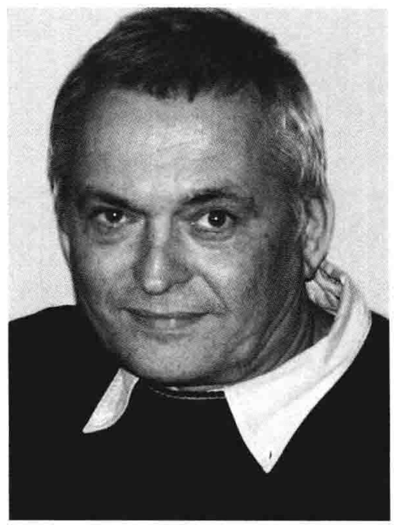
I believe that this series will be of interest of all who work or plan to work in the field of chemical sensor design. The chapters in this series have been prepared by well-known persons with high qualification in their fields and therefore should be a significant and insightful source of valuable information 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.

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Contents

Preface ix

About the Editor xiii

Contributors xv

6 Modeling Interactions of Metal Oxide Surfaces with Water 217

L. Vlcek
P. Ganesh
A. Bandura
E. Mamontov
M. Predota
P. T. Cummings
D. J. Wesolowski

1 Introduction 217

2 Metal Oxide–Water Interactions and Their Study 219
2.1 General Oxide Properties and Surface Processes 220
2.2 Experimental Methods 223
2.3 Computer Simulations 224
2.4 Theoretical Models 228

3 Electronic Structure and Surface Reactions 229
3.1 TiO_2 229
3.2 SnO_2 233
3.3 ZnO 237

4 Thermodynamic and Structural Aspects of Adsorption 240
4.1 TiO_2 240
4.2 SnO_2 243
4.3 ZnO 245

5 Dynamics of Adsorbed Water 246
5.1 Fast Processes—Proton Motion 247
5.2 Slow Processes—Molecular Motion 248

6 Perspectives 251

7 Acknowledgments 252

References 252

7 Density Functional Theory Study of Water Dissociative Chemisorption on Metal Oxide Surfaces 263

C. Zhou
H. Cheng

1 Introduction 263

2 Catalytic Water Dissociation on Metal Oxide Surfaces 265

2.1 Water Dissociative Chemisorption on $Fe_3O_4(111)$ Surfaces 266

2.2 Water Dissociative Chemisorption on Rutile-$TiO_2(110)$ Surfaces 275

2.3 Water Dissociative Chemisorption on α-$Al_2O_3(100)$ Surfaces 280

4 Summary 285

5 Acknowledgments 285

References 286

8 First-Principles Studies of Hydrogen Spillover Mechanisms on Metal Oxides 293

L. Chen
M. Yang
H. Cheng

1 Introduction 293

2 General View of Spillover 294

2.1 Mechanism of Hydrogen Spillover on Metal Oxide 294

2.2 The Role of Noble Metals in the Spillover Effect 295

2.3 The Role of Spillover in Chemical Sensors 296

2.4 Experimental Confirmations of the Presence of Spillover Effect 296

3 Computational Approach 297

4 Hydrogen Spillover in MoO_3 297

5 Hydrogen Spillover in Al_2O_3 306

6 Hydrogen Spillover in WO_3 309

7 Summary 312

References 313

9 Adsorption and Diffusion of Adatoms and Small Clusters on Metal Oxide Surfaces **317**
R. Ferrando
A. Fortunelli

1 Introduction 317

2 Theoretical Methods and Concepts in Metal/Oxide Interaction 320
2.1 Theoretical Methods 320
2.2 Concepts in Metal/Oxide Interaction 322

3 Diffusion of Isolated Adatoms 324
3.1 Energy Barriers for Isolated Adatoms on Flat MgO(001) 324
3.2 Long Jumps in Adatom Diffusion 326
3.3 Diffusion in the Presence of Defects 329

4 Diffusion of Dimers, Trimers, and Tetramers 330
4.1 Dimers 330
4.2 Trimers 333
4.3 Tetramers 334

5 Adsorption and Diffusion on Exotic (Ultrathin) Oxide Substrates 338
5.1 Adsorption 341
5.2 Diffusion 347

6 Conclusions 352

References 353

10 Effect of Size on the Phase Stability of Nanostructures **363**
S. Li
Q. Jiang

1 Introduction and Motivation 363

2 Phase Stability and Structural Phase Transition 367
2.1 Crystals and Crystalline Structures 368
2.2 Factors Triggering Phase Transitions 369
2.3 Size Effect on Phase-Transition Pressure and Temperature of Nanostructures 370
2.4 Research on the Thermodynamics of Solid Structural Nanophase Transitions 370
2.5 Effect of Surface: Surface Energy and Surface Stress 371
2.6 Effect of Shape on Phase Stability 372

3 Theoretical Methods for Size-Dependent Phase Stability 372
3.1 Simulation Techniques 373
3.2 Thermodynamics 374
3.3 Applications: Case Studies 382

4 Concluding Remarks 389

References 390

11 Segregation-Induced Grain-Boundary Electrical Potential in Ionic Oxide Materials: Simulation Approaches and Pending Challenges 397

R. L. González Romero
J. J. Meléndez Martínez
F. L. Cumbrera Hernández
D. Gómez García

1 Introduction: General Ideas About Segregation Effects in Oxide Materials 397

2 Modeling of Segregation to the Grain Boundaries: Analytical (or Continuum) Approach 398

3 Atomistic Approach: Molecular Dynamics Modeling 408

4 Mesoscopic Approach: Phase-Field Models 414

4.1 Topological Evolution of a Collective of Many Grains 415

4.2 Microstructural Evolution Coupled with Chemical Segregation 417

5 Pending Problems and Future Prospects 418

6 Acknowledgments 419

References 419

Index 425