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

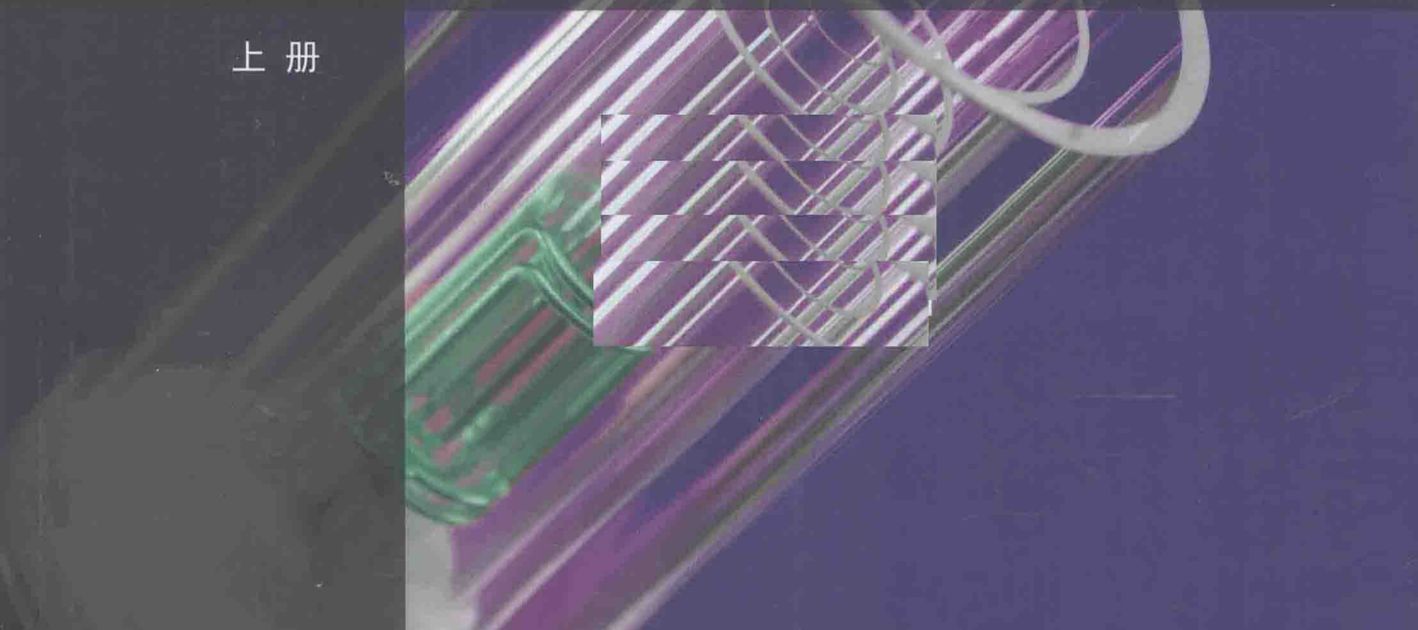
EDITED BY GHENADII KOROTCENKOV

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

上 册



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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.

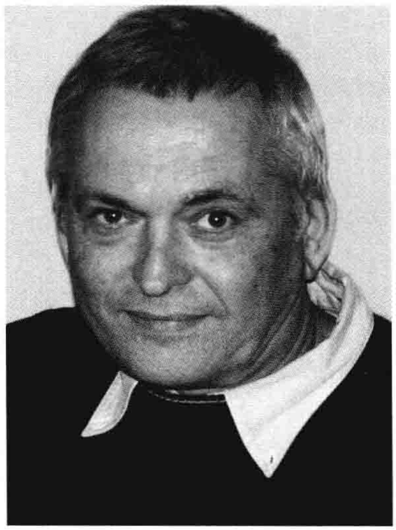
I believe that this series will be of interest of all who work or plan to work in the field of chemical sensor design. The chapters in this series have been prepared by well-known persons with high qualification in their fields and therefore should be a significant and insightful source of valuable information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

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1. INTRODUCTION

Semiconductor oxides are fundamental to the development of smart and functional materials, devices, and systems (Wang 1998; Pan 2001; Chen 2006a). These oxides have two unique structural features, mixed cation valences and an adjustable oxygen deficiency, which are the bases for creating and tuning many novel material properties, from chemical to physical (Chen et al. 2004). Because of the increasing importance of air pollution and the need to monitor concentration levels of gases such as CO, CO_2, NO_x, O_3, SO_2, etc., the development of many kinds of sensors and control systems has been jolted into action in recent years (Dai 2002; Ng 2003; Wang 2003; Cheng 2004). Microstructure variations will inevitably change their physical and chemical properties. Therefore, study of the microstructure of the

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