7 月 31 日，我院 2017 级医学影像学专业本科生陈小波，以第一作者身份在《ACS Sensors》杂志（中科院分区化学大类一区，Top 杂志，IF：7.3）上发表了题为《Effective and Robust Parameter Identification Procedure of a Two-site Langmuir Kinetics Model for a Gas Sensor Process》的学术论文。

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Effective and Robust Parameter Identification Procedure of a Two-Site Langmuir Kinetics Model for a Gas Sensor Process

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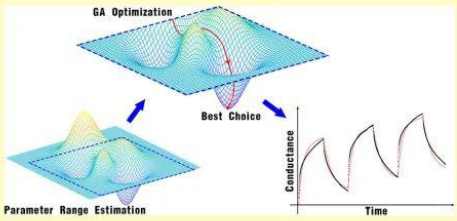
ABSTRACT: Gas sensors have received plenty of attention due to various applications, and the methods to model the kinetic processes and estimate the corresponding parameters play a critical role in characterizing the sensor response behavior. In this work, a two-site Langmuir kinetics model is applied to describe the adsorption/desorption response processes of a SnO_2/reduced graphene oxide resistive gas sensor and the pertinent kinetic parameters are optimized based on the genetic algorithm (GA). For the robustness and fast convergence of the GA, the initial values and ranges of kinetic parameters are obtained step-by-step. This a priori knowledge is sufficient to guarantee reasonable parameter identification from experimental data. Moreover, the kinetics model and GA are integrated into graphical user interface software for subsequent application. Eventually, the exploration of improvements to experimental design is uncovered to increase the accuracy and reliability of the estimation.



KEYWORDS: *gas sensor, Langmuir kinetics model, parameter identification, genetic algorithm, GUI*

Resistive semiconductor gas sensors can trigger the interaction between a sensor and gas molecules by changing the conductivity characteristic of the carrier movement.[1−3] Due to its high sensitivity in the detection of combustible, toxic, and harmful gases, the gas sensor has widespread applications in various fields.[4,5] If there is no general quantitative understanding of the sensor responses, then it is difficult to determine the relationship between the gas concentration and sensor response.[6−8] Therefore, a method to establish the kinetic models to characterize the dynamical behavior of the gas sensor and determine the crucial kinetic parameters to describe the mechanism responsible for gas sensing is vital in the field of sensors in recent years.[9−11]

The mathematical models based on these responses have been the aim of researchers, much effort has been made, and various kinetic models are constantly proposed. First, the Freundlich isotherm was proposed in 1909.[12] As an empirical equation, it can fit the majority of gas sensing data. Nonetheless, in many cases, empirical equations are insufficient to demonstrate the physical mechanisms underlying gas sensors.[12] Then, the Langmuir model was theoretically derived in 1916 from monolayer adsorption, which quantifies the coverage of molecules on a substrate surface as a function of the gas concentration at a fixed temperature.[13,14] The BET model, which supposes that the occupied adsorption sites can continue to adsorb, is derived from the multilayer adsorption study in 1938. Later, a nonlinear diffusion reaction model of electrical conduction was proposed by Gardner.[11] Based on the electron theory of chemisorption, a microscopic model of a thin-film gas sensor was developed by Geistlinger.[15] Currently, the adsorption−desorption kinetics curves and transient response curves are widely analyzed by the modified single-exponential Langmuir kinetic model,[8,16−19] although increasingly many studies indicate that other less known techniques outperform it in many cases.[20] Considering the difference in energy on the film surface, the phenomenon of two adsorption sites and a multi-exponential kinetic model were proposed by Hu et al.[21] and have been successfully applied in diverse senors.[22−25] Recently, one more form of a two-site kinetic model was established to provide microscopic information[26] and an intermolecular-force-based model was proposed to analyze the gas response process.[27] Undoubtedly, the mathematical modeling of gas sensors has remained the focus of this research field.

Given a model expression and sensing experimental data, it is well known that the model parameter estimation is of great significance to reveal the characteristics of the gas sensor response.[6] Many different software tools and optimizing

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该文章采用双位点 Langmuir 动力学模型描述了一类气体传感器的吸附/解吸响应过程，基于模型特点结合数据分析逐步识别参数的取值范围，并运用遗传算

法设计了一套具有高效性、鲁棒性的参数识别方法。文章还将动力学模型和相应算法集成到可视化图形用户界面软件中，并进行了公开发布以供科研工作者下载使用。

陈小波是我院 2017 级医学影像专业 1 班学生。该同学刻苦勤勉，曾凭借优异的成绩获得国家奖学金、校一等奖学金；综合素质良好，曾获三好学生荣誉称号。大一时就加入校数学建模协会，在指导老师的悉心指导下，认真学习 Matlab、Python 等数据处理软件，研修《医学统计学》、《机器学习》等教程，为之后的科研实践奠定基础。

学院一直以来高度重视本科生科研素养的培养。在大一、大二阶段，鼓励学生积极参加校级数学建模等协会，大三大四阶段，鼓励学生参加学校和附属医院老师的课题研究，从而提高学生的科研实践能力和创新能力，提升本科生的综合素质。

陈小波个人简介：

陈小波，男，共青团员，入党积极分子，2017 级医学影像专业学生。主持或参与了多项基金课题和论文的撰写，包括省级新苗人才计划课题 3 项，校级课题 4 项；获得了十余项国家级或省级荣誉。同时，还在杭州某生物科技公司的 8 个月实习期间独立开发了可视化交互软件并完成了 4 项软件著作专利和 1 项国家发明专利的申报。

主要荣誉：

1、2018~2019 年获得国家奖学金、一等奖学金、三好学生等荣誉称号。

2、美国大学生数学建模竞赛二、三等奖。

3、全国大学生服务外包竞赛三等奖。

4、全国大学生数学建模竞赛浙江赛区一等奖、二等奖。

5、全国中医药高等院校大学生课外学术科技作品一等奖。

6、浙江省第十六届“挑战杯”大学生课外学术科技作品一等奖。

7、主持或参与省级新苗人才计划课题三项，校级课题四项。