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Analytical expression for concentration and sensitivity of a thin film semiconductor gas sensor

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Abstract In this paper, a mathematical model for gas sensing thin film semiconductor at an internal diffusion limitation for non-steady-state conditions is discussed. The model is based on diffusion equations containing a linear term related to the reaction processes. Analytical expressions for concentrations are derived using Laplace transformation. The gas sensitivity for both actual and equivalent models has been reported for all the values of reaction parameters such as rate constant and film thickness. Furthermore, in this work a complex inversion formula is employed to solve the boundary value problem. An excellent agreement with simulation data is observed. The dependence of sensitivity on temperature, film thickness and time are discussed for both actual and equivalent models.

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1. Introduction

Gas sensor technology has already been grown as in dispensable practice in various aspects in our life. Yet further advancements in the technology are required in order to improve sustainability of our society and quality of human life. Gas sensors play vital role in detecting, monitoring and controlling the presence of hazardous and poisonous gases in the atmosphere. It is well known fact that the gas adsorption on the surface of a semiconductor can influence its electrical conductivity [1].

Semiconductor based gas sensor can be fabricated into three types of devices, i.e., sintered block, thick film and thin film, of these sintered block and thick film devices are commercialized successfully [2]. Even though thin film devices are brought into practical use, they have remarkable characteristic features such as, fast response, low fabrication cost, ease of miniaturization, and compatibility with microelectronic circuitry [3]. Thong et al. [4] have compared gas sensor performance of SnO_2 nanowires and their hierarchical nanostructures. Every semiconductor gas sensor is provided with a porous sensing layer (resistor) of a semiconducting oxide. Under the steady-state condition, the gas concentration inside the sensing layer would decrease with increasing diffusion depth, resulting in a gas concentration profile which depends on the rates of diffusion and surface reaction [5]. Semiconductor sensors can be produced in arrays to allow sensing of

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Symbol			
a	sensitivity coefficient, ppm^{-1}	r	pore radius, nm
a_0	pre-exponential constant, ppm^{-1}	R	gas constant, J K^{-1} mol^{-1}
$A = \left(\frac{3k_0}{4r}\right)^{\frac{1}{2}}\left(\frac{\pi M}{2R}\right)^{\frac{1}{4}}$	constant, nm^{-1} $K^{1/4}$	R_a	resistance of the film in air, none
C	concentration of target gas, ppm	R_g	resistance of the film in gas, none
C_s	target gas concentration outside the film, ppm	S	sensitivity, none
D	diffusion coefficient, nm^2 s^{-1}	t	time, s
D_k	Knudsen diffusion coefficient, g/mol	u	dimensionless concentration, none
E_a	apparent activation energy, kJ mol^{-1}	x	depth from the film surface, nm
E_k	activation energy, kJ mol^{-1}	x	distance, nm
k	rate constant, s^{-1}		
k_0	pre exponential constant, none	*Greek symbols*	
L	film thickness, nm	χ	dimensionless distance, none
M	molecular weight, Amu	τ	dimensionless time, none
$m = L\sqrt{k/D}$	Hatta number, none	$\sigma(x)$	sheet conductance under exposure to the gas, none
		σ_0	sheet conductance normalized in air, none

multiple species simultaneously with advances in sensitivity and detection limits which approaches parts-per-million (ppm) levels for some species. Tin oxide semiconductor gas sensors patented in 1962 by Taguchi [6]. Korotcenkov and Cho [7] analyzed the influence of film thickness of SnO_2 films deposited by a spray pyrolysis method on the operating characteristics of gas sensors. Since then stannic oxide gas sensors have undergone extensive research and development. Nowadays, Tin dioxide (SnO_2) is the most important material for use in gas sensing applications [8].

Gas sensor technology has played an important role in various fields such as in the automation of industrial processes, emission control for automobiles, and gas leakage detection in home and workplace. Specifically, the research work done on gas sensors based semiconducting metal oxides has made remarkable progress in detecting various kinds of gas molecules such as H_2, CO, hydrocarbons, NO_x, SO_x, CO_2, VOCs, and odors [9,10]. The pioneering works of Taguchi [6] in the early 1960s supported the same. Among semiconducting metal oxides, the gas sensing properties and sensing mechanism of SnO_2 have been well studied by many workers due to their excellent ability for gas sensing [11–15]. However, the understanding of working principles needs further exploration in order to develop high-performance semiconductor gas sensors required for practical applications.

Several attempts have been made to analyze/improve semiconductor gas sensors based on diffusion equations by many researchers [16–25]. Need of a sensing body with the well-defined geometry and porous structure with proper initial and boundary conditions are found to be important from the existing analysis reports [5]. Gas diffusion dynamics of a thin film semiconductor gas sensor is investigated by solving the relevant diffusion equation using the explicit finite difference method [26]. Liu et al. [27] proposed the probable application of the modified expression on explaining response of thin films to various reducing and oxidizing gases. Hosein-Babaei and Orvatinia [28] presented a mathematical model for simulation of the steady state gas sensitivity ($s = G_g/G_a$) of a thin film resistive gas sensor. Yamazoe and Shimanoe [29] discussed the gas response of oxide semiconductor film devices under control of gas diffusion and reaction effects. It is found that no rigorous analytical expressions for the concentrations of target gas and sensitivity inside the thin film semiconductor gas sensor for all values of reaction parameters have been reported so far. Hence an attempt has been made, in this paper to come up with, approximate analytical expressions for the concentrations and sensitivity of both actual and equivalent models using Laplace transformation method. In addition the dependence of gas sensitivity on film thickness and temperature is also reported.

2. Mathematical modeling

A thin film semiconductor gas sensor is usually fabricated by depositing a porous thin layer of a semiconducting oxide on a dense substrate. The target gas molecules diffuse in the thin layer while reacting with the surface oxygen of the oxide grains. Generally, Scanning electron micrographs (SEM) demonstrate information about the surface homogeneity, surface morphology like crack free nature, pinholes, grain size, nature of the film and smoothness of the films. In optimized conditions, Metal oxide (Tin oxide thin films) illustrates a well defined and smooth uniform surface with uniform grain distribution or high crystalline nature. It provides good sensing behavior. As the layer thickness is far smaller than the layer width, the gas diffusion can be taken as one-dimensional along the direction of depth, as illustrated in Fig. 1(a) for actual

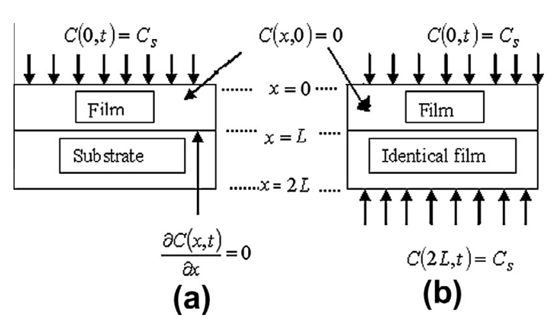

Figure 1 Modeling of thin film device: (a) for actual model (b) for equivalent model.

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