engineering proceedings

MDPI

Proceeding Paper

Elaboration of Undoped ZnO Nanowires for Use as Acetone Gas Sensors †

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† Presented at the 2nd International Electronic Conference on Chemical Sensors and Analytical Chemistry, 16–30 September 2023; Available online: https://csac2023.sciforum.net/.

Abstract: The objective of our work is to provide an advantage for designing new, more efficient sensors using undoped ZnO nanowires. Nanostructures based on ZnO have demonstrated improved sensor performance, thanks to their excellent chemical and thermal stability, as evidenced by their high melting temperature. We have utilized the Schottky defect model to simulate the behavior of free carriers in ZnO semiconductors. Additionally, we have investigated the theoretical model of oxygen molecule adsorption and desorption. Furthermore, we have examined the adsorption of reducing gases, with acetone gas being used as an example. By employing the Comsol software, we have discovered that the solid–gas interaction is significantly reduced at a temperature of 295 °C for ZnO nanowires compared to bulk ZnO, which typically requires a temperature of 500 °C. This reduction can be attributed to the predominant behavior of the side surfaces $(10\bar{1}0)$ in ZnO nanostructures, as well as the lower activation energy of these surfaces compared to the (0002) surfaces. These ZnO nanowire nanostructures provide numerous active and thermodynamically favorable surfaces for the adsorption of reducing gases. The simulation method using Comsol is one of the means to achieve improved design and offer optimal device operation.

Keywords: semiconductor; ZNO; nanostructure

Citation: Zeboudj, A.; Hamzaoui, S.; Zardali, M.; Tadji, A. Elaboration of Undoped ZnO Nanowires for Use as Acetone Gas Sensors. *Eng. Proc.* **2023**, *48*, 51. https://doi.org/10.3390/CSAC2023-14925

Academic Editor: Nicole Jaffrezic-Renault

Published: 7 October 2023

1. Introduction

Natural occurrences of ZnO are commonly found in ruby-red minerals, whereas artificially synthesized ZnO appears colorless or white [1]. It finds applications in diverse fields such as solar cells, light-emitting diodes, and gas sensors.

Gas sensors play a crucial role in various applications, from environmental monitoring to detecting toxic gases in industries. In recent years, ZnO nanofils have garnered significant attention due to their unique properties [2], such a high surface area and sensitivity. Our goal is to provide added value to the design of more efficient sensors with a resistance-based configuration using nanostructures. We pursue this objective by developing ZnO nanowires through a hydrothermal method, followed by studying their detection properties. These nanowires are characterized by multiple active surfaces that are thermodynamically favorable for gas adsorption. However, the challenge we face is to find ways to further enhance the sensitivity of ZnO nanowires towards acetone by exploring configuration modifications.

2. Materials and Methods

2.1. Growth of ZnO Nanostructures

ZnO nanowires have a significant impact in diverse domains including environmental monitoring, security, and healthcare. They are widely employed for manufacturing gas sensors, pressure sensors, and humidity sensors due to their exceptional characteristics. Their remarkable specific surface area and heightened sensitivity enable them to detect minute concentrations of gases and chemical compounds [3].

2.2. Practical Realization

There are several methods commonly used for growing ZnO nanowires. In this part, we are interested in various synthesis methods and chemical bath deposition (CBD) stands out as a promising technique for the fabrication of ZnO nanowires.

The CBD method presents a simple and cost-effective approach for synthesizing ZnO nanowires, making it highly attractive for large-scale production [4]. This part aims to delve into the details of the CBD technique for the elaboration of ZnO nanowires, focusing on the crucial parameters and their influence on the growth process.

2.3. Solution Preparation

The CBD process begins with the preparation of a chemical solution containing ZnO precursors. This section discusses the selection of precursors, solvent choice, and their concentrations.

We utilize a fixed reaction medium consisting of an equimolar mixture at a concentration of 0.3 mol/L of zinc nitrate ($Zn(NO_3)_2$) and HMTA l'hexaméthylènetétramine dissolved in deionized water.

2.4. Substrate Treatment

Prior to the deposition of ZnO nanowires, the substrate undergoes a thorough cleaning process to eliminate impurities and establish an optimal surface for nanowire growth. This involves meticulous cleaning steps to ensure a pristine substrate surface.

To promote the growth of ZnO on a substrate, we first apply an initial layer called a "seed layer".

2.5. Subtract Trap

Seed layer deposition is the initial step in the growth of subsequent layers, providing a foundation or template for desired properties. In the case of the ZnO layers deposited through a dipping process using an equimolar mixture of zinc acetate and MEA, their morphology is significantly influenced by the concentration of the solution, the withdrawal speed of the sample, and the number of deposition cycles performed. To investigate the impact of solution concentration, a series of four samples were prepared with concentrations of 0.1, 0.3, 0.5, and 0.7 mol/L. These layers were deposited onto silicon substrates, with a constant withdrawal speed of 10 mm/s. Subsequently, the annealing process was carried out conventionally in two stages: 20 min at 300 °C, followed by 1 h at 500 °C on a hot plate.

The substrate is immersed in the chemical bath solution, where a chemical reaction takes place to form ZnO nanowires. The Zn^{2+} ions from the ZnO precursor react with the OH- ions present in the solution to form ZnO nuclei on the substrate surface.

3. Results and Discussion

The morphology of the obtained ZnO structures was analyzed using Scanning Electron Microscopy SEM) utilizing a Hitachi type S-2600N instrument from Japan. Each ZnO nanorod exhibited unique configurations. Figure 1 depicts the diverse morphologies of individual ZnO nanorods.

The crystallinity of nanomaterials was followed by X-ray diffraction (DRX).

The morphological and structural properties of ZnO nanowires deposited via a chemical bath on layers S1 to S4 are shown in Figure 1 and Table 1. For all samples, the nanowires exhibit a wurtzite crystal structure and are oriented along the c-axis. As expected, the diameter, length and density are strongly influenced by the morphology of the seed layer used (see Figure 2).

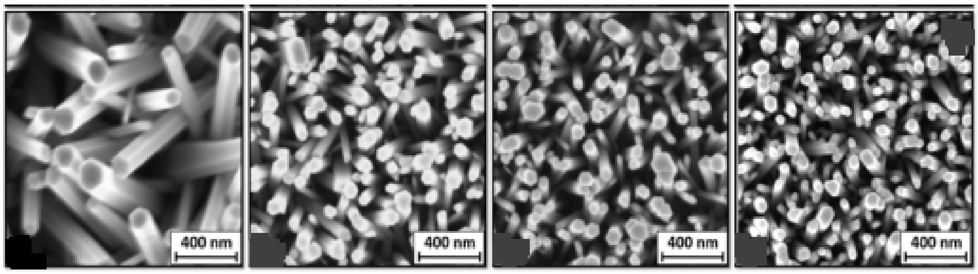

Figure 1. Image MEB presents morphological and variable structural characteristics of ZnO nanofils deposited on a chemical bath under strictly identical experience conditions.

Table 1. Morphological and structural characteristics of ZNO nanowires deposited in a chemical bath.

	Average Diameter (nm)	Medium Length (nm)	Density (μm^{-2})
s_1	115	1400	23
s_2	77	1060	60
s_3	60	960	112
s_4	58	840	100

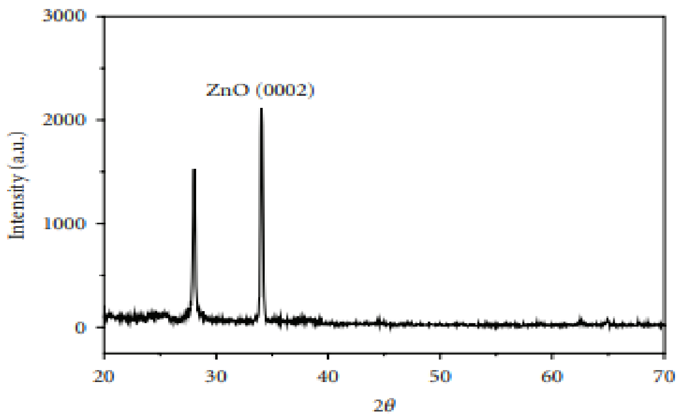

Figure 2. XRD pattern of the ZnO nanowires.

4. Gas Responses of the Undoped ZnO

The sensitivity was calculated using [5]: s = R_a/R_g

In the above equation, R_a is the film conductance under air and R_g is the film conductance under gas.

Our sample demonstrated its highest sensitivity at a temperature of 295 °C. As the temperature increased beyond this point, the ZnO nanorod exposed to acetone gas underwent a noticeable color change. This change in color is attributed to the adsorption of reduced acetone gas, which leads to an increase in the film's conductance and a shift in the plasmon frequency from the infrared to the visible region [6]. Notably, the electrical properties of pure ZnO are significantly influenced by the adsorption of oxygen on their surfaces. This oxygen adsorption affects the electrical conduction and results in an increase in the resistance of ZnO. Our experimental findings indicate that the specimen exhibits sensitivity to acetone only within the temperature range of 295 °C, as illustrated in Figure 3.

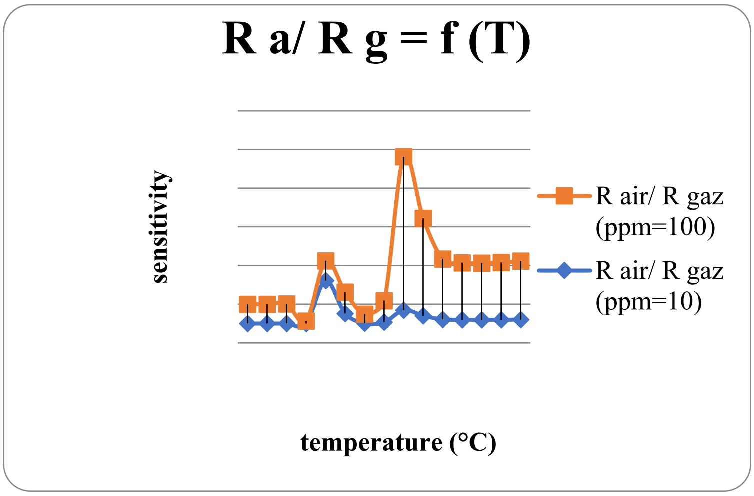

Figure 3. The relationship between the responses to 10 ppm and 100 ppm acetone gas and working temperature of undoped ZnO.

5. Conclusions

The elaboration of ZnO nanowires through chemical bath deposition is a versatile method that enables control over the morphology, density, and orientation of the nanowires. By varying the growth parameters and experimental conditions, nanowires of different shapes can be formed, including straight nanowires, helical nanowires, and branched nanowires. This flexibility allows for tailoring the nanowires to meet specific requirements and optimize their performance in various applications.

Adequate substrate pretreatment is of paramount importance in promoting nucleation and controlling the growth orientation of ZnO nanowires. Among these techniques, substrate cleaning and the use of a seed layer are included.

The influence of substrate properties on nanowire growth is also addressed, emphasizing the importance of substrate selection for specific applications.

Author Contributions: A.Z. wrote the main manuscript text, prepared the figures and performed all the experiments. S.H. and M.Z. oversaw the project and assisted with the writing of the overall manuscript, alongside M.Z. and A.T. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data are provided in the figures of the article.

Acknowledgments: We would like to thank the LMESM Laboratory, Physics Department, University of Science and Technology Mohamed Boudiaf in "Instrumentation aux limites".

Conflicts of Interest: The authors declare no conflict of interest.

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