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Proceeding Paper

Simulation ZnO Nanofils Application Acetone Gas Sensor †

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Abstract: Our objective is to present a valuable contribution towards designing more efficient sensors using undoped ZnO nanofils. The utilization of nanostructures based on ZnO has shown significant enhancements in sensor performance due to the excellent chemical and thermal stability exhibited at its high melting temperature. In our work, we focused on modeling the behavior of ZnO semiconductors by employing the Schottky defect model as a source of free carriers. Specifically, we examined the theoretical model of oxygen molecule adsorption and desorption. We explored two types of molecules responsible for adsorbing reducing gases, taking acetone gas as an example. Through the use of the Comsol software, we found that the interaction between the solid and gas occurs at a considerably lower temperature of 295 °C, compared to ZnO thin films, which typically require temperatures as high as 500 °C. This outcome can be attributed to the behavior of ZnO nanostructures, where the influence of side surfaces ($10\bar{1}0$) is predominant, along with their lower activation energy compared to (0002) surfaces. These ZnO nanofils exhibit numerous active and thermodynamically favorable surfaces, which facilitate the adsorption of reducing gases. Employing simulation methods, such as Comsol, offers an effective approach for achieving optimal device design, thereby ensuring superior device performance. This research demonstrates the potential of using undoped ZnO nanofils for the development of highly efficient sensors with enhanced operational characteristics.

Keywords: semiconductor; ZNO; nanostructures; the Schottky defect; adsorption; desorption; acetone gas

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1. Introduction

this research lies in the development of environmentally-conscious materials with strong capabilities in gas detection. This poses a significant challenge for scientists who are aiming to create durable solutions in the realm of material science. Among the various possibilities offered by metal oxides, those that exhibit semi-conductive properties have emerged as particularly promising candidates for gas sensing applications.

One standout example within this category is zinc oxide (ZnO), which has garnered substantial attention due to its wide-ranging potential, spanning applications in both renewable energy and environmental preservation. ZnO, found abundantly in vivid ruby-red ores, possesses remarkable attributes that make it highly suitable for gas sensing purposes. Moreover, ZnO's versatility extends to pioneering novel materials for the realm of renewable energy.

While naturally occurring ZnO displays a distinctive ruby-red color, artificially synthesized versions appear colorless or white. This compound finds practical utility across various domains, encompassing solar cell technology, light-emitting diodes (LEDs), and the field of gas sensors the main objective of this study is to develop sensors based on these nanowires for their potential use in medical devices enabling early diagnosis of certain conditions, including the measurement of acetone in the urine of diabetic individuals.

2. Materials and Methods

- **Nanowire-Based Sensors: Configurations and Operations:**

Sensors constructed using solid metal oxide materials typically comprise [1]: A sensitive layer of oxide/semiconductor that directly interacts with the targeted gas. Electrodes that facilitate electrical measurements and monitor the interaction process.

An optional heating system to manage and regulate the temperature of the sensitive layer. Nanowires have garnered substantial interest in the realm of gas detection applications due to their elevated surface-to-volume ratio, which holds the promise of achieving ultra-sensitivity. This emphasis on nanowires has underscored that the operational efficacy of these sensors is intricately tied to both the selection of material for the nanowires and the specific configuration chosen [2,3].

In our specific context, we are focusing on the resistance-based configuration for fabricating gas sensors utilizing ZnO nanowires (Figure 1).

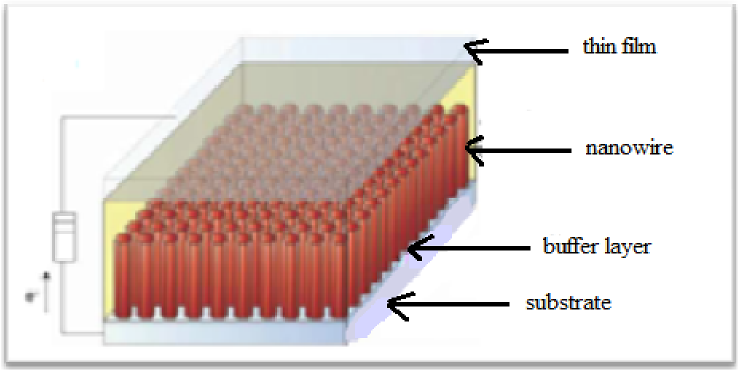

Figure 1.: Schematic representation of the ZnO nanowire-based sensor [5].

In this arrangement, the nanowire functions as a channel, with its ends connected to the source and drain. Upon exposure of the ZnO nanowires' surface (0002) to the gas, a distinct reaction ensues, inducing alterations in their electrical behavior and generating an electrical signal that correlates with the gas detection phenomenon.

- **Gas Detection Principle**

The fundamental principle of gas detection relies on the alteration of semiconductor surface resistance, typically involving modifications in the conductivity of the sensor's constituent materials. This change originates from fluctuations in the density of electron species caused by the adsorption of gas molecules onto the surface of the host material [4,5]. In our context, we are particularly concerned with detecting Acetone gas.

Acetone, a commonly used solvent in research laboratories and the paint and adhesive industry, falls into the category of highly volatile organic compounds (VOCs) and is recognized as a toxic compound. Its high volatility is concerning due to its significant absorption rate (approximately 75%) through human respiratory pathways [6]. Exposure to concentrated Acetone poses risks to living organisms.

The detection of Acetone using a semi-conductive surface has been extensively explored in existing literature. When ZnO is exposed to the reducing gas Acetone

(CH_3COCH_3), Acetone molecules react with adsorbed oxygen (O) species on the surface of ZnO (0002), resulting in the formation of CO_2 and H_2O. This chemical reaction leads to an increase in carrier concentration and a subsequent reduction in electrical resistance.

$$CH_3\,COCH_3 + 8O^- \rightarrow 3CO_2 + 3H_2O + 8e^-$$

3. Results and Discussion

We utilized the COMSOL software to develop our research. Our primary objective was to design an undoped ZnO nanowire gas sensor, where the nanowire size is defined as 100 nm. This sensor was integrated with an embedded mini furnace crafted from platinum and deposited onto a glass wafer. The integration aimed to efficiently control and regulate the temperature. Moreover, we positioned a sensitive ZnO layer between two titanium electrodes. The ZnO layer's thickness was established at 0.5 µm.

Table 1. Compiles the various concentrations employed to ascertain their response concerning gas concentrations.

V_{in}	T (°C)	R_a (ppm=0)	R_a/R_G (ppm=10)	R_a/R_G (ppm=100)	R_a/R_G (ppm=500)
1	56	1.24×10^9	1.00	1.00	1.01
2.5	187	4.69×10^6	3.22	1.02	1.08
2.6	198	5.14×10^6	1.52	1.11	1.71
3.5	295	2.46×10^6	1.69	7.93	$3.57*10^1$
4.8	444	1.87×10^3	1.19	2.95	$1.07*10^1$
5	468	8.99×10^2	1.19	2.93	$1.07*10^1$

The R_a/R_G ratio illustrates the sensor's sensitivity or response to the detected gas.
knowing that:
V_{in}: input voltage
R_a: air resistance
R_G: gas resistance

The data is translated into a profile illustrating the sensor's temperature against the R_a/R_G response.

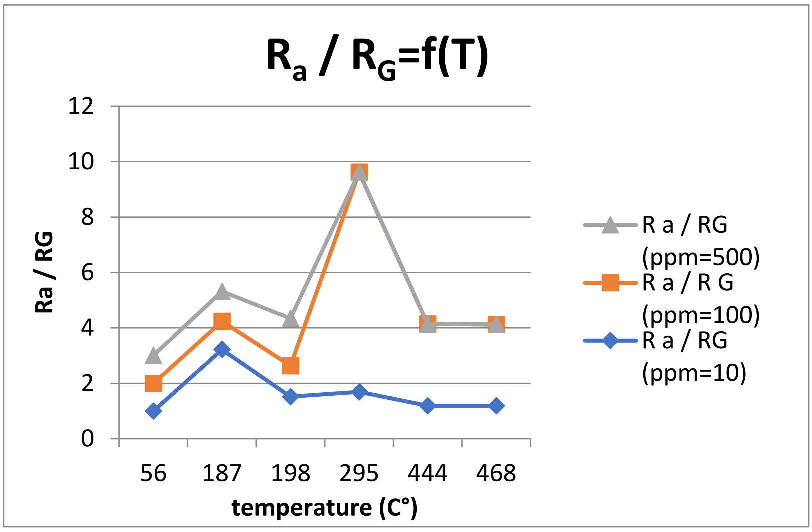

Figure 2. The sensitivity of gas sensors based on ZnO nanowires in relation to temperature.

The figure depicts how temperature influences the sensitivity of undoped ZnO nanowires to different levels of Acetone gas. The profile clearly demonstrates that the sensitivity of the sensor, as indicated by the ratio of resistances, varies with rising temperature. The sensor's sensitivity is quantified by the specific Acetone-driven ratio, Ra/Rs (air resistance/gas resistance). The sensor maintains a consistent response relative to air across temperatures, but its sensitivity becomes more pronounced around Ts = 295 °C for the various Acetone concentrations simulated.

4. Conclusions

ZnO a non-toxic semiconductor, is gaining increasing significance within the scientific community. This is primarily due to its remarkable physicochemical properties, making it a promising material for metal oxide gas sensors. In this context, it is utilized to optimize sensor components through electrical measurements (I-V) conducted using multiphysics simulation software (COMSOL). We studied the effect of operating temperature on the sensitivity of ZnO nanowires to Acetone. The results clearly demonstrate that this temperature plays a major role in determining the film's sensitivity to different concentrations of Acetone.

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