Solid-State Electronics 204 (2023) 108641

Contents lists available at ScienceDirect

Solid State Electronics

journal homepage: www.elsevier.com/locate/sse

Compact model of a metal oxide molecule sensor for self-heating control

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ARTICLE INFO

Keywords:
Compact model
Molecule sensor
Self-heating
Sensor array
Metal oxide
SPICE

ABSTRACT

Metal oxide molecular sensors have notable advantages in their low cost and small size, and they are useful to establish a low-power sensory system for massive data accumulation. However, most of them require high temperatures to cause chemical reactions, and an external heater is needed. Thus, their sensory system consumes around 1 W or higher power for operation. A candidate solution to decrease power consumption is using self-heated sensors. Since the heating area is limited in the sensor itself, mW-order and quick operation are possible. Since the sensors need careful temperature management, a dedicated analog circuit is demanded. Therefore, it is important to create their compact models in MATLAB or Verilog-A and predict the performance of the system as a whole with simulations. In this paper, an experimental self-heated sensor and its compact model are developed. To check the model's validity, some critical model parameters are determined firstly by experiments without self-heating. Then, the simulation outputs are compared with experimental results with self-heating. The comparison shows that the model predicts the saturation value and transient time constant of the gas reaction well. In addition, the error caused by the sensor's drift increases particularly if the sensor is operated in an inert gas.

1. Introduction

Compared with most conventional semiconductor molecule sensors, self-heated molecule sensors are beneficial for developing low-power systems because they consume small power to increase sensing temperature [1,2]. In addition, there have been some reports that the sensor configured to different temperature reacts to different molecules [3–5]. A self-heated sensor only heats a limited sensing area, thus short time constant for controlling temperature can be realized. If the temperature of those sensors is controlled precisely, the number of detectable molecules will increase. One of the main obstacles to realizing the system is to control sensor temperature by feedback power from the interface circuit. The main operation of the circuit is keeping the sensitivity and controlling temperature by feedback voltage or current while consuming a small amount of power. Designing the dedicated circuit for the self-heated sensor, and making compact models of the sensor for circuit simulation is inevitable. Moreover, compact modeling is highly useful for analyzing sensor data in advance by integrating many sensors into a simulation environment (Fig. 1). Sensor experiments with many different types of molecules require precise and complicated setups. Also, the sensor's reaction to molecules usually takes around a few minutes. Self-heating sensors will be driven under various temperature conditions in one experiment operation. Building a sensor's compact model helps us to conduct advanced research on data classification with circuit-level reliability.

In this paper, the metal oxide sensor was introduced, which could generate Joule heating under 5–15 V. The model of the sensor response to NO_2 and the heated temperature was created and the fitted parameters were obtained with the experiment data. The optimized function was applied to the same condition as dynamic response experiments and both results were compared.

2. Developed sensor

In Fig. 2, the microscope image of the developed self-heated sensor and its measured I-V characteristics are shown. The I-V curve indicates

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https://doi.org/10.1016/j.sse.2023.108641

Available online 21 March 2023

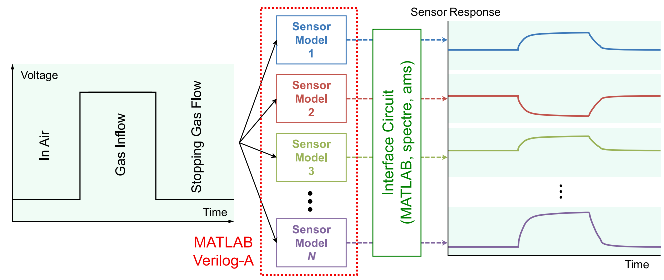


Fig. 1. Simulated sensor response.

that the sensor is an ohmic device. SnO_2 thin film (20 nm) is used as the sensing material, and an electrode is made of Ti/Pt. The resistance of SnO_2 film is changed if it adsorbs certain molecules. The narrow sensor shape and 20 nm thinness enable it to operate as a self-heated sensor. To verify the self-heated characteristics, a thermal simulation was carried out with COMSOL Multiphysics software, and it was verified that only the sensor spot reached a high temperature of around 420 K as shown in Fig. 3. In the thermal simulation, the sensor's electrical resistivity was set to 0.05 Ω·cm, and 10 V was biased. It should be noted that the sensor's resistivity has variation due to a fabrication process and the value was just selected out of possible values. The sensor film thickness was 20 nm, the cross-sectional area was 0.1×10^{-8} cm^2, and the length was 10 μm. Thus, the sensor resistance was calculated as around 50 kΩ. The resistance value was fixed during the simulation, then nearly 2 mW of heating was generated in the sensor device.

3. Compact modeling

The developed block diagram of the self-heated sensor is shown in Fig. 4. While the sensor's temperature was controlled with an external heater in the previous works [6], the feedback loop to cause temperature fluctuation derived from its own resistance change was added. To simplify the model, the number of input gas was limited to one. The gas flow system and the dynamic response filter were represented as low-pass filters. In this work, the gas flow system was removed because the dynamic response filter was dominated filter in our laboratory setup. The dynamic response filter consists of a 2nd-order filter. Values of two poles and one zero were fitted with System Identification Toolbox in MATLAB from experiment data plots. The static response gain and temperature-dependent gain are represented as follows:

$$G_{gas} = k_{1T} \bullet e^{-E_{A1}/kT} \bullet C^{n_1 kT} \quad (1)$$

$$G_{base} = G_{0T} \bullet e^{-E_{A0}/kT} \quad (2)$$

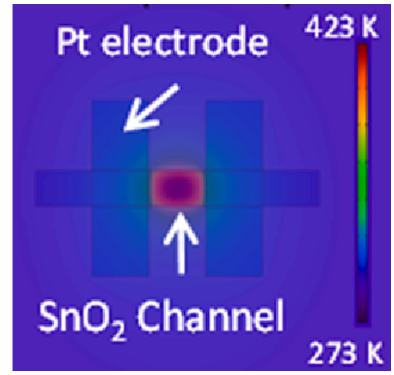


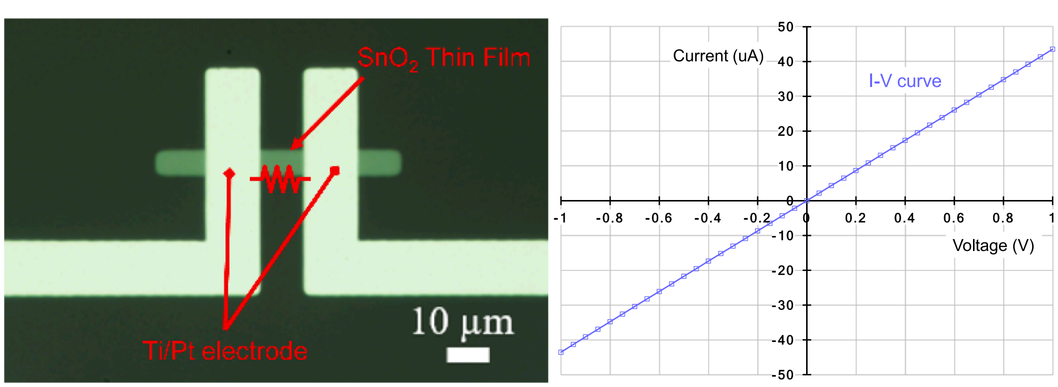
Fig. 3. Thermal simulation results run in COMSOL.

where k and T represent Boltzmann constant and absolute temperature. E_{A0} and E_{A1} are activation energies of the baseline conductance and of the change conductance by a target gas. k_{1T}, G_{0T}, and n_1 are coefficients. C represents the concentration of input gas. The thermal circuit consists of the thermal resistance R_{heat} and the thermal capacitance C_{heat}. Since it is quite difficult to measure the precise thermal circuit parameters, simulation results obtained from COMSOL Multiphysics software were substituted. The input voltage representing 1 ppm gas concentration corresponds to 1 V and the voltage follows linearly to the gas concentration. Temperature-dependent gain has a time delay until it is reflected on the sensor resistance change. However, the time constant was much smaller than that of the molecule's dynamic response because of the small sensor size. Thereby, the delay for the temperature-dependent gain was not taken into account.

4. Experiment and simulation results

The unknown model parameters: E_{A0}, E_{A1}, k_{1T}, G_{0T}, and n_1 were determined by fitting them to experimental data with Eqs. (1), (2). In the experiment, the target gas was NO_2, and the surrounding gas was N_2. In the experiment, resistance was measured under different temperatures of 150, 200, and 250 °C. Since it was difficult to monitor the sensor's surface temperature accurately, an external heater was used. Then, the bias voltage was set to 1 V so as not to cause self-heating. In each temperature condition, gas concentration was set to 0, 10, 20, 50, and 100 ppm, and a steady-state value was measured. Table 1 shows adjusted parameters. In Fig. 5, the comparison between experimental data and calculated data from the determined parameters is shown.

With determined parameters in the above experiments, the dynamic responses were compared. The ambient temperature was set to 100 °C and the sensor was biased with 9 V and 10 V. Fig. 6 shows the resistance



(a) (b)

Fig. 2. (a) Microscope image of the self-heated sensor device. (b) I-V curve of the self-heated sensor.

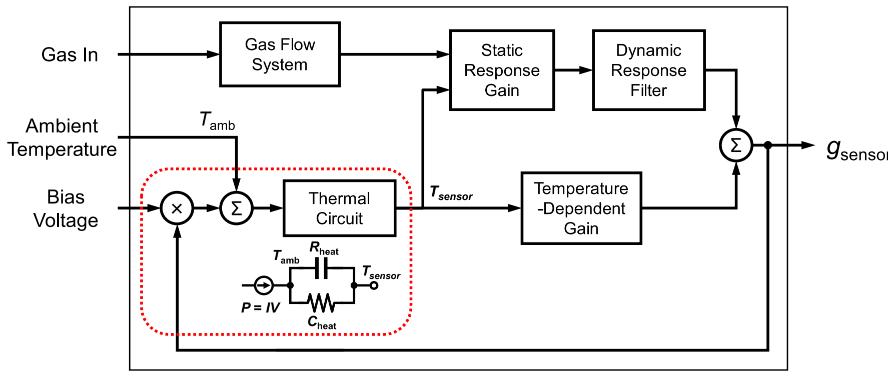


Fig. 4. Self-heated molecule sensor model.

Table 1
Parameters determined by experiments and COMSOL Multiphysics software.

Parameters	Values
G_{0T}	0.0001095[S]
K_{1T}	−0.003043[S/ppm]
E_{A0}	0.01567[eV]
E_{A1}	0.2334[eV]
n_1	3.176[eV^{-1}]
R_{heat}	29.7[K/mW]
G_{heat}	0.0297[uJ/K]

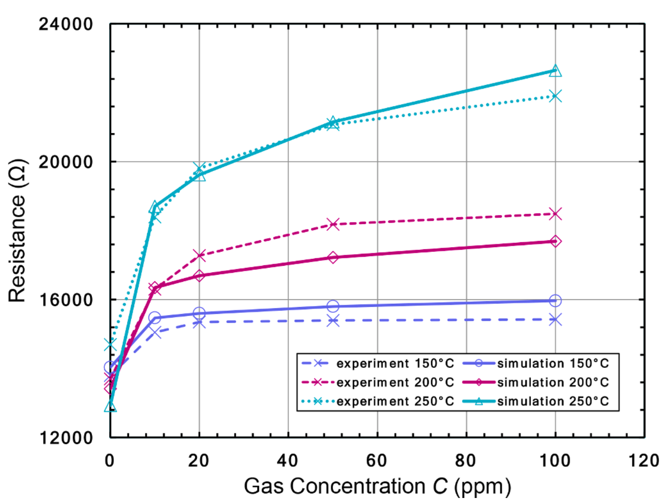


Fig. 5. Comparison of the static responses between the simulated values with the fitting parameters and experiment data.

comparison between simulation and experiment data. Although the sensor drift effects were seen in the no gas phase, the static sensor response value in the simulation followed the experiment resistance change. It was also shown that sensing temperature in the simulations was fluctuate as high as 90 °C when the sensor reacted to NO_2 under a constant bias voltage condition.

5. Conclusion

The self-heated molecular sensor and its compact model were developed. The resistivity of the developed sensor was confirmed by the electrical measurement, and the self-heating effect was ascertained with the thermal simulation in COMSOL Multiphysics. The model parameters were fitted with the results of the thermal simulation and the experimental static responses. The static response gain and temperature-dependent gain were determined by the experimental results, in which the sensor's temperature was configured by the external heater. Even though most of the model parameters were determined without the self-heating effect, the outputs of the simulation model followed the sensor response affected by self-heating. It was also found that there is relatively a large gap between the simulated resistance and a measured sensor resistance due to a drift particularly if the sensor is operated under an inert gas.

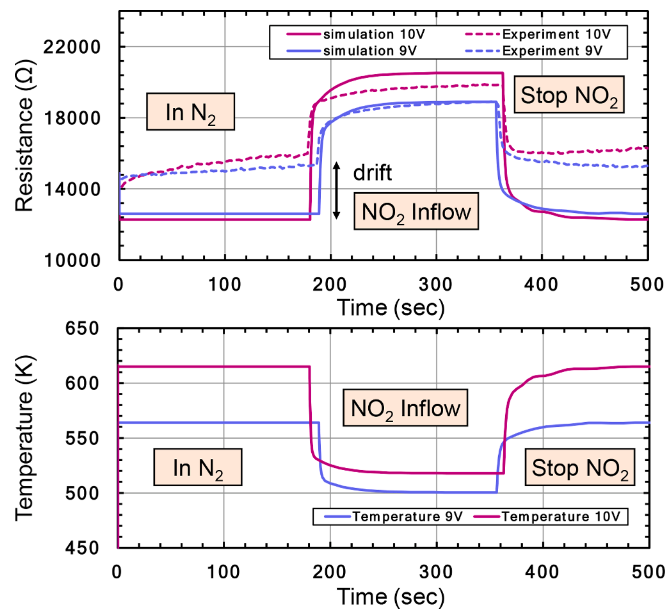


Fig. 6. Comparison of the dynamic responses between the simulated values with the fitting parameters and experiment data.

Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Yohsuke Shiiki reports financial support was provided by Japan Science and Technology Agency. Tsunaki Takahashi reports financial support was provided by Japan Science and Technology Agency.

Data availability

Data will be made available on request.

Acknowledgment

This work has supported by JST SPRING, Grant Number JPMJSP2123. T.T. was supported by JST PRESTO Grant Number JPMJPR19M6, Japan.

References

[1] Tanaka T, Tabuchi K, Tatehora K, Shiiki Y, Nakagawa S, Takahashi T, et al. Low-Power and ppm-Level Multimolecule Detection by Integration of Self-Heated Metal Nanosheet Sensors. IEEE Trans Electron Dev Dec. 2019;66(12):5393–8.

[2] Fàbrega C, Casals O, Hernández-Ramírez F, Prades JD. A review on efficient self-heating in nanowire sensors: Prospects for very-low power devices. Sens Actuators B Chem 2018;256:797–811.

[3] Liu H, Meng G, Deng Z, Nagashima K, Wang S, Dai T, et al. Discriminating BTX Molecules by the Nonselective Metal Oxide Sensor-Based Smart Sensing System. ACS Sens 2021;6(11):4167–75.

[4] Liu H, He Y, Nagashima K, Meng G, Dai T, Tong B, et al. Discrimination of VOCs molecules via extracting concealed features from a temperature-modulated p-type NiO sensor. Sens Actuators B Chem 2019;293:342–9.

[5] Hossein-Babaei F, Amini A. A breakthrough in gas diagnosis with a temperature-modulated generic metal oxide gas sensor. Sens Actuators B Chem 2012;166–167: 419–25.

[6] Llobet E, Vilanova X, Brezmes J, López D, Correig X. Electrical equivalent models of semiconductor gas sensors using PSpice. Sens Actuators B 2001;77:275–80.

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