PSpice Model of Hydrogen Nanosensors and Ultraviolet Photodetectors

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***Abstract* — In this work is presented PSpice circuit models of hydrogen gas nanosensor using individual zinc oxide nanowire with fast response at room temperature and of an individual ZnO microwire-based ultraviolet (UV) photodetector. The model of hydrogen nanosensor depicts the dynamic response to 100 ppm gas concentration at room temperature and influence of the UV irradiation on electrical resistance of the material. The model of photodetector depicts the transient response to UV light (365 nm) and variation of the electrical resistance in the dark and under UV illumination for different relative humidity RH values. The models have been studied using Cadence software student version, and are based on the physical and chemical proprieties of the metal oxide sensing material.**

***Index Terms* — Equivalent Circuit, Nanosensor, Photodetector, PSpice, ZnO.**

I. INTRODUCTION

In the past decade, ultraviolet rays reaching the earth's surface have intensified due to increasing stratospheric ozone depletion, and they may cause adverse effects on the human body, like high skin cancer rates, etc.

In this connection there is a strong motivation for the development of small, low-cost, robust, and efficient UV detectors able to work in diverse conditions and that can be installed in different customer electronic devices easily, and the development of highly sensitive, selective, reliable, and compact sensing devices to detect flammable, toxic, chemical and biological agents [1-8]. However, to integrate such detectors with driving circuits and to simulate it is important to develop its PSpice model. PSpice models makes easy to study characteristics of sensors and can be used to create efficient applications, it helps in the design of new devices and in the interpretation of experimental data [3-4]. These models are based on the physical and chemical proprieties of the sensing nanomaterial. The main feature of the PSpice models presented here is that they can simulate photodetector properties, either when the UV irradiations and relative humidity are modulated using arbitrary functions (concentration pulses, irradiation pulses, etc).

In this work we report on developed PSpice circuit models of hydrogen gas nanosensor using individual zinc oxide nanowire and of an individual ZnO microwire-based UV photodetector. The modes are implemented in Cadence software student version together with associated Schematics, Model Editor and PSpice A/D.

II. SENSING MATERIAL PROPRIETES

In work [1] was developed and studied experimentally the gas response and selectivity of ZnO nanowires to H_2, NH_3, *i*-Butane, CH_4 gases at room temperature. According experimental results as can be seen from Figure 1 gas response of ZnO nanowire is a curve. UV radiation procedure is used to facilitate desorption of gas species from the surface and to improve the recovery time of the nanosensor. Figure 1 (curve 2) demonstrates that the recovery time of the UV radiated sensor is much shorter than that of curve 1 (Fig. 1).

In Figure 2 the device was subjected to irradiation with 365 nm UV light in ambient air with electrical resistance monitoring [2]. The background atmosphere was ambient air with relative humidity (RH) of 53%.

Figure 3 presents the variation of the electrical resistance of ZnO microwire-based detector in the dark and under UV illumination for different RH values.

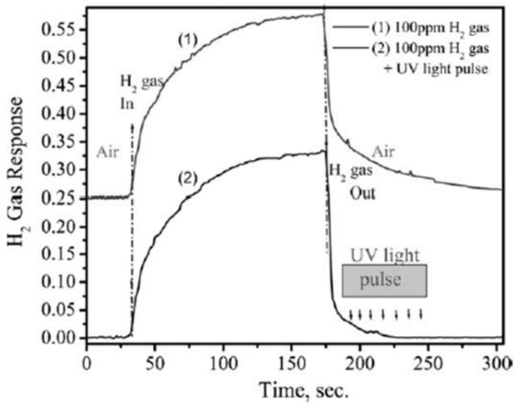

Fig. 1. Gas response curves of the 100 nm ZnO nanowire-based gas sensor under exposure to 100 ppm of H_2 gas at room temperature. Curve (1) is displaced upward by 0.25 to avoid overlapping with curve (2) [1].

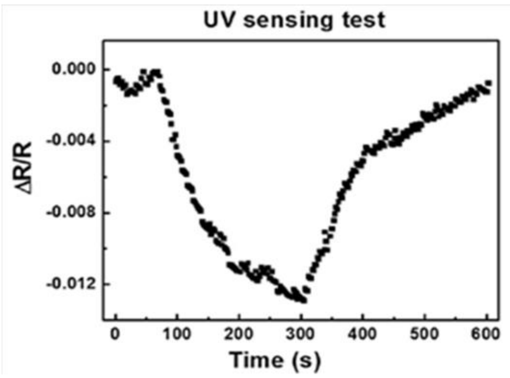

Fig. 2. UV sensitivity measurement of the fabricated single ZnO microwire device structure [2].

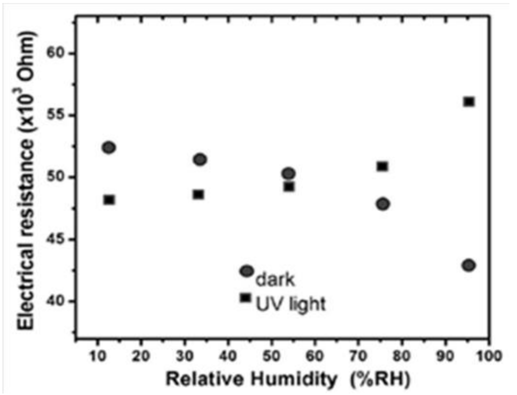

Fig. 3. Dependence of the electrical resistance versus relative humidity in the dark and under UV light [2]

III. EQUIVALENT CIRCUIT

In work [1] the gas response was defined as the ratio:

$$S \approx \left|\frac{\Delta R}{R}\right| \quad (1)$$

where $|\Delta R| = |\Delta R_{air} - R_{gas}|$ and R_{air} is the resistance of the sensor in dry air and R_{gas} is resistance in the test gas.

Figure 4 shows the basic structure of the proposed model for UV photodetector [2], comprising three blocks that represent UV irradiation transfer, influence of relative humidity and adder block. The model has one input V_{uv} for UV light, one input V_{rh} for relative humidity and one input V_{ref} is used for voltage reference.

In Fig. 5 is represented a schematic view of the UV photodetector. For simulation purposes and simplicity reasons, a voltage source emulates the UV irradiation where it is assumed that 1 V corresponds to 1 eV, for instance, the UV irradiation with wavelength range 365 nm, corresponding to photon energy 4.2 eV, can be simulated by supplying a pulse of 4.2 V from pulse source. The relative humidity RH is simulated by supplying a d.c. voltage. The output voltage indicates electrical resistance ratio, where it is assumed that 1 V corresponds to 1 % of relative humidity RH.

The UV block emulates the dynamic sensor response to gas pulses from pulse source V_{uv} and it consist from passive integrator circuit, the RH block simulated influence of relative humidity (RH), because dependence of electrical resistance of photodetector versus relative humidity under the irradiation and in the dark are different (Fig. 3), RH block consist from two voltage controlled switches and two function blocks, UV_Light block simulating dependence of the electrical resistance of photodetector under UV light, and DARK block in the dark. The SUM block evaluates response as a function of the UV irradiation, effects of RH and voltage reference V_{ref} and it consist from a simple adder block. UV sensitivity was defined as 1 % = 1V.

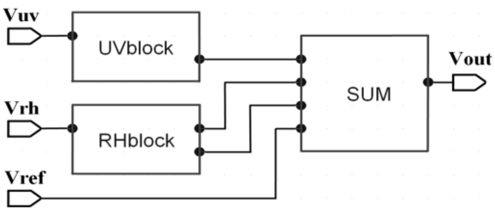

Fig. 4. Block diagram of the purposed model for the UV photodetector.

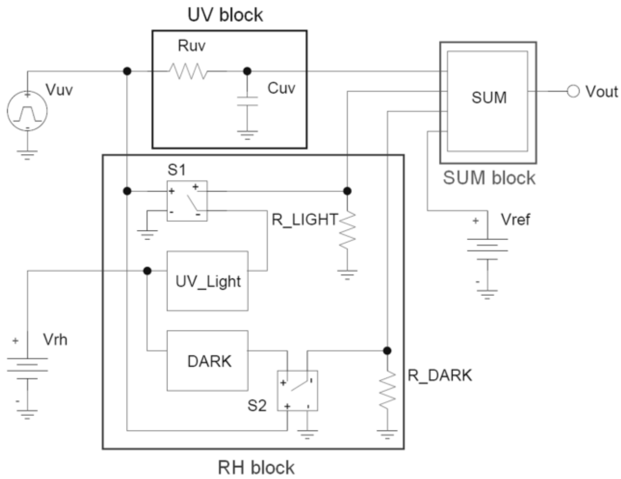

Fig. 5. Bloc diagram and schematic view of the UV photodetector.

In Fig. 6 is represented a developed bloc diagram of the nanosensor [1]. The model has one input V_{gas} for gas concentration, one input for UV irradiation and one input for voltage divider V_{REF}. A voltage divider configuration has been chosen here in order to convert the sensor resistance into a voltage that can be further processed, amplified or interfaced to other devices [3]. For simulation purposes and simplicity reasons, a voltage source emulates the gas concentration where it is assumed that 1 V corresponds to 1 ppm of gas concentration. For instance, the injection of 100 ppm of hydrogen (H_2) gas in air can be simulated by supplying a pulse of 100 V from voltage source. UV source is simulated by PULSE source.

In Figure 7 is represented a schematic view of the gas nanosensor model. The block ns01 that simulates gas transfer (V_{gas}) behavior is also included in the model, and consist from passive integrator circuit and pulse source. The block ns02 simulated UV irradiation (UV) that consist from passive derivative circuit, a simple rectifier diode for exclude a positive pulses after derivation of pulses of UV light and a resistive divider. The block sum evaluate response as a function of the gas concentration and UV irradiation, the block ns03, that represents a integrator circuit and a diode for excluding negative values of the final response, emulates the dynamic sensor response to gas pulses. Due for R_{fil} it is possible to set the gas response.

The gas response was defined as 1 % = 1 V. Experimental deduced formula for gas response S:

$$S = \frac{1}{2} \cdot \left(V_{gas} \cdot \frac{R_{FIL}}{R_{REF} \cdot R_{FIL}} \right) \quad (2)$$

where S is gas response, V_{gas} is gas concentration pulse

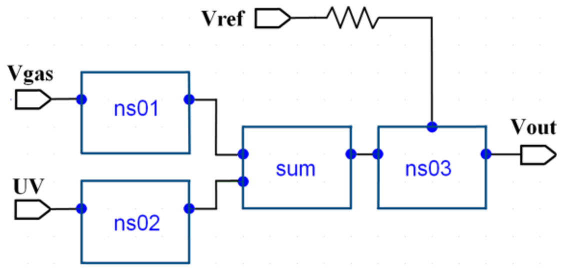

Fig. 6. Block diagram of the purposed model for the gas nanosensor.

value (parameter V2 from Table II), R_{FIL} is value of resistance from block ns03 and R_{REF} is a value of reference resistance. Formula 2 is available if $R_{REF} = R_{FIL}/2$.

IV. PSPICE MODEL

On the base of equivalent circuit shown on Fig. 5 and Fig. 7 were created subcircuit files SUBCKT and included in the library of PSpice A/D with extension .lib for each model (not shown).

UV photodetector model

The voltage controlled switch is a special kind of voltage controlled resistor. The voltage between the <(+) switch node> and <(-) switch node> depends on the voltage between the <(+) controlling node> and <(-) controlling node>. The resistance varies between the R_{ON} and R_{OFF} model parameters.

Values of the model parameters used for the simulation:

UV photodetector

TABLE I. VALUES OF MODEL PARAMETERS FOR THE UV PHOTODETECTOR

Parameter	SIGNIFICATION	Value
RH	relative humidity	53
R_UV	resistance from UVblock	1×10^3
C_UV	capacitance from UVblock	3×10^{-4}
DARK_S	dark sensibility	1×10^{-6}
UV_S	UV light sensibility	5×10^{-3}
UV	UV irradiation	4.2
R_0dark	electrical resistance when RH is 0 % under the light	5.2×10^{-2}
R_0light	electrical resistance when RH is 0 % in the dark	4.2×10^{-2}

Selective hydrogen nanosensor

TABLE II. VALUES OF MODEL PARAMETERS FOR NANOSENSOR

Parameter	SIGNIFICATION	Value
UV	UV irradiation source	50
TD	delay time from time zero of the first rising edge of V_{gas}	10
PW	pulse width for V_{gas}	100
PER	period	145
V2	gas concentration	100
T	rise and fall time	1×10^{-6}
Cgas	capacitance from block ns01	2.5
C_UV	capacitance from block ns02	0.15
C_fil	capacitance from block ns03	2×10^{-3}
R_gas	resistance from block ns01	10
R_UV	resistance from block ns02	100
R_fil	resistance from block ns03	2×10^3
V2_gas2	pulse value for source Vgas2	{V2 × 0.5}
TD_gas2	delay time for source Vgas2	{TD + PW}
TF_gas2	fall time for source Vgas2	{PER-PW+TD}
PW_gas2	pulse width for source Vgas2	{TF_gas2×0.1}
R_refer	Reference resistance R_{REF}	{R_fil/2}

Parameters for voltage controlled switches (Fig. 5):

S1 – $R_{ON} = 0.1$, $R_{OFF} = 1\cdot10^9$, $V_{ON} = -0.2$, $V_{OFF} = 0$;

S2 – $R_{ON} = 1\cdot10^9$, $R_{OFF} = 0.1$, $V_{ON} = -0.2$, $V_{OFF} = 0$;

where R_{ON} – on resistance (units in Ohm), R_{OFF} – off resistance, V_{ON} – control voltage for on state (units in Volts), V_{OFF} - control voltage for off state.

When value of PULSE voltage source V_{UV} is 0 V resistance of both switches are totally different, S1 have a minimal value (0.1 Ω), S2 have a maximal value (1 MΩ).

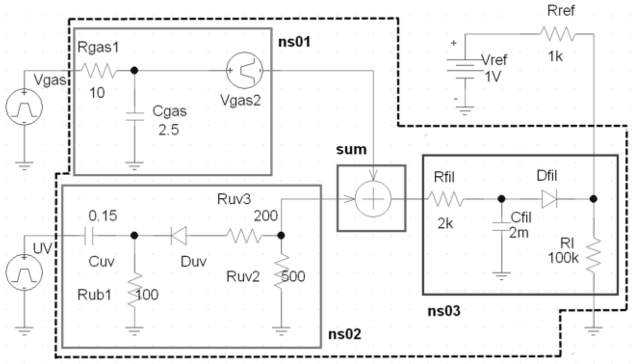

Fig. 7. Bloc diagram and schematic view of the nanosensor PSpice model and the potential divider circuit used to test the nanosensor in simulation process.

From these considerate signal will flow through UV_light to SUM block. When value of source is less than 0.2 V resistance of switch S1 will change to maximal value and resistance from S2 to minimal value, signal from V_{RH} source will flow through DARK block. Each block from RH_block cell processed signal by a particular function. UV_Light cell function from RH block it's an exponential function:

$$R = R_{0light} + S_{light} \cdot exp(V \cdot k) \quad (3)$$

where R is electrical resistance under UV light, R_{0light} is electrical resistance when RH is 0 % under the light, S_{light} is UV light sensibility, V is the voltage value and k is an experimental coefficient. DARK cell function:

$$R = R_{0dark} + S_{dark} \cdot V^2 \cdot V \quad (4)$$

where R is electrical resistance in the dark, R_{0dark} is electrical resistance when RH is 0 % in the dark, S_{dark} is dark sensibility, V is the voltage value.

With R_{0light} and R_{0dark} parameters is possible to install the photodetector resistance under the radiation and respectively in the dark environment, with S_{ligh} and S_{dark} parameters is installed influence of relative humidity.

V. RESULTS

To check the validity of the developed PSpice models it was used to simulate the responses of UV photodetector to UV irradiation and selective hydrogen nanosensor to 100 ppm of H_2 concentration. First was checked the photodetector. The pulse with width 75 s was applied from V_{UV} source and 53 V was applied from V_{RH} source.

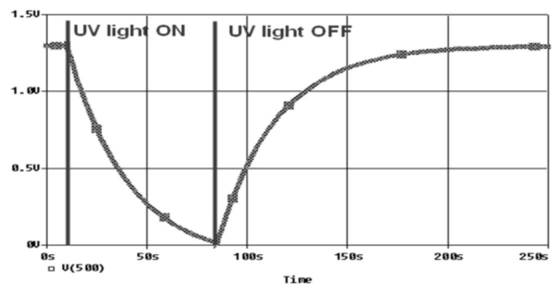

Fig. 8. Results of simulation UV photodetector PSpice model.

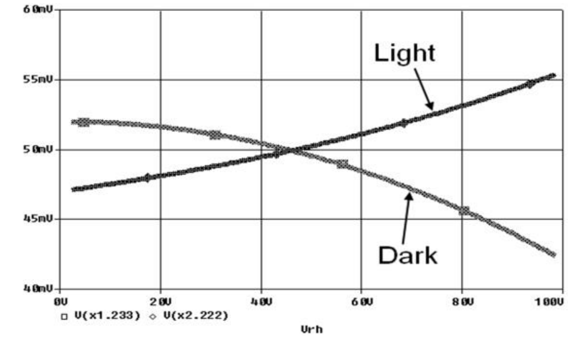

Fig. 9. Results of simulation electrical resistance versus RH in the dark and under UV light.

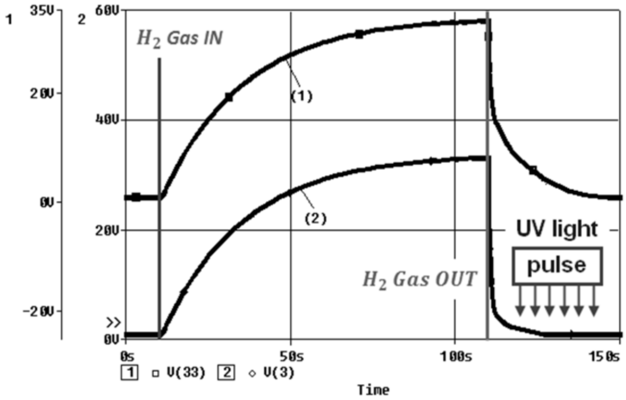

Fig. 10. Results of simulation gas nanosensor PSpice model. (1) 100 ppm H_2 gas, (2) 100 ppm H_2 gas + UV light pulse. Curve (1) is displaced up to

Fig. 8 demonstrates that the PSpice model accurately depicts the dynamic response of a model to irradiation exposure. Dependence of the electrical resistance versus RH in the dark and under UV light is represented in Fig. 9. It can be seen that results are in conformity with physical proprieties of sensing material (Fig. 3). Developed model permits to simulate photodetector curves in PSpice software. The ability of the nanosensor model to emulate the response in the presence of 100 ppm hydrogen concentration was also checked. The pulse with width 100 s and value of 100 V was applied from V_{GAS} source. After gas pulse ends, it was applied a pulse with width 45 s from UV source. Results of simulation nanosensor are presented in Fig. 10, curve 2 demonstrates that the recovery time of the UV radiated nanosensor is much shorter than that of curve 1. Model of nanosensor displayed the gas response of about 34% to 100 ppm hydrogen gas. It can be seen that proposed and developed PSpice model of H_2 nanosensor is able to depict the nanosensor transient and to reproduce experimental curves presented in Figure 1.

VI. CONCLUSION

It was developed PSpice circuit models for hydrogen gas nanosensor and for UV photodetector. To verify the validity of the developed PSpice models it was simulated the responses of UV photodetector to UV irradiation and hydrogen nanosensor to 100 ppm of H_2 concentration.

It was demonstrated that simulations results are in good agreement with the experimental data. Proposed models can be used in studying of gas nanosensor based on individual ZnO nanowire and an individual ZnO microwire-based UV photodetector in different circuit with PSpice models. The PSpice tool and, particularly, its analog behavioral model blocks are shown to be very effective and flexible for model building [9].

ACKNOWLEDGMENTS

This research was performed with the financial support of the STCU and ASM through Grant 09 STCU.A/5833.

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