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Analysis of nanowire transistor based nitrogen dioxide gas sensor – A simulation study

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ABSTRACT

Sensors sensitivity, selectivity and stability has always been a prime design concern for gas sensors designers. Modeling and simulation of gas sensors aids the designers in improving their performance. In this paper, different routes for the modeling and simulation of a semiconducting gas sensor is presented. Subsequently, by employing one of the route, the response of Zinc Oxide nanowire transistor towards nitrogen dioxide ambient is simulated. In addition to the sensing mechanism, simulation study of gas species desorption by applying a recovery voltage is also presented.

1. Introduction

Since their invention, semiconductor gas sensors has been actively investigated and groups worldwide have been reporting their findings on the improvement in sensors sensitivity, selectivity and stability [1,2]. Some of theses reports, includes mathematical modeling and simulation studies which elaborate upon the sensing mechanism of semiconducting sensors [3–5]. Supan et al. developed a theoretical model to understand the chemical reaction taking place on titanium nitride based ammonia sensor and derives adsorption and desorption reaction rate equations [4]. Guerin et al. developed a dynamic model for the tungsten oxide based ozone sensors. The model takes semiconductor surface modification upon ozone exposure into consideration and allows the calculation of the conductivity according to the ozone concentration present in the atmosphere [6]. In a different modeling and simulation approach, Soares et. al develops a model for a three terminal nanowire field effect transistor (FET) sensor. While Supan and Guerin considered the surface modification causing the response, Soares et al. developed the model by considering the semiconductor device physics to explain the device response in the presence of analytes [7]. It may be infer that the modeling or simulation of semiconducting sensors enables the sensor designers in understanding the sensing mechanism. Moreover, it aids sensor designers in deciding the structure and its parameters such as contact material, channel dimensions, semiconductor doping and biasing conditions for achieving maximum sensitivity. In this paper, the various routes for simulating and modeling a semiconducting gas sensor response is presented. Subsequently, by employing one of the route, response of a field effect transistor based device is simulated and compared with the experimental results reported elsewhere. Electrodesorption is sensors recovery method [8] in which the adsorbed gas molecules on the semiconductor surface are removed by applying a voltage at gate terminal, simulation results are presented to elaborate upon the mechanism behind this method of recovery, such a study will help the potential sensors designers in designing an efficient semiconducting gas sensor with an effective electrodesorption based recovery mechanism.

2. Various modeling and simulation routes

In Fig. 1 the various routes for modeling/simulation of a gas sensor are identified. Computational software program such as Matlab/Mathematica can be used for simulating chemisorption induced surface bending, surface potential and theoretical verification of current through sensor. For analyzing the field effect based sensors response in steady state, Technology Computer Aided Design (TCAD) software such as SILVACO or Sentaurus can be used. Whereas, for the transient analysis of these field effect based sensors, one can use simulation packages such as COMSOL and Matlab in conjunction.

The various method of simulating a gas sensor can be classified into three paths, and each path includes the device physics involved when a sensor is exposed to a gas. Exposure of semiconductor surface to target gas will induce chemisorption effect, which leads to the change in device characteristics such as

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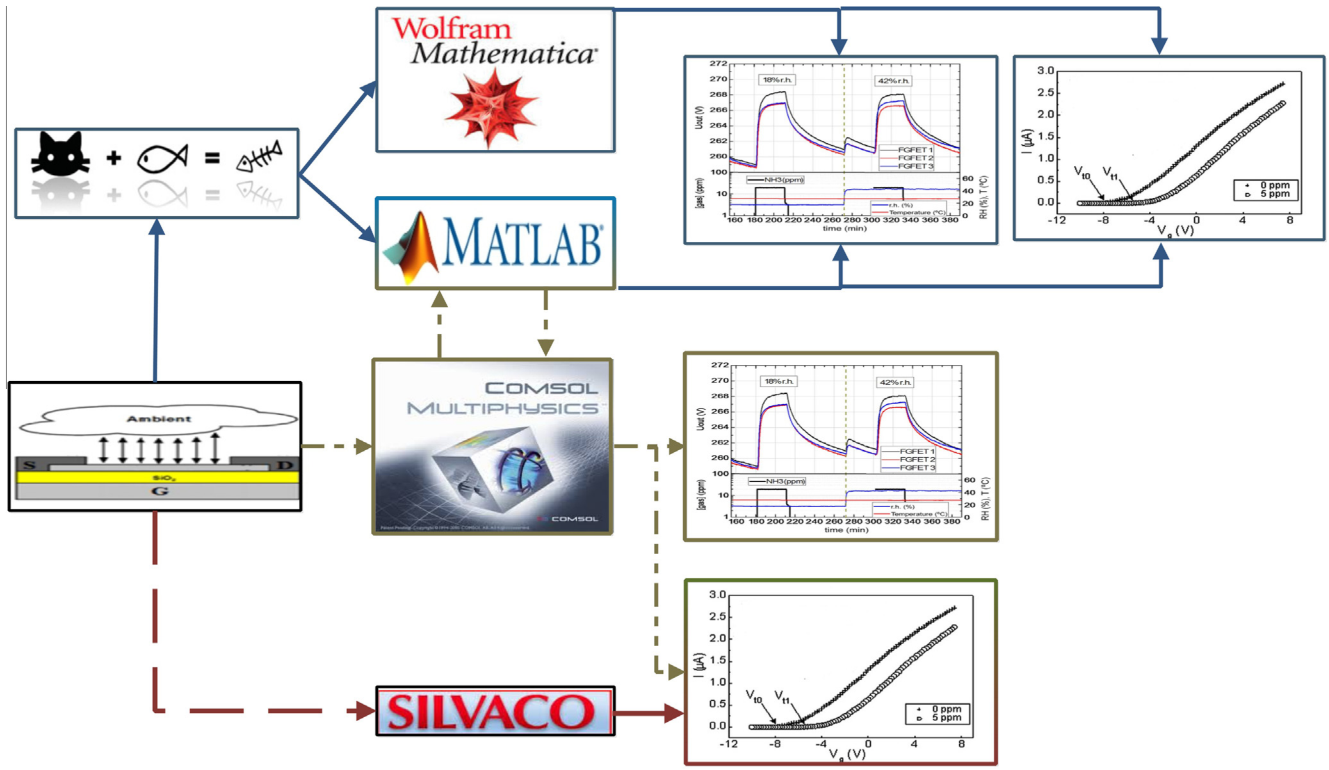

Fig. 1. Various simulation/modeling methods for gas sensor. Identified paths I, II and III are shown in blue, green and red color respectively. Transient and steady state responses are for illustration only [4,8] and all computational packages mentioned, are proprietary software. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

channel/carrier concentration modulation, Schottky barrier formation or contact transformation. As shown in Fig. 1, path one involves, the sensor's governing equations which are often solved simultaneously to analyze the device response to the targeted ambient. These coupled equations can be solved iteratively using mathematical packages such as Mathematica or Matlab. The second path identifies an another possible approach, in which, the influence of ambient gas on the semiconductor surface can be analyzed in the steady or transient state. The second path defines the method to simulate the sensor characteristics by combining finite element analysis (FEA) and/or finite difference method (FDM)/finite element method (FEM) simulations. The surface bending and chemisorption effect is captured using mathematical packages such as Matlab/Mathematica. And the device equations can be handled with a FEA simulators such as COMSOL [9]. By using both the computational packages in conjunction, where the surface bending results from the mathematical package will be called to the FEA simulator for obtaining the sensor response. Therefore, this path can lead to the extraction of both steady state and transient response. In the third path, the gas sensing response can be obtained by defining the sensor structure and material properties in a TCAD simulator and considering the steady state surface bending which may lead to the sensor's steady state response.

3. Device structure

The device structure investigated in this section is a back gated field effect device reported in [8] (Fig. 2(a)), an n-type Zinc Oxide (ZnO) nanowire as the sensing layer. A heavily doped p-substrate act as gate, silicon dioxide (SiO_2) as gate oxide and Ni/Au metal is used for source and drain contacts. The work function difference between the contact metal and the ZnO leads to the formation of non-ohmic contacts with depletion widths (d_{SC} and d_{DC}). The depletion width due to the oxide-semiconductor work-function difference is depicted as d_2 in Fig. 2(b).

4. Result and discussion

By following the third route which is depicted in Fig. 1, the structure described in [8] is simulated in a TCAD software [10] for its change in the threshold voltage with exposure to target NO_2 gas. When the ZnO nanowire surface is exposed to the oxidizing gas (NO_2 in this case) the surface depletion width increases and the effective channel thickness reduces and therefore the voltage required to deplete the channel reduces. Figs. 3 and 4 shows the simulated transfer ($I_D - V_{GS}$) and output ($I_D - V_{DS}$) characteristics respectively. As can be seen from the figure, upon an exposure to 5 ppm of NO_2, a 2.5 V shift in the threshold voltage can be observed in simulated results. The device parameters used for the simulation study are depicted in Table 1.

4.1. Concept of recovery: electrodesorption effect

Electrodesorption is a self-contained method of sensor's recovery in which sensor does not require any other means such as UV illumination or sensors heating, to desorb [8]. Electrodesorptions takes advantage of the FET device structure and simplifies the design of chemical sensors. In this method, a high gate potential is applied to refresh the surface of exposed nanowire chemical sensor. For the device structure under consideration, sensors surface is refreshed by applying a large negative gate voltage (Fig. 5), by which bands are moved temporarily such that the channel is p type and the surface electrons are desorbed and returns to the channel. It is know that, the maximum surface band bending at which the