Simulation of ZnO/Si Nanowires p-n Heterojunction Microarrays Diode Based Gas Sensor

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INTRODUCTION: In recent years, gas sensors are commercially available for use in healthcare as new vistas for technological application. In this work we report ZnO/Si NWs hetero-junction array based NO gas sensor operating at room temperature with extremely high response (noise limited response ~ 10 ppb). We observe that the heterostructure leads to a synergetic effect where the sensing response is more than the sum total of the individual components, namely the ZnO and the Si NWs. We make a physical electrical circuit model for simulation by COMSOL Multiphysics®

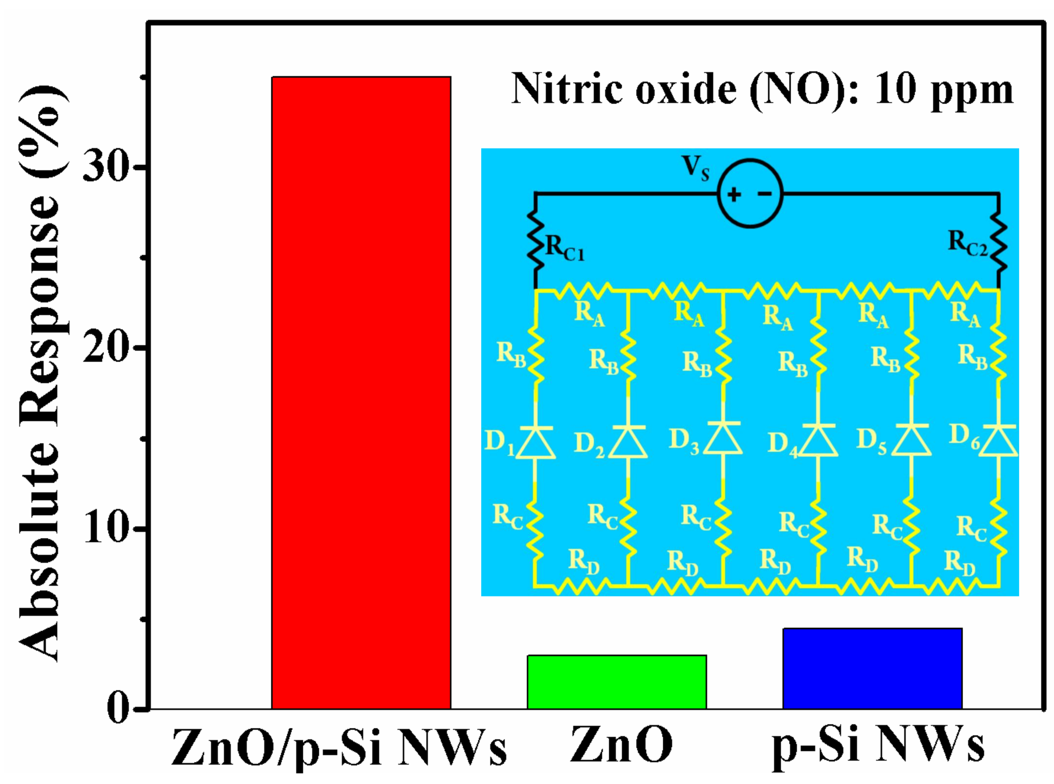

Figure 1. Comparison of absolute gas sensing response |Ř| of ZnO/p-Si NWs, ZnO and p-Si NWs to 10 ppm of NO gas at room temperature with electrical circuit model

COMPUTATIONAL METHODS: For simulation of device parameters we make electrical circuit (Fig 2) based on physical geometry of p-n heterojunction with analysis of cross-sectional electron microscopy of device with Electrical circuits (cir) interface of AC/DC module based COMSOL Multiphysics®. The electrical model analysis is based on finite number of resistors and p-n junctions which are meant to capture the essential physical process. In real device there are larger number of resistors and p-n junctions. Thus the quantification of parameters from the model that we obtained from finite number of circuit elements will be treated as suggestive than rigorous.

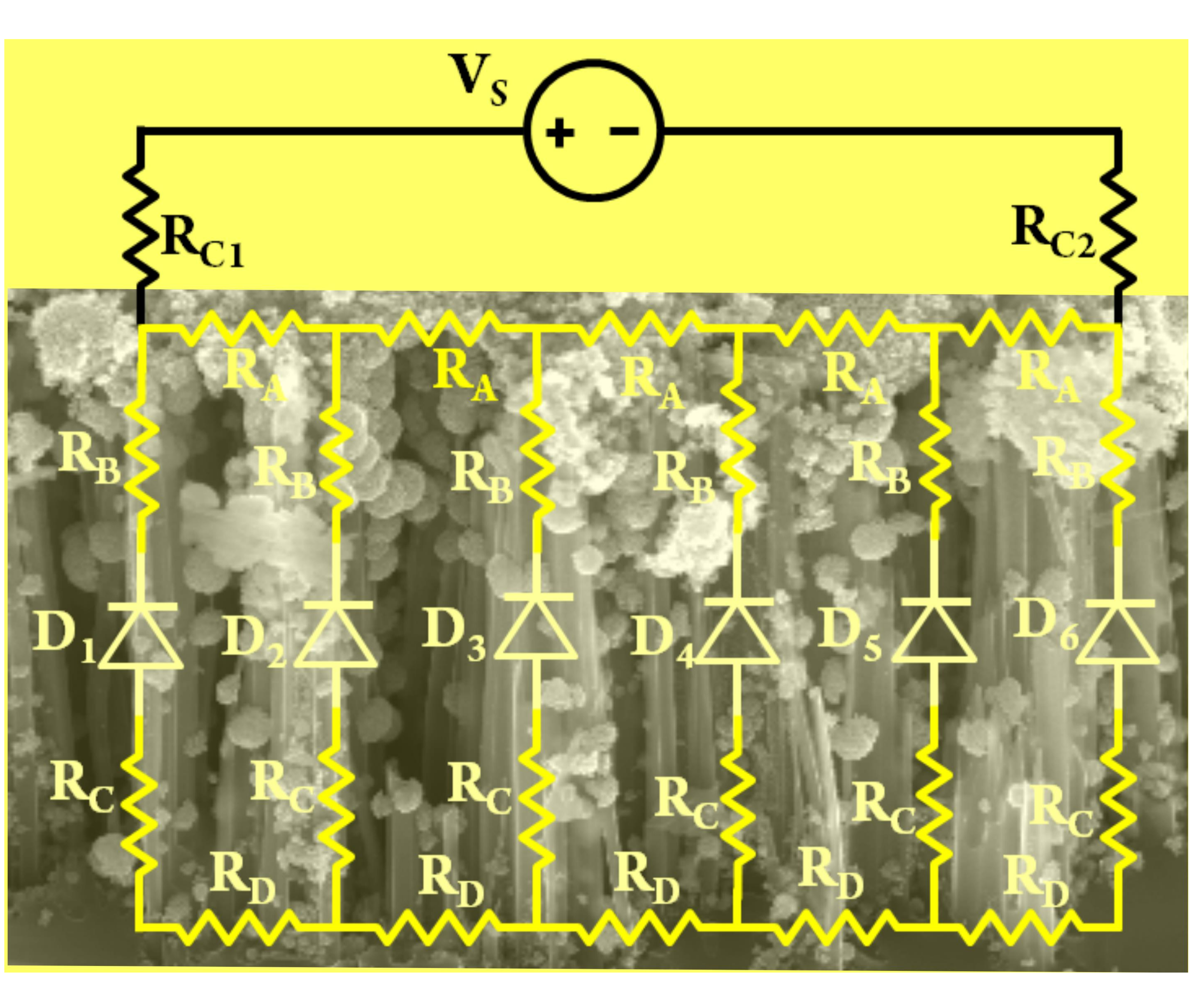

Figure 2. A physical model of the sensor with schematic of the electrical model embedded on SEM with it.

RESULTS: The comparison of the simulation results with the experiment identifies the materials parameters that enhance the device response. The characteristics values of the parameters for the best fits obtained from the simulation are given in Table 1.

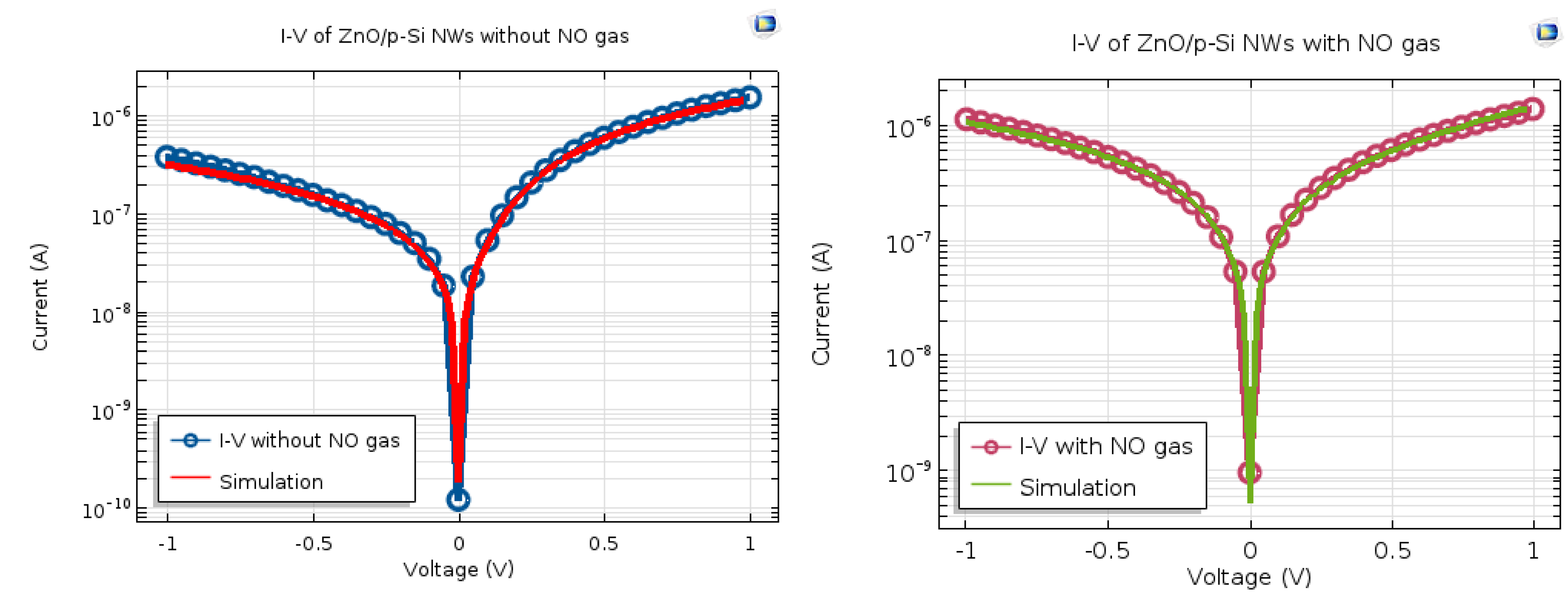

Figure 3. (a) Simulation I-V data fitted with experimental data before NO gas exposure. (b) after NO gas exposure of ZnO/p-Si NWs sensor.

Characteristics of p-n junction	Before gas expose	After gas expose	Percentage change
Saturation current (I_0)	5.34x 10^{-9} Amp	9.05 x 10^{-9} Amp	70 %
Resistance of ZnO (R_A)	785 kΩ	295 kΩ	62 %
Series resistance of p-n junction (R_B)	130 kΩ	70 kΩ	46 %
Series resistance of p-n junction (R_C)	100 kΩ	40 kΩ	60 %
Resistance of Si NWs arrays (R_D)	25 kΩ	20 kΩ	20 %

Table 1. Characteristics value of ZnO/Si NW p-n heterojunction before and after Nitric oxide (NO) gas exposure of 5 ppm

From Table 1, it can be seen that all the parameters undergo change in the electrical model and this leads to enhancement of current in the device on gas exposure. Note: The main inference from the simulation is that the observed high performances of the sensor device depends on change in resistances of the constituents as well change in the reverse saturation current at the ZnO/p-Si NW p-n junction.

CONCLUSIONS: In this section we make an electrical model of the device and then make an analysis of the device model by simulation of the device electrical characteristics using COMSOL Multiphysics® software. The physical model proposed is given in Figure 2 that has been obtained from detailed cross-sectional microscopy. The electrical model is laid out on the same figure, which is an array of p-n junctions and resistor arrays.

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