

# HYDROGEN SENSOR BASED ON SILICON CARBIDE (SiC) MOS CAPACITOR

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**Abstract**—Silicon carbide (SiC) based MOS capacitor devices are used for gas sensing in high temperature and chemically reactive environments. A SiC MOS capacitor structure used as hydrogen sensor is defined and simulated. The effects of hydrogen concentration, temperature and interface traps on C-V characteristics were analysed. A comparison between structures with different oxide layer types (SiO<sub>2</sub>, TiO<sub>2</sub> and ZnO) and thicknesses (50..10nm) was conducted. The TiO<sub>2</sub> based structure has better performance than the SiO<sub>2</sub> and ZnO structures. Also, the performance of the SiC MOS capacitor increases at thinner oxide layers.

**Keywords:** SiC, MOS capacitor, hydrogen sensor

## 1. INTRODUCTION

MOS capacitors based on silicon carbide are widely used as hydrogen and hydrocarbon sensors in high temperature and chemically reactive environments. The use of silicon carbide enables the sensor to operate at temperatures in excess of 1200K because of its large band gap (2.86eV in the case of 6H-SiC). In addition, silicon carbide is chemically stable making it well suited for harsh environment sensing applications [1, 2].

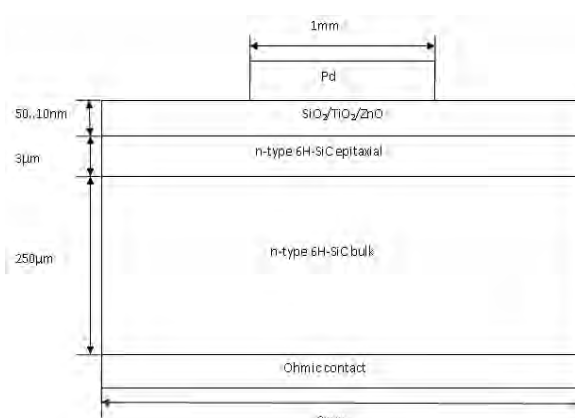
This paper presents the performance of a silicon carbide MOS capacitor used as a hydrogen sensor. Different oxides and oxide layer thicknesses were employed. The change in C-V characteristics due to hydrogen concentration, temperature and interface states have been obtained by extensive simulations.

## 2. SIMULATION METHODS

The general SiC MOS capacitor structure used to simulate the hydrogen sensors is

illustrated in Fig. 1. It consists of a 250μm 6H-SiC substrate with a doping of  $5 \times 10^{18} \text{ cm}^{-3}$ . On top of the bulk, an epitaxial layer is considered with a concentration of  $2 \times 10^{16} \text{ cm}^{-3}$ . Over the epitaxial layer a 50nm oxide is deposited. Different oxides were employed: SiO<sub>2</sub>, TiO<sub>2</sub> and ZnO. In the SiO<sub>2</sub> case, several thicknesses between 50nm and 10nm were also considered. The metal electrode is Pd because hydrogen has a high solubility in this material.

When the structure is introduced in hydrogen environment, the gas molecules dissociate in contact with the Pd electrode at temperatures as low as 150°C. A part of the hydrogen atoms are absorbed at the metal surface and some diffuse into the metal until they reach the metal-oxide interface. Here, they produce a dipole layer that decreases the work function of the metal. This reduces the flat band voltage of the MOS capacitor which results in a parallel shift of the sensor C-V characteristic towards negative voltages [3].



**Fig. 1.** General structure of simulated SiC MOS capacitor hydrogen sensor.

At temperatures above 700K, the hydrogen atoms diffuse through the insulator too until they reach the oxide-semiconductor interface. Here, these atoms passivate the interface state charges. This passivation reduces the concentration of traps and causes a shorter transition from accumulation to inversion on the sensor C-V characteristic [3]. The process is reversible but not very stable [4].

The sensor response to gas ambient (hydrogen) is obtained by keeping the device at a constant capacitance in the depletion region and measuring the voltage needed to maintain that capacitance [4].

First, the influence of oxide type and oxide layer thickness on the MOS capacitor C-V characteristic was analyzed. The simulations were performed in MEDICI [5] at a temperature of 1000K, in an inert environment and with interface states of  $1 \times 10^{12} \text{ cm}^{-2}/\text{eV}$  [6].

Then, the change in the C-V characteristics with hydrogen concentration was investigated. MEDICI does not offer the possibility to simulate different gas concentrations in the external environment. Thus, in order to simulate a hydrogen environment, the work function of the metal was changed in accordance with the experimental C-V characteristics shifts published in literature [2, 7, 8]. A reduction of the work function from 5.12eV (the value for Pd in inert environment) to 4.12eV was employed in order to simulate the entire hydrogen concentration range in the environment. The same hydrogen absorption was considered for all structures. The simulations were performed at a temperature of 1000K.

The influence of temperature on the C-V characteristics was investigated. Simulations were performed at 700K and 1000K in inert environment.

The influence of interface states concentration on the C-V characteristic was also analyzed. Simulations were conducted with concentrations of  $1 \times 10^{12} \text{ cm}^{-2}/\text{eV}$  and  $6 \times 10^{10} \text{ cm}^{-2}/\text{eV}$ , at the temperature of 1000K in inert environment.

Because MEDICI is a 2D simulator, the capacitance values of the simulated MOS structures are expressed in  $\text{F}/\mu\text{m}$ . The difference between the dielectric constants of the oxides tested (3.9 for  $\text{SiO}_2$ , 31 for  $\text{TiO}_2$  and 10 for  $\text{ZnO}$ ) causes a large variation of the accumulation region capacitance values. In order to compare these oxides performance the  $C/C_{\text{OX}}$  ratio as a

function of bias voltage was preferred. The same technique was used for the structures based on  $\text{SiO}_2$  layer with different thickness.

### 3. RESULTS

#### 3.1. Oxide Type and Thickness Variation

The C-V characteristics of  $\text{SiO}_2$ ,  $\text{TiO}_2$  and  $\text{ZnO}$  based MOS capacitor structures with the same geometry are illustrated in Fig. 2. It can be observed that the transition from accumulation to inversion shortens as the dielectric constant increases. Thus, the largest depletion region slope is found at the SiC MOS structure with  $\text{TiO}_2$  oxide layer.

In Fig. 3 the simulated C-V characteristics of the structures with  $\text{SiO}_2$  thickness between 50nm and 10nm are evinced. The change in the C-V curves is similar to the one in Fig. 2. As the oxide thickness decreases, the transition from accumulation to inversion shortens.

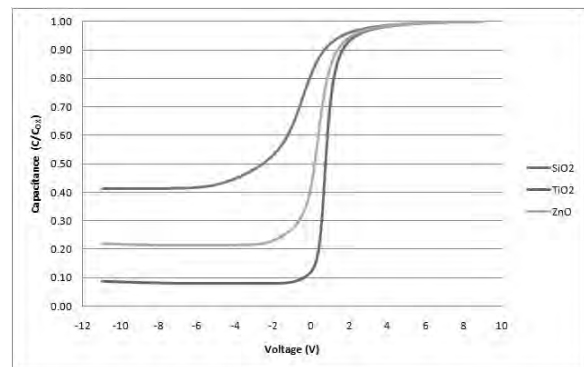


Fig. 2. C-V characteristics of  $\text{SiO}_2$ ,  $\text{TiO}_2$  and  $\text{ZnO}$ -based SiC MOS capacitors

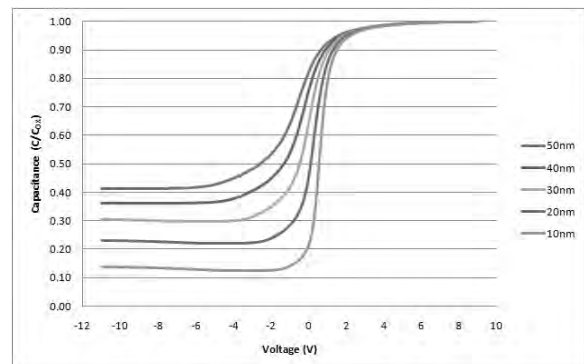


Fig. 3. C-V characteristics of  $\text{SiO}_2$ -based SiC MOS capacitors with different oxide thickness

From both figures it can be concluded that the slope of the depletion region increases with the oxide capacitance.

### 3.2. Work Function Variation

The changes in the C-V curves of the structures with different oxide layer type and thickness are shown in Figs. 4-5. The interrupted lines signify an environment with hydrogen (a value of 4.12eV of the work function was used in the simulation). The continuous lines represent the inert environment with a value of 5.12eV for the metal work function.

By comparing the course from Figs. 4-5, one can observe the same voltage shift induced in the C-V characteristics. This means that the oxide type and oxide layer thickness respectively do not influence the change in the C-V curves when the same hydrogen absorption is considered. Thus, the only phenomenon responsible for the different voltage shifts in the real MOS capacitor structures, for the same environmental gas concentration, is the absorption capacity of the metal and oxide layers employed.

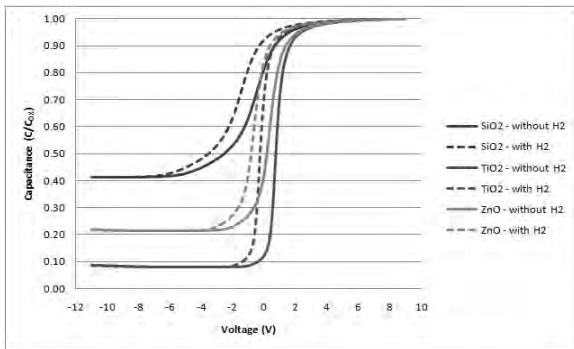


Fig. 4. C-V characteristics of SiO<sub>2</sub>, TiO<sub>2</sub> and ZnO-based SiC MOS capacitors in inert and hydrogen environments.

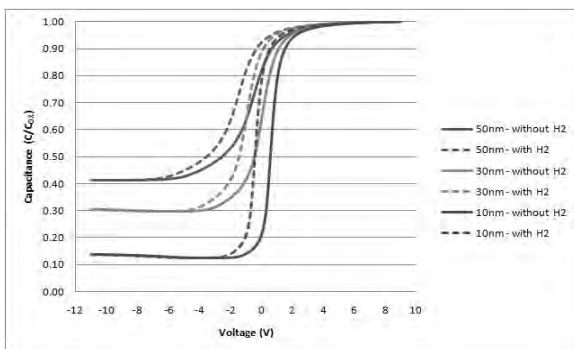


Fig. 5. C-V characteristics of SiO<sub>2</sub>-based SiC MOS capacitors with different oxide thickness in inert and hydrogen environments.

### 3.3. Temperature Variation

The C-V characteristics of MOS structures at temperatures of 700K and 1000K are depicted in

Figs. 6-7. TiO<sub>2</sub> has the smallest variation with temperature among the three oxides investigated. A high deviation with temperature is observed for ZnO structure (Fig. 6). Also, when the oxide thickness decreases, the temperature variation also decreases (Fig. 7). Note that the change in the depletion region of 50nm TiO<sub>2</sub> structure (Fig. 6) is smaller than the one of SiO<sub>2</sub> structure with only 10nm thickness. Instead, this SiO<sub>2</sub> structure has a smaller change of the capacitance in the inversion region. As mentioned before, the hydrogen concentration measurement implies keeping the sensor at a constant capacitance in the depletion region while measuring the voltage necessary to keep that capacitance. Thus, the change with temperature in the depletion region of C-V characteristic has to be as small as possible, like in the case of 50nm TiO<sub>2</sub> structure.

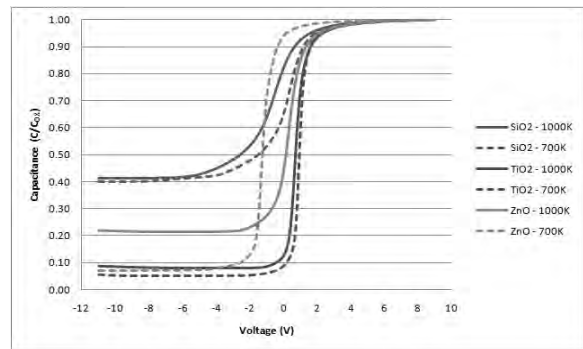


Fig. 6. C-V characteristics of SiO<sub>2</sub>, TiO<sub>2</sub> and ZnO-based SiC MOS capacitors at temperatures of 700K and 1000K.

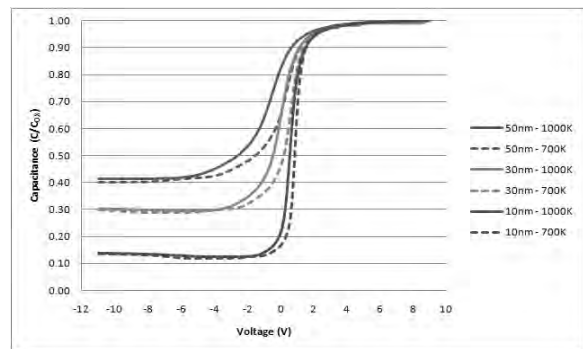


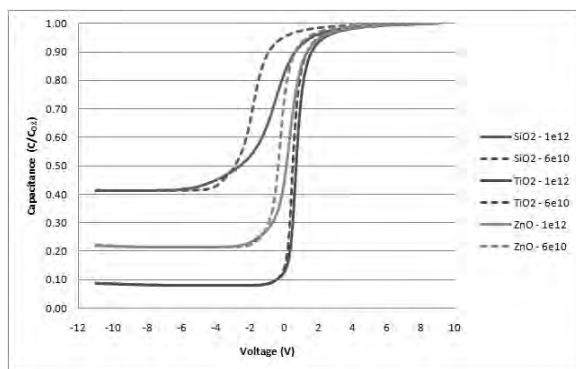
Fig. 7. C-V characteristics of SiO<sub>2</sub>-based SiC MOS capacitors with different oxide thickness at temperatures of 700K and 1000K.

### 3.4. Interface States Variation

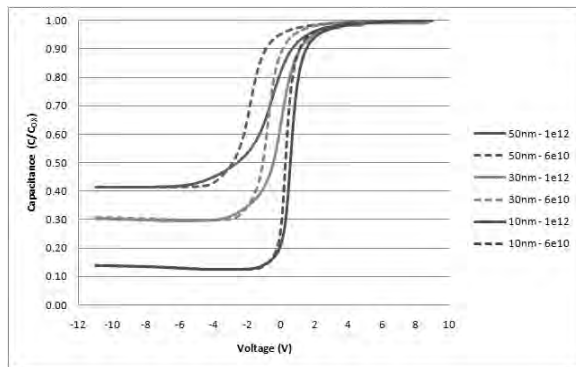
The change in C-V characteristics with oxide-semiconductor interface traps concentration is presented in Figs. 8-9. Since the passivation of interface traps by hydrogen atoms is not a stable

process, it is desired that the influence of interface states concentration on C-V characteristic to be as small as possible [4].

TiO<sub>2</sub> has the slightest variation with interface states concentration, while the SiO<sub>2</sub> structure has the largest one. When the thickness of the oxide layer decreases, the change in the C-V plots is diminished (Fig. 9). Thus, it can be concluded that the influence of interface states on MOS capacitor C-V characteristic decreases with the increase of the oxide layer capacitance. If we also compare the variations of 50nm TiO<sub>2</sub> (Fig. 8) and 10nm SiO<sub>2</sub> (Fig. 9) structures, we can observe that TiO<sub>2</sub> structure has a smaller shift in the C-V curve.



**Fig. 8.** C-V characteristics of SiO<sub>2</sub>, TiO<sub>2</sub> and ZnO-based SiC MOS capacitors with interface states concentrations of  $1 \times 10^{12} \text{ cm}^{-2}/\text{eV}$  and  $6 \times 10^{10} \text{ cm}^{-2}/\text{eV}$



**Fig. 9.** C-V characteristics of SiO<sub>2</sub>-based SiC MOS capacitors of different oxide thickness with interface states concentrations of  $1 \times 10^{12} \text{ cm}^{-2}/\text{eV}$  and  $6 \times 10^{10} \text{ cm}^{-2}/\text{eV}$ .

#### 4. CONCLUSIONS

The influence of oxide layer type and thickness on SiC MOS capacitor hydrogen sensor performance was investigated.

Simulations of the C-V characteristics in hydrogen environment, at different temperatures and interface states concentrations were performed.

Results obtained by extended simulations show that the shift of the C-V curves is similar for all oxide types and thicknesses investigated when considering the same hydrogen absorption.

The best performance on temperature and interface states concentration variation is obtained by 50nm TiO<sub>2</sub> structure. The change of the oxide layer thickness does not produce a performance as good as the one produced by the change of the oxide type. As a conclusion, a SiC MOS capacitor with a 50nm TiO<sub>2</sub> oxide is recommended for hydrogen detection at elevated temperatures up to 1000K.

#### References

- [1] P. Tobias, B. Golding, R.N. Ghosh, "Sensing Mechanisms of High Temperature Silicon Carbide Field-Effect Devices", in *Proc. of 12<sup>th</sup> International Conference on Solid State Sensors, Actuators and Microsystems*, pp. 416–419, Boston, June 8-12, 2003.
- [2] Adrian Trinchi, Sasikaran Kandasamy, Wojtek Wlodarski, "High temperature field effect hydrogen and hydrocarbon gas sensors based on SiC MOS devices", *Sensors and Actuators B* **133**, pp. 705–716, Elsevier, 2008.
- [3] Mun Teng Soo, Kuan Yew Cheong, Ahmad Fauzi Mohd Noor, "Advances of SiC-based MOS capacitor hydrogen sensors for harsh environment applications", *Sensors and Actuators B* **151**, Elsevier, pp. 39–55, 2010.
- [4] Ruby N. Ghosh, Peter Tobias, Sally G. Ejakov, Brage Golding, "Interface States in High Temperature SiC Gas Sensing", *Proceedings of IEEE Sensors*, **2**, pp. 1120–1125, 2002.
- [5] Synopsys, Inc., "Taurus Medici User Guide", Version Y-2006.06, June 2006
- [6] W. J. Choyke, H. Matsunami, G. Pensl, "Silicon Carbide: Recent Major Advances", *Springer-Verlag Berlin Heidelberg*, 2004.
- [7] Md H. Rahman, Jagdish S. Thakur, Lajos Rimai, Soma Perooly, Ratna Naik, Linfeng Zhang, Gregory W. Auner, Golam Newaz, "Dual-mode operation of a Pd/AlN/SiC device for hydrogen sensing", *Sensors and Actuators B* **129**, Elsevier, pp. 35–39, 2008.
- [8] Sasikaran Kandasamy, "Investigation of SiC Based Field Effect Sensors with Gas Sensitive Metal Oxide Layers for Hydrogen and Hydrocarbon Gas Sensing at High Temperatures", *Doctor of Philosophy Thesis*, School of Electrical and Computer Engineering, RMIT University, Melbourne, Australia, December 2007.