

# Determination of face terminated wet thermal oxidation rates in 4H-SiC substrate

Sanjeev K. Gupta<sup>1,2</sup>, A. Azam<sup>2</sup>, R.R. Bhatia<sup>1</sup>, R.N. Soni<sup>1</sup> and J. Akhtar<sup>1</sup>

<sup>1</sup>Sensors and Nano-Technology Group, Semiconductor Devices Area  
Central Electronics Engineering Research Institute (CEERI)/ Council of Scientific and Industrial Research (CSIR)  
Pilani-333 031, India

<sup>2</sup>Center of Excellence in Materials Science (Nanomaterials), Department of Applied Physics  
Z. H. College of Engg. & Tech. A.M.U. Aligarh-202002, India

The thermal oxidation rate constants on both polar faces (Si-face and C-face) of 4H-SiC have been experimentally investigated. The thermal oxidation was performed in horizontal quartz furnace at different temperature for different oxidation time. The growth rate constants were calculated by fitting the experimentally measured curve ( $X_0$  versus  $t/X_0$ ) to the frame of Deal and Grove model. It has been observed that the value of A (one rate constant) increases with decreasing oxidation temperature while the slope of curve B (another rate constant) increases with oxidation temperature. The reported work has significance in the development of 4H-SiC oxidation mechanism for device application. The relevant details are discussed and reported in this paper.

*Index Terms*—4H-SiC, Oxidation mechanism, Rate constants, Si-face and C-face.

## I. INTRODUCTION

SILICON CARBIDE is one of the most promising semiconductor materials in the development of devices for high power, high temperature, high frequency and harsh environment application. It has enormous electronic properties beyond the limit of silicon and other semiconductor material such as wide band gap energy, high thermal conductivity, high saturation velocity of electron and high breakdown electric field. These existing marvelous properties stand this material in the queue of third generation electronics market. Among the group of wide bandgap semiconductors, Silicon Carbide is the only material, which can be thermally oxidized similar to silicon growth mechanism. This unique capability of oxidation in the form of SiO<sub>2</sub> making it an obvious choice for the replacement of silicon MOS devices with excellent characteristics. The full reaction kinetics of the oxidation process is not yet fully understood.

A number of recent publications in order to develop the oxidation mechanism [1]-[6] clearly indicate not well understood phenomenon of SiC oxidation. The reported work is an experimental addition in the development of thermal oxidation mechanism of one of the commercially available device grade polytypes of SiC; 4H-SiC. The faces of all hexagonal polytypes of Silicon Carbide are always terminated into silicon rich and carbon rich faces resulting into Si-face and c-face surfaces. The oxidation mechanisms on Si-face and c-face have been found very different however still maintaining SiO<sub>2</sub> composition on both the faces [1]. The growth of the oxidation mechanism on the two faces, therefore, becomes interesting for exploration [5]. Efforts have been made to understand the oxidation phenomenon by doing dry oxidation [3], ultra thin oxide [6] etc. This paper deals with the determination of thermal oxidation rate constants for both faces of thick epitaxial (on Si-face) of device grade 4H-SiC substrate.

Experimental details of sample preparation, fabrication of MOSiC structures and electrical characterization methodology is given in the next section. Current conduction mechanisms, extraction of different MOSiC parameters acquired results with discussion are mentioned in the section thereafter, which is followed by conclusions.

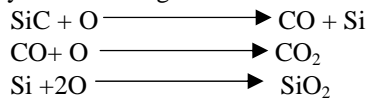
## II. EXPERIMENTAL DETAILS

A 2" diameter 4H-SiC (0001) epitaxy wafer of n/n<sup>+</sup> type 8° off-axis oriented has been cut into several pieces using special dicing blade from M/s DISCO Japan [7]. Prior to loading in a quartz furnace for the oxidation, RCA chemical cleaning treatment was given to all the samples. Thermal oxidation is accomplished using an oxidation furnace (or diffusion furnace, since oxidation is basically a diffusion process involving oxidant species), which provides the heat needed to elevate the oxidizing ambient temperature. A furnace typically consists of a cabinet, a heating system, a temperature measurement and control system, fused quartz process tubes where the wafers undergo oxidation, a system for moving process gases into and out of the process tubes and, a loading station used for loading (or unloading) wafers into (or from) the process tubes. The heating system usually consists of several heating coils that control the temperature around the furnace tubes. The wafers are placed in quartz glassware known as boats, which are supported by fused silica paddles inside the process tube. A boat can contain many wafers. The oxidizing agent comes with the contact of wafers and diffusion take place at the interface. In this experiment wet Thermal oxidation is divided in six groups. Thermal oxidation was performed at 1000°C, 1050°C, 1110°C and 1150°C for different oxidation time (30, 60, 90, 120, 150 and 180 minutes). Samples were loaded for oxidation at 800°C with a flow of nitrogen. Temperature of the furnace was increased to desired temperature and nitrogen flow was stopped while wet O<sub>2</sub> was flown for the required

time of oxidation. Temperature of the furnace was decreased to 800 °C and the samples were unloaded. This was repeated for each batch of samples with varying oxidation time. Oxide thickness on each sample was recorded using ellipsometer [8].

### III. RESULTS AND DISCUSSIONS

The thermal oxidation mechanism of SiC is described by same rules as Si, which is explained by Deal and Grove [9]. During thermal oxidation of silicon carbide most of the excess carbon is believed to be removed from the interface through the formation of CO<sub>2</sub>, which diffuses through the oxide and is thereafter released from the sample surface. However, some of the carbon can remain within the oxide and form carbon clusters or graphitic regions. Such regions near the SiO<sub>2</sub>/SiC are expected to be electrically active and could give rise the interface states [10]. The Process of SiC thermal oxidation can be divided into three steps. First, the oxidation of the SiC surface occurs through the interaction of an oxygen atom into the chemical bond of a SiC molecule. This Oxygen insertion creates a Si-O-C species, which then splits into a CO molecule and a Si atom with a dangling bond. These CO molecules diffuse through the oxide of the oxide surface and react with an oxygen atom, creating CO<sub>2</sub>. Second the Si atom reacts with oxygen atoms, which are at the SiC surface in the initial oxidation or diffuses through the oxide to the oxide SiC interface, forming SiO<sub>2</sub>. These three processes can be summarized by the following reactions



As opposed to the relatively simple oxidation of Si, there are five steps in the thermal oxidation of SiC.

1. transport of molecular oxygen gas to the oxide surface
2. in-diffusion of oxygen through the oxide film
3. reactions with SiC at the oxide/SiC interface;
4. Out-diffusion of product gases (e.g., CO<sub>2</sub>) through the oxide film; and
5. removals of product gases away from the oxide surface.

The last two steps are not involved in the oxidation of Si. The oxidation of SiC is about one order of magnitude slower than that of Si under the same conditions. The first and last steps are rapid and are not rate-controlling steps. But among the remaining steps, the rate-controlling step is still uncertain as discussed in several articles. It has been reported in various research paper that the thermal growth kinetics of SiC is governed by linear parabolic law of Deal and Grove, as derived for Silicon.

$$X_0^2 + AX_0 = B(t + \tau) \quad (1)$$

In above equation X denotes oxide thickness where as t is oxidation time. The quantity  $\tau$  corresponds to a shift in the time coordinate that correct for the presence of the initial layer of oxide thickness and A and B are constants. The above equation is a quadratic equation. The solution of equation can be written as

$$\frac{X_0}{A/2} = \left( 1 + \frac{t + \tau}{A^2/4B} \right)^{1/2} - 1 \quad (2)$$

There are two limiting case of equation 2

For long oxidation time i.e. thick oxidation Equation 2 becomes

$$X_0^2 = Bt \quad (3)$$

This relation is called parabolic law and B is called parabolic rate constant. This limiting case is diffusion controlled case because diffusion flux become small compared to the substrate surface reaction flux. Here the rate of oxidation is limited by the availability of oxidant at the Si rich interface as well as c rich interface, which is controlled by the diffusion process.

For short oxidation time i.e. thin oxide Equation 2 can be written as

$$X_0 = \frac{B}{A}(t + \tau) \quad (4)$$

This relation is called linear law and the quantity B/A is called the linear rate constant because in this case enough oxidant is transported across the oxide layer, and the oxidation rate is controlled by concentration of oxidant at the surface [11].

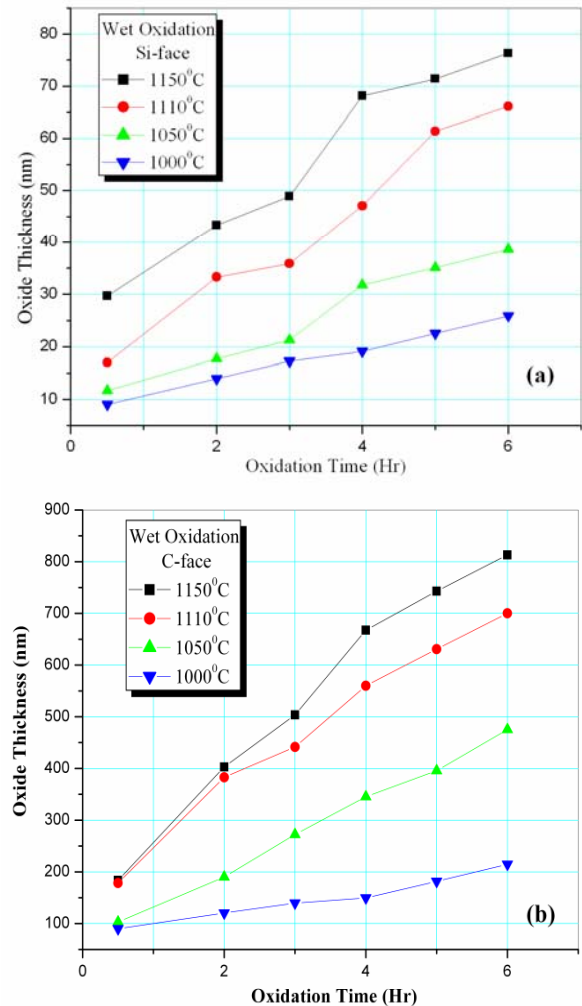


Fig.1. (a) Variation of oxide thickness on Si-face of 4H-SiC at different temperature while (b) shows the distribution of oxide thickness on C-face

Thermal oxide growth rate constants have been determined by fitting the experimentally measured curve to the measurement made by Deal and Grove (as explained above) of oxide thickness as a function of oxidation time at various oxidation temperatures. In this experiment wet thermal oxidation has been performed (as explained in section 2.3) at  $1000^{\circ}\text{C}$ ,  $1050^{\circ}\text{C}$ ,  $1110^{\circ}\text{C}$  and  $1150^{\circ}\text{C}$  for different oxidation time. In each individual experiment, the value of  $\tau$  has been fixed to zero for all temperature range. A plot of oxide thickness ( $X_0$ ) versus  $t/X_0$  from equation 1 should yield a straight line with intercept  $-A$  and slope  $B$ . Fig. 2. (a) and Fig. 2 (b) shows the  $X_0$  versus  $t/X_0$  plots of wet oxidation on Si-face (figure a) and C-face (figure b) of 4H-SiC respectively. It has been observed that the absolute value of  $A$  increasing with decreasing oxidation temperature. At the same condition, the slope of the plots increases with increasing temperature.

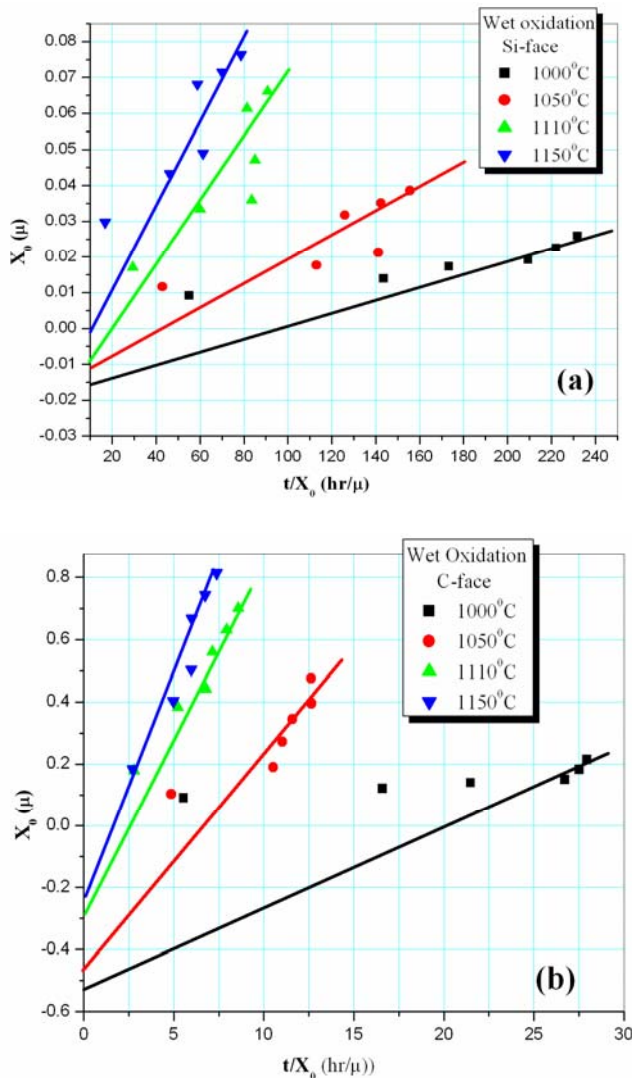


Fig.2. (a) Determination of rate constants on Si-face while (b) shows the determination of rate constants on C-face of 4H-SiC

## IV. CONCLUSION

This article reports an experimental study of the face terminated wet thermally grown  $\text{SiO}_2$  and determination of face terminated wet thermal oxidation rate constants. Deal and Grove model has been used in the calculation of rate constants. It has been reported that the value of  $A$  (one rate constant) increases with decreasing oxidation temperature while the slope of curve  $B$  (another rate constant) increases with oxidation temperature. These experimental results will be used as an input parameter in the modeling of oxidation mechanism in 4H-SiC.

## ACKNOWLEDGMENT

Authors are grateful to the director, Dr. Chandra Shekhar, CEERI Pilani, for his kind approval to carry out this work. The financial support through Senior Research Fellowship (SRF) of Council of Scientific and Industrial Research (CSIR), India to one of the authors (SKG) is gratefully acknowledged.

## REFERENCES

- [1] I.C. Vickridge, J.-J. Ganem, G. Battistig, E. Szilagy, "Oxygen isotopic tracing study of the dry thermal oxidation of 6H-SiC", Nuclear Instruments and Methods in Physics Research B Vol. 161, pp. 462-466, 2000.
- [2] Y. Song, S. Dhar, L.C. Feldman, G. Chung, J.R. Williams, "Modified Deal Grove model for the thermal oxidation of silicon carbide" J Appl. Phys., Vol-95, No.9, pp.4953-4957, 2004.
- [3] J.M. Knaup, P. Deak, T. Frauenheim, A. Gali, Z. Hajnal, W.J. Choyke, "Theoretical study of the mechanism of dry oxidation of 4H-SiC" Phys. Rev. Vol. B71, p. 235321, 2005.
- [4] K.-C. Chang, Y. Cao, L.M. Potter, J. Bentley, S. Dhar, L.C. Feldman, J.R. Williams, "High resolution elemental profiles of the silicon dioxide /4H-Silicon carbide interface" J Appl. Phys., Vol.97, pp.104920 2005.
- [5] M. Schuermann, S. Dreiner, U. Berges and C. Westphal, "Structure of the interface between ultrathin  $\text{SiO}_2$  films and 4H-SiC (0001)", Phys. Rev. B Vol. 74, p. 035309, 2006.
- [6] P. Fiorenza and V. Raineri, "Reliability of thermally oxidized  $\text{SiO}_2$ /4H-SiC by conductive atomic force microscopy", J. Appl. Phys. Letts., Vol. 88, p. 212112, 2006.
- [7] J. Akhtar et. al. "Design and fabrication of 4H-SiC Schottky Diode Detector", CEERI/MTG/RR- 1/2007.
- [8] Sanjeev Kumar Gupta, Ameer Azam and Jamil Akhtar, "Wet thermal oxidation of epitaxial 4H-SiC: an experimental process for devices fabrication. ICFAI Univ J. Sci. Tech., Vol. 5, No. 1, pp. 7-15, 2009
- [9] B.E. Deal and A.S. Grove, "General relationship for the thermal oxidation of Silicon", J. Appl. Phys. 36, p. 3770 1965.
- [10] Eckhard Pippel and Woltersfordf, "Interfaces between 4H-SiC and  $\text{SiO}_2$ : Microstructure, nanochemistry, and near-interface traps", J. Appl. Phys. 97, p. 034302 2005.
- [11] Sanjeev K. Gupta, A. Azam and J. Akhtar, "Surface topographical analysis face terminated wet thermal oxidation of 4H-SiC substrate", Int. J. Chem. Sci., Vol. 7, No. 3, pp. 1987-1999, 2009.