

# Generation and Suppression of Oxidation Byproducts at 4H-SiC C-face / SiO<sub>2</sub> Interface Characterized by Infrared Spectroscopy

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## Abstract

We found that infrared spectroscopy is able to detect an unexpected structure at 4H-SiC/SiO<sub>2</sub> interface, by focusing on the wavenumber region of 2100 - 2150 cm<sup>-1</sup>. This absorption should be attributed to oxidation byproducts at the interface. Its intensity is significantly dependent on oxidation temperature and oxidant. These results indicate that selection of oxidation conditions is inevitably important for the suppression of interfacial byproducts.

## 1. Introduction

It is widely discussed that defects at 4H-SiC/SiO<sub>2</sub> interface are responsible for the deterioration of MOSFET performance[1]. Some studies have clarified that changing oxidation process[2][3] or post-oxidation annealing[4][5] are effective to improve the SiC-MOS properties, but mechanisms of improvement by such techniques have not been clarified. We investigated the 4H-SiC/SiO<sub>2</sub> interface formed by thermal oxidation paying attention to the interfacial byproducts with infrared (IR) spectroscopy, which is useful to analyze microscopic structures and chemical states.

## 2. Experimental

N-doped ( $\sim 1 \times 10^{16} \text{cm}^{-3}$ ) 4H-SiC(000 $\bar{1}$ )C-face epitaxial wafers were cleaned by RCA and HF, followed by oxidation under dry or wet ambient. Dry oxidations were performed at 500 or 1000°C. Wet oxidations were conducted at 1000°C by bubbling gases through 60°C de-ionized water, which yields water vapor of 0.2 atm. O<sub>2</sub>, N<sub>2</sub> and 5%-H<sub>2</sub> (diluted with Ar) were employed for the carrier gasses. We denoted these conditions as wet-O<sub>2</sub>, wet-N<sub>2</sub> and wet-H<sub>2</sub>, respectively. Some samples were annealed in H<sub>2</sub> at 1000°C for 1 hour. To investigate interfacial byproducts, we decreased the oxide film thickness by HF etching, as shown in Fig. 1. The attenuated total reflection technique with a crystalline Ge prism was applied to IR measurements. The

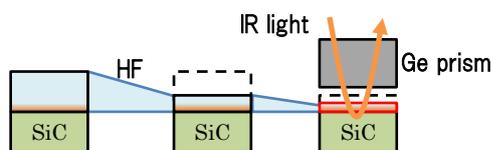


Fig. 1. Schematic of the experimental procedure. Decrease film thickness with HF and analyze the interface by the ATR technique.

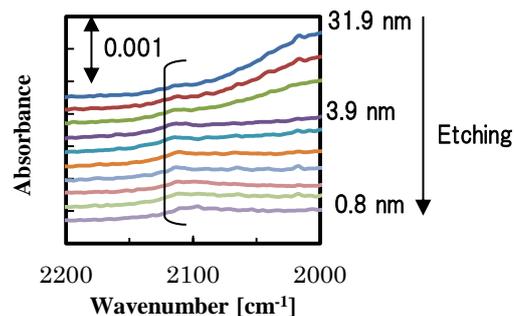


Fig. 2. The IR peak detected within 2100 - 2150 cm<sup>-1</sup> for the oxide grown in wet-O<sub>2</sub> with various thicknesses.

incident angle was 45° and resolution was set to 4 cm<sup>-1</sup>. The film thickness was determined by either X-ray reflectivity or Si2p XPS.

## 3. Results and discussions

### (1) Detection of oxidation byproducts at the interface

When we analyze thermally-grown oxide on 4H-SiC, we can detect strong absorption peaks which are attributable to SiC and Si-O-Si vibrations. In addition to these peaks, we also detected an unidentified peak within 2100 - 2150 cm<sup>-1</sup> in the cases of dry-O<sub>2</sub> and wet-O<sub>2</sub>. IR spectra of this region are shown in Fig. 2. As we decreased the film thickness, the peak became obvious. This behavior can be explained due to the geometric effect of ATR, rather than products of SiO<sub>2</sub> etching, taking account of the exponential decay of the evanescent wave intensity. To eliminate this SiO<sub>2</sub>-thickness effect, we evaluate the peak intensity by normalizing with SiC substrate peak intensity. Fig. 3 shows

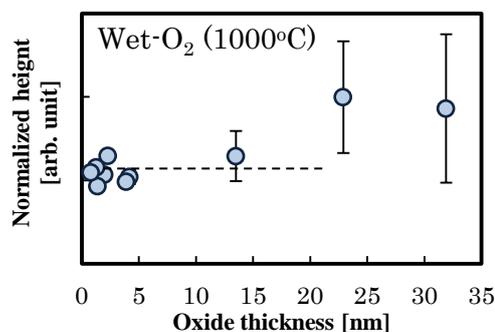


Fig. 3. Normalized intensity of the peak within 2100 - 2150 cm<sup>-1</sup>. Unchanged intensity by HF etching indicates that the responsible structures should locate at the interface.

the film-thickness dependence of the normalized peak intensity. The intensity did not change when we decrease the film thickness, indicating that this peak should be attributed to structures which locate at the interface.

### (2) Intensity difference among dry-oxidation conditions

In order to clarify how the structure forms, we investigated 4H-SiC/SiO<sub>2</sub> interfaces for some dry-oxidation conditions. Samples in this experiment were separately prepared using a cold-wall furnace with a cooling rate of ~100°C/min to avoid the ambiguity of oxidation temperature. Fig. 4 shows the peaks for the oxides grown at 500 and 1000°C. The identical film thicknesses of ~1 nm were employed for the fair comparison of the intensity. It is clearly observed that the peak intensity of 500°C-oxide is stronger than that of 1000°C. We also investigated a “slow-cooling” sample which was grown at 1000°C followed by slower cooling (~10°C/min), without gas displacement. Slow-cooling resulted in enhancing the intensity. From these results, we concluded that the structure is likely formed at low temperature.

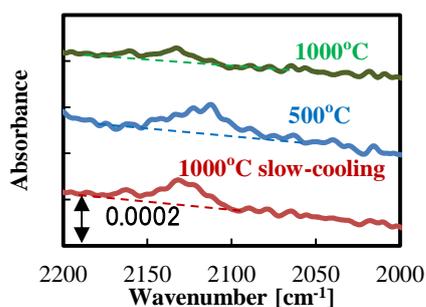


Fig. 4. The intensity change of the peak within 2100 – 2150 cm<sup>-1</sup> for different oxidation conditions. It is indicated that low-temperature oxidation induces the formation of the structure.

### (3) Effects of oxidants and H<sub>2</sub> annealing

We also found that changing oxidant from O<sub>2</sub> to H<sub>2</sub>O is an effective way to suppress the intensity of the peak. Fig. 5 shows the comparison between oxidation conditions with O<sub>2</sub> (dry-O<sub>2</sub> and wet-O<sub>2</sub>) and without O<sub>2</sub> (wet-N<sub>2</sub> and wet-H<sub>2</sub>) and H<sub>2</sub> annealing.

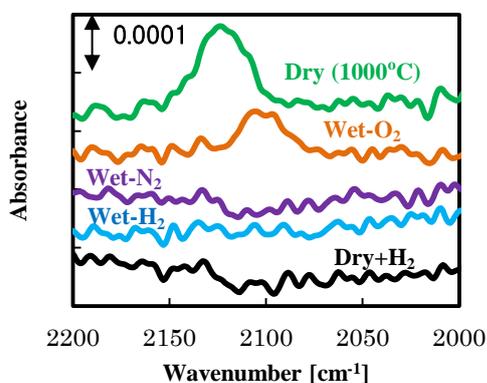


Fig. 5. Intensity changes of the peak within 2100 – 2150 cm<sup>-1</sup> by wet-oxidation and H<sub>2</sub>-annealing. H<sub>2</sub>O oxidation and H<sub>2</sub> annealing are the effective ways to suppress the peak.

wet-H<sub>2</sub>) in the ambient. Note that according to the thermodynamic equilibrium at 1000°C, oxygen partial pressures of wet-N<sub>2</sub> and wet-H<sub>2</sub> are negligibly low: 10<sup>-6</sup> and 10<sup>-13</sup> atm, respectively. From these results, we found that oxidant is an important factor to suppress interfacial byproducts. To examine the effect of hydrogen, we analyzed H<sub>2</sub>-annealed oxide grown in dry-O<sub>2</sub> (dry + H<sub>2</sub>). As a result, we found that the peak completely disappeared. Though wet-N<sub>2</sub> did not include atmospheric hydrogen, the hydrogen generated at the interface during interfacial reactions should affect the structure. The fact that not only wet-H<sub>2</sub> but also wet-N<sub>2</sub> is effective on suppression reveals that such slight amount of hydrogen is sufficient to suppress the structure efficiently. Next, we discuss the possible structure attributable to the peak. It is well known that Si-H bonds appear at around 2100 cm<sup>-1</sup>[6], but this assignment seems controversial to our result that H<sub>2</sub>-annealing eliminates the peak. We speculate that another candidate structure is carbon related one since it has been reported that C≡C related structures appear around 2100 cm<sup>-1</sup>[7][8].

### 4. Conclusions

We have investigated oxidation byproducts at 4H-SiC/SiO<sub>2</sub> interface. We clearly detected an absorption peak within 2100 – 2150 cm<sup>-1</sup> with IR spectroscopy, which should be attributable to byproducts at the interface. A comparison among dry-oxidation conditions revealed that the byproduct is mainly formed by oxidation at low temperature such as 500°C. H<sub>2</sub>O oxidation and H<sub>2</sub> treatment are effective ways to suppress this structure at the interface. As schematically shown in Fig. 6, oxidation condition and oxidants are the important factors to suppress the interfacial byproducts.

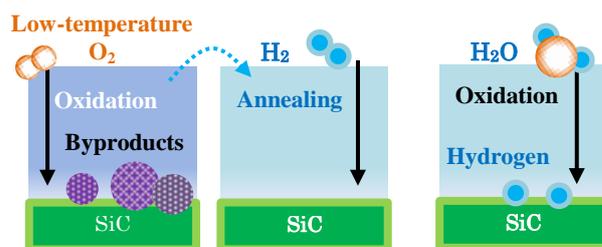


Fig. 6. Schematic of interfacial byproducts suppression of 4H-SiC C-face investigated with IR spectroscopy. We clarified that oxidation temperature and oxidant are the important factors to suppress the unexpected structure.

### References

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