

## Surface orientation dependence of SiC oxidation process studied by *in-situ* spectroscopic ellipsometry

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**Abstract.** We performed real-time observations of SiC oxidation at various temperatures by *in-situ* spectroscopic ellipsometry using a Si-face, an a-face and a C-face substrates. We calculated oxide growth rates based on “Si-C emission model,” taking into account the emission of interfacial Si and C atoms from the SiC–SiO<sub>2</sub> interface. The calculated values well reproduced the oxide thickness dependence of oxide growth rates. We discussed the SiC oxidation mechanism using the parameters deduced from the calculations.

### Introduction

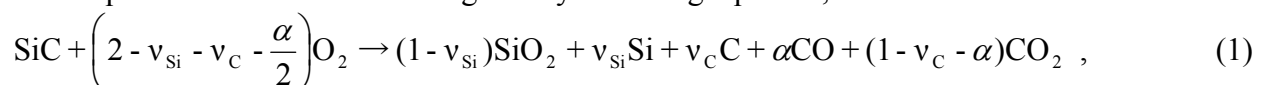
For practical use of SiC-MOSFETs, it is an essential problem to reduce their on-resistance. Since the increase of on-resistance is chiefly due to the reduction of channel mobility at the inversion layer, to control the SiC–SiO<sub>2</sub> interface is the key technology. Because the oxidation mechanism should be closely related to the oxide and interface quality, we have performed real-time observations of SiC thermal oxidation process using an *in-situ* spectroscopic ellipsometer [1]. As a result, we found for the first time that oxide growth rate decelerates rapidly in the initial oxidation stage, which cannot be explained by Deal-Grove model [2]. This initial deceleration has been pointed out also in the Si oxidation and physically explained by “Si emission model” [3-5].

To describe the initial deceleration phenomenon of SiC oxidation, we have proposed a kinetic model of SiC oxidation, termed “Si-C emission model [6].” According to this model, the interfacial Si and C atom emissions into the oxide accompanied by the oxidation of SiC are taken into account.

We have been doing various discussions on the SiC oxidation mechanism based on the Si-C emission model in previous works [7,8]. In order to further understand the oxidation mechanism, it is effective to investigate differences in the surface orientations. Thus, in this study, we performed real-time observations of the SiC oxidation process using a (0001) Si-face, (11–20) a-face and (000–1) C-face and surveyed parameters related to Si-C emission model.

### Calculation method

Consider the Si and C emission during the oxidation based on the Si-C emission model [6]. The reaction equation for SiC oxidation is given by following equation,



where  $\nu$  is the emission ratio,  $\alpha$  is the production ratio of CO, and the subscript means the value for corresponding atom. According to the Si-C emission model, the interfacial reaction rate is lowered by accumulation of Si and C interstitials at the SiC–SiO<sub>2</sub> interface since such an accumulation of interstitials inhibits new emission of interstitial and limits the oxidation reaction. Therefore,

concentrations of emitted interstitials at the interface dominate the oxide growth rate in the initial oxidation stage. We introduced the following equation as the interfacial reaction rate  $k$ ,

$$k = k_0 \left( 1 - \frac{C_{Si}^I}{C_{Si}^0} \right) \left( 1 - \frac{C_C^I}{C_C^0} \right), \quad (2)$$

where  $k_0$  is the initial interfacial reaction rate,  $C^0$  is the solubility limit in  $\text{SiO}_2$ , and  $C^I$  is the concentration of interstitials at the interface. From eq. (2), increase of  $C^I$  due to Si and C emission leads to decrease of  $k$ . The detailed calculation method of oxide growth rate is described elsewhere [6].

## Experiments

4H-SiC (0001) Si-face ( $n$  type,  $1.0 \times 10^{16} \text{ cm}^{-3}$ ,  $8^\circ$  off), 6H-SiC (11-20) a-face ( $n$  type) and 4H-SiC (000-1) C-face ( $n$  type,  $5.0 \times 10^{15} \text{ cm}^{-3}$ ,  $0.5^\circ$  off) substrates were used in this study. Spectroscopic polarization parameters ( $\Psi$ ,  $\Delta$ ) were recorded with real-time using an *in-situ* spectroscopic ellipsometer connected to a furnace. Dry oxidation was carried out at various oxidation temperatures and at oxygen partial pressure of 1.0 atm. Oxide thicknesses were calculated from ( $\Psi$ ,  $\Delta$ ) spectra obtained, where we used an analysis model that is composed of a SiC/interface layer/SiC structure [9]. Oxide growth rates were determined from relationships between oxidation time and oxide thickness. Parameters related to growth rate calculations were determined by fitting the calculated oxide growth rates to the observed ones.

## Results and discussion

Figure 1 shows the oxide thickness dependence of oxide growth rates for (a) Si-face, (b) a-face and (c) C-face at various temperatures. As can be seen from these figures, the oxide growth rate decelerates rapidly in the thin oxide region and then it levels out. It is found that the oxide growth rate for C-face is faster than that for Si-face, and that for a-face is between them at same temperature. The broken curves in Figs. 1 mean calculated oxide growth rates using the Si-C emission model. It is found from the figures that the calculated oxide growth rates well reproduce the experimental values including the initial deceleration region.

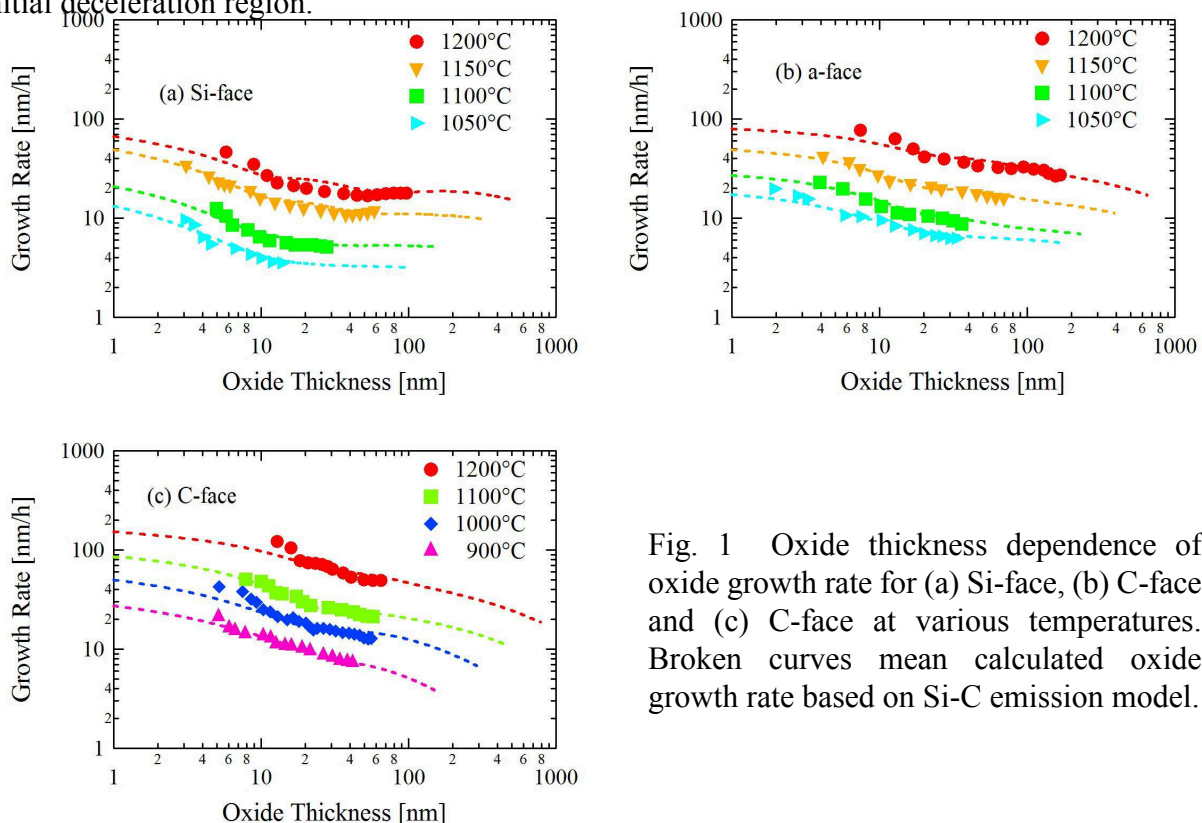


Fig. 1 Oxide thickness dependence of oxide growth rate for (a) Si-face, (b) C-face and (c) C-face at various temperatures. Broken curves mean calculated oxide growth rate based on Si-C emission model.

Figure 2 shows the temperature dependence of initial interfacial reaction rate  $k_0$ . The ratio of activation energy for C-face, a-face and Si-face is found to be nearly equal to 1:2:3. When Si atoms in SiC substrate are oxidized, it is necessary to break one Si-C back-bond in C-face, two Si-C back-bonds in a-face and three Si-C back-bonds in Si-face. Therefore,  $k_0$  might relate to the surface structure of SiC substrate. However, though absolute values of  $k_0$  for Si-face are considered to be the smallest of three, experimental values are large. This is for further study. Figure 3 shows the temperature dependence of Si and C emission ratio ( $v_{Si}$  and  $v_C$ , respectively.) It is found that  $v_{Si}$  in the case of Si-face that has the lowest growth rate is the highest of the three faces and the case of C-face is the reverse situation. On the other hand,  $v_C$  hardly depends on surface orientation. Namely, only  $v_{Si}$  depends on surface orientation and chiefly determines the oxide growth rate.

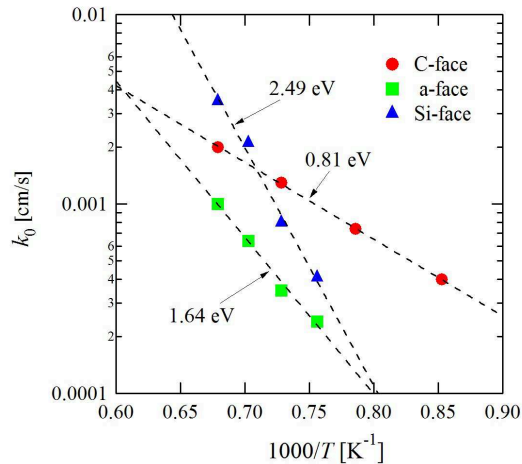


Fig. 2 Temperature dependence of initial interfacial reaction rate  $k_0$

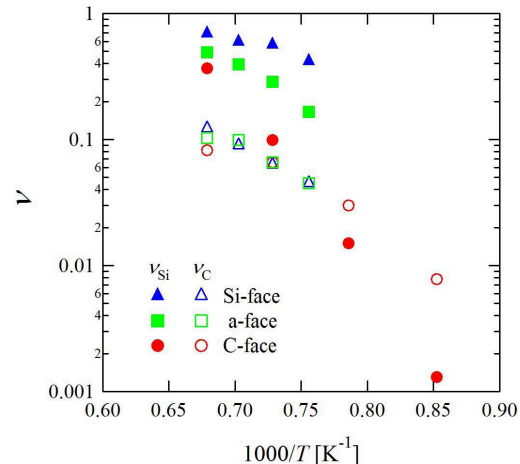


Fig. 3 Temperature dependence of emission ratio  $v_{Si}$  and  $v_C$

Figure 4 shows the calculated oxide thickness dependence of concentration of Si interstitials at the SiC-SiO<sub>2</sub> interface  $C_{Si}^I$  for (a) Si-face, (b) a-face and (c) C-face. From this figure, it is found that only  $C_{Si}^I$  for C-face reduces after oxide growth of about 100 nm. This is because the oxide growth rate decelerates due to the diffusion rate-limiting step and as a result the emission rate of Si interstitials decreases.

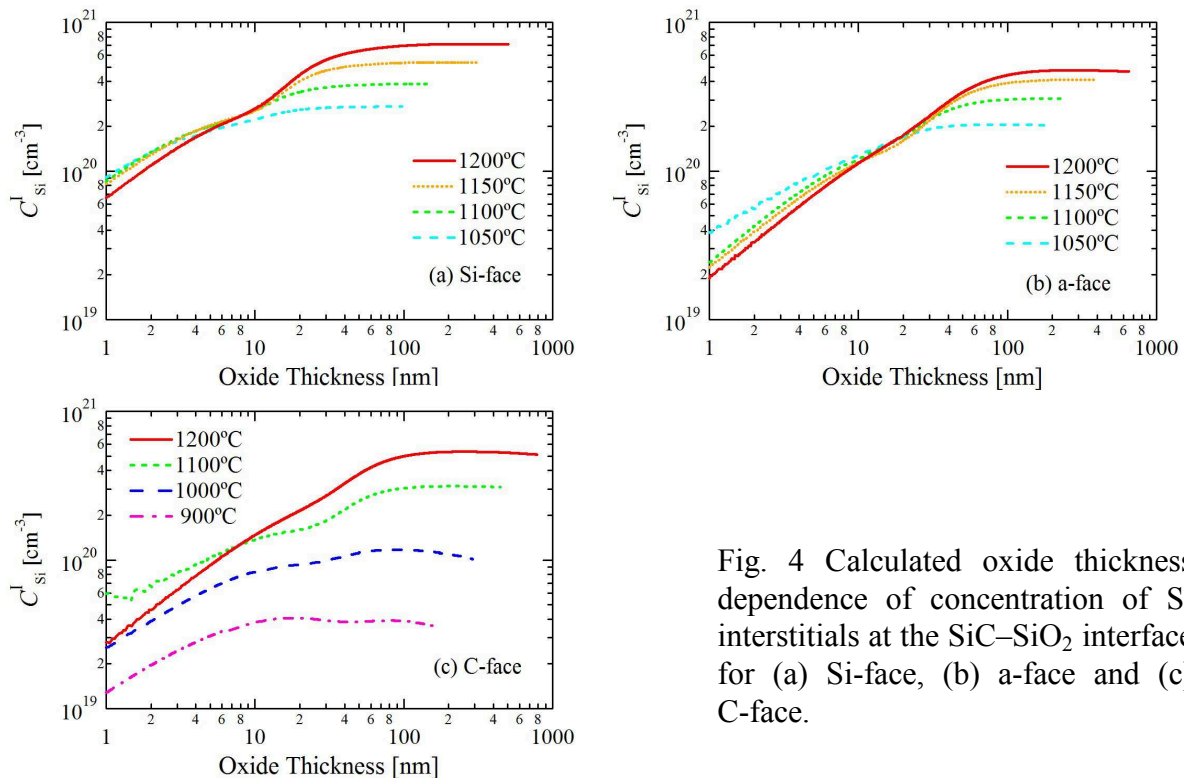


Fig. 4 Calculated oxide thickness dependence of concentration of Si interstitials at the SiC-SiO<sub>2</sub> interface for (a) Si-face, (b) a-face and (c) C-face.

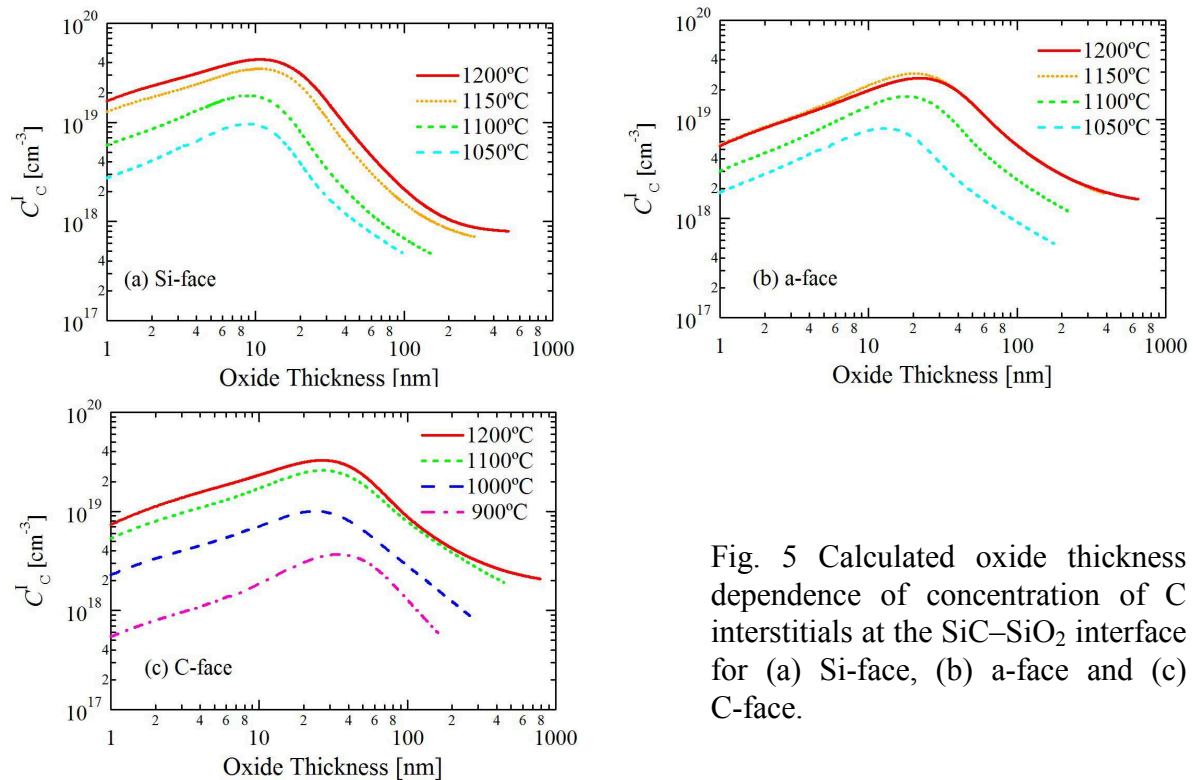


Fig. 5 Calculated oxide thickness dependence of concentration of C interstitials at the SiC–SiO<sub>2</sub> interface for (a) Si-face, (b) a-face and (c) C-face.

Figure 5 shows the calculated oxide thickness dependence of concentration of C interstitials at the SiC–SiO<sub>2</sub> interface  $C_C^I$  for (a) Si-face, (b) a-face and (c) C-face. As clearly seen in the figure, the variation of  $C_C^I$  exhibits a peak around several tens nm. This peak can be explained as follows: since the accumulation of C interstitials is earlier than that of Si interstitials, after the saturation of C interstitials, Si interstitials still remain increasing. As a result, the emission rate of C interstitials starts to decrease because the oxidation rate decreases.

## Summary

We performed real-time observations of SiC oxidation of various surface orientations using an *in-situ* spectroscopic ellipsometer to understand the oxidation mechanism of SiC. We surveyed oxidation parameters based on Si-C emission model by fitting calculated growth rate to experimental values obtained. As a result, we found that the initial interfacial reaction rate  $k_0$  depends on surface orientation and that the ratio of activation energy of  $k_0$  corresponds to the number of back-bond of Si atom in SiC substrate. We performed the simulations of oxide thickness dependence of Si and C interstitial concentration at the SiC–SiO<sub>2</sub> interface. It was found that, in contrast to  $C_{Si}^I$ ,  $C_C^I$  starts to decrease after oxide growth more than several tens nm. It can be said that this time important information to control the physical properties of the interface was acquired.

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