Model Calculation of SiC Oxide Growth Rate Based on the Silicon and Carbon Emission Model

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Abstract. We proposed a kinetic model for SiC oxidation, named 'silicon and carbon (Si-C) emission model', taking into account the emission of Si and C atoms from the SiC–oxide interface, which suppresses the oxidation rate at the interface. Based on the model, we calculated oxide growth rates for SiC (0001) Si- and (000–1) C-face and found that the calculated values exhibit good fits to the measured ones in the entire oxide thickness range for both faces. We also calculated depth profiles of Si and C interstitials and oxidants, and discussed the oxidation mechanism of SiC as well as the difference in the oxidation process of Si-face and C-face.

Introduction

Silicon carbide (SiC) is an attractive material for applying to electron devices because it can be thermally oxidized and SiO_2 layers, known as a superior insulator for metal-oxide-semiconductor (MOS) applications, can be formed. However, despite many researches and developments have been done, SiC MOSFETs still have serious problems, such as a higher on-resistance than those expected from the physical properties of SiC and a short-term reliability of oxide layers. Little is known about the oxidation mechanism of SiC compared with that of Si, which should bring about the difficulty in the solution of these problems.
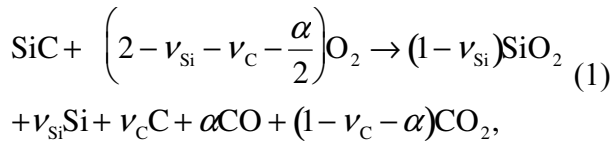
In previous works, we have successfully performed a real time observation of SiC oxidation by using an *in-situ* spectroscopic ellipsometer [1–4] and found that the oxide growth rate increases in the thin oxide regime (< *ca.* 20 nm) [2–4], which cannot be explained by Deal-Grove model [5], as in the case of Si oxidation [6]. For the explanation of the growth enhancement phenomena in Si oxidation, the interfacial Si emission model has been proposed [7,8]. According to the model, Si atoms are emitted into the oxide layers accompanied by oxidation of Si, caused by the stain due to the expansion of Si lattices during oxidation. The oxidation rate at the interface is primarily large and is suppressed by the accumulation of emitted Si atoms with the increase of oxide thickness, i.e., the oxidation rate is not enhanced in the thin thickness regime but is suppressed with increase of thickness. Because the density of Si atoms in SiC ($4.9{\times}10^{22}$ cm^{-3}) is almost equal to that of Si, an interfacial stretch strain should be generated, and, as a result, interfacial Si emission is considered to occur also in SiC oxidation. Thus, we have applied the Si emission model to SiC C-face oxidation [9] and found that the model well explains the thickness dependence of oxidation rate, including the high growth rate in the thin oxide regime. However, there exist some issues in the application of Si-emission model for SiC oxidation from the physical viewpoints, for instance, oxygen diffusivity in SiO_2 that is different from that of Si oxidation is required to explain SiC oxidation, which are considered to be due to the ignorance of the presence of carbon atoms.

In this report, we proposed a kinetic model for SiC oxidation, named 'silicon and carbon (Si-C) emission model', derived by introducing C oxidation and emission processes to the interfacial Si emission model for Si [7,8]. Based on the model, we calculated growth rates at various oxide

thicknesses and depth profiles of the concentration of Si and C interstitials and oxidants in the oxides, and discussed the difference in the oxidation process between (0001) Si-face and (000–1) C-face.

Basis of calculation

Figure 1 shows schematic illustrations of Si-C emission model and concentration profiles of Si and C interstitials and oxidants, where C, x and X denote concentration of interstitials, distance from the interface and oxide thickness, respectively. The subscripts, Si, C and O, denote the values for corresponding atoms. Considering Si and C atom emission from the interface during oxidation, a reaction equation for SiC oxidation can be written as,

$$\text{SiC} + \left(2 - \nu_{\text{Si}} - \nu_{\text{C}} - \frac{\alpha}{2}\right)\text{O}_2 \rightarrow (1 - \nu_{\text{Si}})\text{SiO}_2 \quad (1)$$
$$+ \nu_{\text{Si}}\text{Si} + \nu_{\text{C}}\text{C} + \alpha\text{CO} + (1 - \nu_{\text{C}} - \alpha)\text{CO}_2,$$

Fig. 1 Schematic illustration of the Si-C emission model.

where ν and α denote the interfacial emission rate and the production rate of CO, respectively. The set of diffusion equations for Si and C interstitials and oxidants are given for the calculation of concentration profiles of them in the oxide. It has been considered that the oxidation rate in thick oxide regime is limited by the in-diffusion of oxidant or out-diffusion of CO. According to the recent works [3,10], the oxide growth rate in the thick oxide regime is proportional to the partial pressure of O_2, which suggests that the oxide growth rate is limited only by the out-diffusion of O_2. Therefore, it is considered that the diffusivity of CO in SiO_2 is much larger than that of O_2. Thus we assumed that CO is quickly diffused out to the oxide surface and ignore the diffusion process of CO for the Si-C emission model.

According to the Si emission model [7,8], the interfacial reaction rate (k) can be written as a decreasing function of the concentration of Si interstitials at the interface (C^{I}_{Si}), i.e., $k = k_0(1 - C^{\text{I}}_{\text{Si}} / C^{0}_{\text{Si}})$, where C^0 is the solubility limit of the corresponding interstitials in the oxide, k_0 is the interfacial reaction rate in the case of no accumulation of interstitials, and the superscript 'I' means the position at the oxidation interface ($x = 0$). We assumed that the interfacial reaction rate for SiC oxidation is suppressed by the accumulation of C atoms as well as that of Si atoms emitted near the interface, and is given by multiplying a decreasing function for Si and that for C, as

$$k = k_0\left(1 - \frac{C^{\text{I}}_{\text{Si}}}{C^{0}_{\text{Si}}}\right)\left(1 - \frac{C^{\text{I}}_{\text{C}}}{C^{0}_{\text{C}}}\right). \quad (2)$$

Oxide growth rates were numerically calculated from the diffusion equations and the boundary conditions for these interstitials by use of the partial differential equation solver ZOMBIE [11]. The parameters related to the properties of Si oxide, *e.g.*, C^{0}_{Si} in Eq. (2), were set to the same values as those obtained for Si oxidation [8], which means that the issue appeared in the application of Si emission model to SiC oxidation has been solved. The parameters concerning C interstitials, *e.g.*, α and ν_{C} in Eq. (1), as well as the values of k_0 and ν_{Si} were determined by fitting the calculated oxide growth rates to the measured ones. Depth profiles of the concentrations of Si and C interstitials and
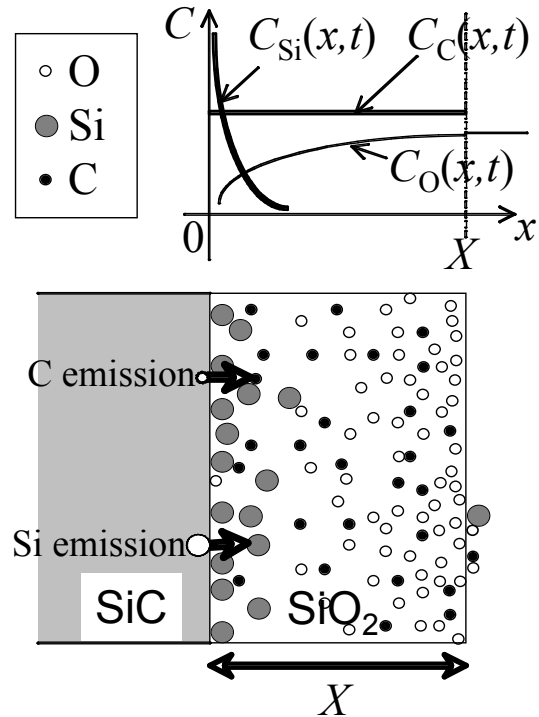
oxidants in the oxide layer were calculated with these parameters. The details of calculations for oxide growth rates will be described elsewhere.

Results and Discussion

Figure 2 shows the oxide growth rates measured for C-face at 1090°C (circles) and Si-face at 1080°C (triangles), and those given by the Si-C emission model (solid lines) and the Si emission model (broken lines). The figure shows that the Si-C emission model reproduces the observed growth rates better than by the Si emission model without carbon emission, especially in the thin oxide regime. Although modifications of the parameters related to the properties of Si oxide are necessary for the Si emission model to account for the rapid growth rate decreasing in the thin oxide regime, the modifications are unnecessary for the Si-C emission model. Hence, the C interstitials as well as Si interstitials are thought to play an important role for the reduction in interfacial reaction rate k. In the case of C-face, the values obtained for α, ν_C and production rate of CO_2 were 0.8, 0.04 and 0.16, respectively. Therefore, at this temperature, most of the C atoms are oxidized to form CO or CO_2 molecules at the SiC–oxide interface. The value of α is determined from the oxide-thickness dependence of growth rates in the parabolic rate regime, in which the growth rate decreases inversely proportional to oxide thickness [5]. However, in the case of Si-face, the influence of the oxygen diffusion is significant in the thickness range more than several μm. Thus we could not determine the value of α for Si-face.

Figure 3 shows the calculated depth profiles of Si and C interstitials and oxidants

Fig. 2 Oxide thickness dependences of measured and calculated growth rates.

Fig. 3 Depth profiles of Si interstitials, C ones and oxidants in the oxide for Si- and C-face at the oxide thickness of 50 nm, oxidation temperature of 1100°C calculated by the Si-C emission model.

(C_{Si}, C_C and C_O, respectively) for Si- and C-face when $X = 50$ nm at the oxidation temperature of 1100°C. Here, we gave the same α value for Si-face as that for C-face. It is noticed that the oxide thickness of 50 nm corresponds to the typical thickness used for the gate oxide of actual SiC MOSFETs. From Fig. 2, the oxide growth rate at this oxide thickness for Si face is around 1/10 times of that for C-face. The oxide growth rate is roughly given by kC_O^I/N_0, where N_0 is the density of Si atoms in SiO_2. As shown in Fig. 3, the concentration of oxidants at the interface for Si-face is higher than that of C-face by a factor of 1.4. Therefore, the k for Si-face is smaller than that for C-face by a factor of 1/14. The k is, as shown in Eq. 2, given by the products of k_0, $(1-C_{Si}^I / C_{Si}^0)$ and $(1-C_C^I / C_C^0)$. The k_0, corresponding to the oxidation rate at the very early stage, for Si-face is smaller than that for C-face by a factor of 1/2.5. Because the interfacial concentration of Si interstitials for
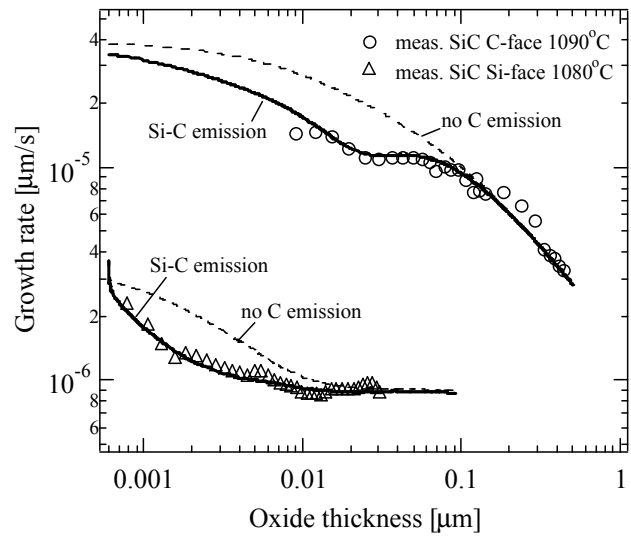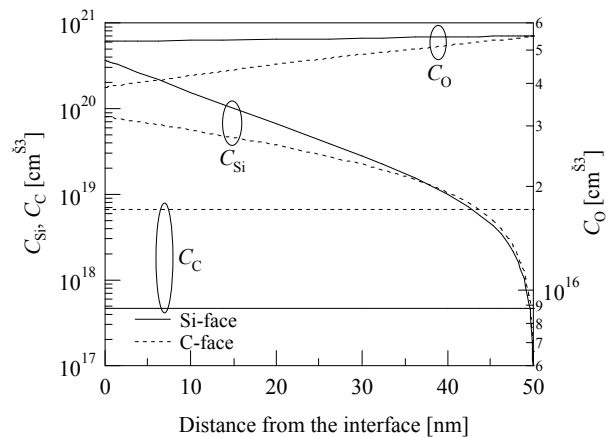
Si-face increases with increase of oxide thickness up to near the solubility limit of Si interstitials (C^0_{Si}: 4.2×10^{20} cm^{-3} at 1100°C), the term ($1 - C^I_{Si} / C^0_{Si}$) indicating the decreasing factor of k for Si interstitials decreases to 0.12 at 50 nm, leading to a remarkable reduction of the oxidation rate. In contrast, the term for C-face is 0.81 at this thickness. The increase in concentration of Si interstitials at the interface can be attributed to the high Si emission rate. The terms ($1 - C^I_C / C^0_C$) indicating the decreasing factor of k for C interstitials are 0.99 for Si-face and 0.84 for C-face (C^0_{Si}: 4.2×10^{20} cm^{-3} at 1100°C), which are not significantly different though the value for C-face a little smaller. Therefore, it is considered that the much lower oxide growth rate at 50 nm for Si-face compared with that for C-face and the rapid reduction in oxide growth rate for Si-face are mainly caused by the accumulation of large number of Si interstitials at the interface.

As mentioned above, most of the C atoms at the interface are oxidized to form CO or CO_2 molecules. Since the diffusivity of CO molecule is very large and CO_2 molecule is unlikely to react with another atom, most of oxidized carbons are diffused out to the oxide surface. The diffusivity of C interstitial is deduced to be also large. Therefore, the results in this study suggest that the concentrations of these carbonaceous species at the SiC–oxide interface are significantly lower than that of Si interstitials.

Summary

We proposed an oxidation model of SiC, named 'Si-C emission model,' by introducing processes of C oxidation and emission to the Si emission model. In comparison to the measured oxide growth rate, our model well reproduces the thickness dependence of growth rate of SiC in the entire oxide regime both for Si- and C-faces. We calculated the depth profiles of Si interstitials, C ones and oxidants in the oxide using our model. The calculation results suggest that the accumulation of large number of Si interstitials near the SiC–oxide interface mainly contribute to the reduction of oxidation rate for Si-face and that carbonaceous species are not accumulated near the interface because of their high diffusivity or high stability in the oxide.

Acknowledgement

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