

Model calculations of SiC oxide growth rates at sub-atmospheric pressures using the Si and C emission model

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Abstract. We found that the ‘Si and C emission model’ that we proposed as an oxidation model of SiC could not reproduce the initial oxide growth rates of SiC at sub-atmospheric pressures. The comparison between calculated and observed growth rates suggests that the oxide growth on the oxide surface is enhanced in the initial oxidation stage and thus our oxidation model is inaccurate in the description of the initial surface oxidation. Accordingly, we have reconsidered the parameters on surface oxidation and, as a result, found that a much enlarged oxygen concentration on the oxide surface is necessary for solving the discrepancy between calculated and observed growth rates.

Introduction

Silicon carbide (SiC) is a unique wide bandgap semiconducting material because a SiO₂ film can be grown on its surface by thermal oxidation similarly to Si. By making a use of superiority in physical properties of SiC, a high-performance power MOSFET is expected to realize with the conventional MOS device technologies. However, despite many active researches, SiC MOSFETs still have serious problems, such as a higher on-resistance than those expected from the properties of SiC and a low long-term reliability of oxide layers [1]. We believed that deeper understanding of the SiC oxidation mechanism leads to the solution of these problems.

In previous work [2], we proposed a kinetic model of SiC oxidation on the basis of the interfacial silicon and carbon emission phenomenon, which we referred to as ‘silicon and carbon emission model,’ (SCEM) derived by adding the processes of C oxidation and emission to the interfacial Si emission model proposed for Si oxidation [3,4]. For another work, we have shown that the initial stage of SiC oxidation at sub-atmospheric pressure is presumably dominant to the oxide growth on the oxide layer, which originates from the oxidation of Si interstitials emitted and transmitted through the oxide [5].

In this report, we try to apply the SCEM to the growth rate data at various oxygen partial pressures and discuss the oxidation mechanism of SiC more in details by making a comparison between calculated growth rate curves and the observed ones.

Experiments

An *in-situ* spectroscopic ellipsometer consisting of an oxidation furnace combined with the ellipsometer arms was employed in this study. The ellipsometric parameters (Ψ , Δ) in the wavelength region between 295 and 370 nm were obtained using a CCD detector and the angle of incidence was 75.8°.

Epitaxial wafers of 4H-SiC with a 0.5° off-oriented (000-1) C-face and a 8° off-oriented (0001) Si-face, both are *n*-types, having a net donor concentration $N_d - N_a = 3 \times 10^{15}$ and $1 \times 10^{16} \text{ cm}^{-3}$, respectively, were used in this study. All oxidations were conducted at the oxidation temperature of 1100°C . Further experimental details are shown elsewhere [5]. The changes in the ellipsometric parameters (Ψ , Δ) were recorded during oxidation of the samples. The obtained (Ψ , Δ) spectra were analyzed using a three-layer structure model, *i.e.*, SiC/interface layer/SiO₂, because excellent fitting with the observed (Ψ , Δ) spectra has been achieved with this structure, as reported in the references [6,7]. The optical constants of the interface layers were assumed to follow the modified Sellmeier's dispersion relation taking a weak optical absorption into account [8], so that we could obtain the thickness and optical constants of the interface layer as well as the SiO₂ layer thickness.

Results and Discussion

The plots in Figs. 1 denote observed oxide growth rates at various oxygen partial pressures on SiC (000-1) C-face (a) and (0001) Si-face (b). Also shown in the figures are the growth rates given by the Si and C emission model (solid lines). The figures indicate that: (1) the observed data show an abrupt reduction in the thickness region less than 10 nm especially in the case of lower partial pressure, (2) after the abrupt reduction they gently reduce, (3) the calculated curves successfully reproduce the observed growth rates though restricted in the mild deceleration region, (4) the calculated curves show the rapid reduction more remarkable as higher partial pressure, which is opposite tendency to that of observed data. The figures and point (1) indicate that the growth rate in the abrupt reduction region slightly decreases with decreasing partial pressure [5]. According to the SCEM, Si and C interstitials are emitted into the oxide layer during oxidation. When the oxide is very thin, the interstitials should be transmitted through the layer and instantly oxidized on the oxide surface. Because the density of oxygen coming from gas phase is enough to instantly oxidize the interstitials on the oxide surface even if the partial pressure is below 0.1 atm, the initial growth rates at low partial pressure are thought to be dominant to the oxide growth on the surface. At present we consider that the discrepancy in point (4) should be solved when calculation using the SCEM exactly takes into account the oxide growth on the oxide surface. The remarkable change in growth rate at low partial pressure, in which the growth rate rapidly decreases at the initial stage and then decreases gently (point (1) and (2)), have also been pointed out in the case of Si oxidation [9]. Also point (4) is thoroughly similar to the tendency of calculation for Si oxidation [9].

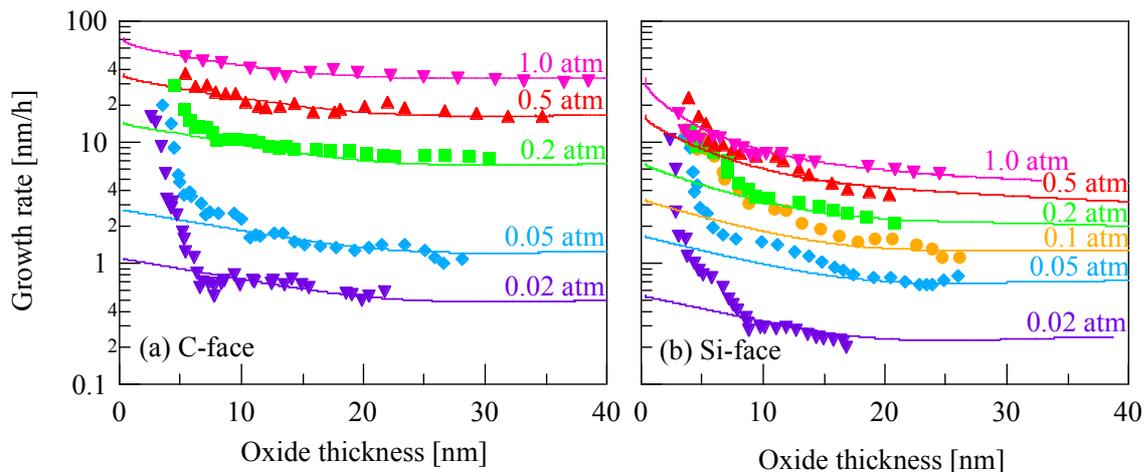


Fig. 1. Oxide thickness dependence of growth rates at various oxygen partial pressures on C-face (a) and Si-face (b). The solid lines are calculated growth rate curves based on the SCEM [2].

We consider that the accurate description for the surface oxide growth may dissolve the disagreement between the calculated and observed oxide growth rates in the cases of low partial pressures. To verify this idea, first of all, we separately calculated the oxide growth rate on the

surface, inside the SiO₂ layer, and at the SiC–SiO₂ interface (denoted as F_{sur} , F_{ox} , and F_{int} , respectively) using the SCEM.

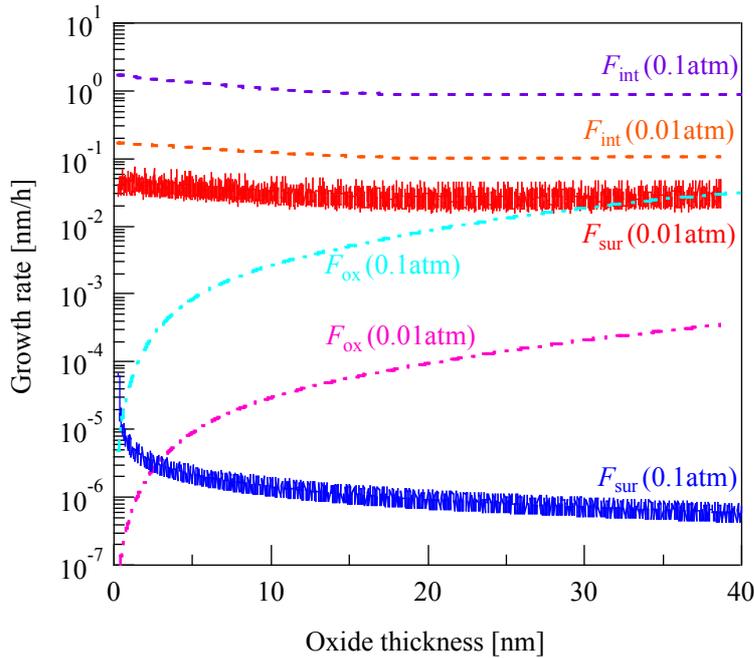


Fig. 2. Simulated oxide growth rates on the surface, inside the SiO₂ layer, and at the SiC–SiO₂ interface (F_{sur} , F_{ox} , and F_{int} , respectively) at 0.1 and 0.01 atm on Si-face.

Figure 2 shows the calculation results of F_{sur} , F_{ox} , and F_{int} at 0.1 and 0.01 atm on Si-face. The figure indicates that the F_{sur} curve for 0.01 atm is much higher than that for 0.1 atm by a factor of approximately 5 orders, though the F_{sur} is still lower than F_{int} . This result confirms that the low-pressure oxidation enhances the oxide growth on the surface, as discussed above, which is probably due to the reduction in the possibility that the emitted Si interstitials encounter oxygen in-diffusing from the oxide surface. Conversely, the F_{ox} and F_{int} curves for 0.01 atm are lower than those for 0.1 atm by factors of 2 orders and 1 order, respectively. From the fact that the F_{int} is generally higher than F_{ox} , it is found that the observed growth rate in the mild deceleration stage to be proportional to pressure [5] is due to the proportional increase in F_{int} .

A careful look confirms the deceleration of F_{int} in the very-thin oxide region (*ca.* < 5 nm) to be enhanced as elevating the pressure, which has been seen as Point (4). In this oxide thickness region, the value of F_{ox} is small enough to be ignored. Therefore, to reproduce the rapid reduction of growth rate, we should reconsider not the oxide growth process of interfacial or internal oxide but the process of surface oxidation of Si interstitials in the SCEM.

According to the SCEM, the oxide growth rate on the oxide surface (F_{sur}) is described as follows [2–4]:

$$F_{\text{sur}} = \eta C_{\text{O}}^{\text{S}} C_{\text{Si}}^{\text{S}} / N_0, \quad (1)$$

where η denotes oxidation rate on the oxide surface, C^{S} concentration of corresponding interstitials on the oxide surface, and N_0 the molecular density of SiO₂. Since the transport coefficient from gas phase to oxide surface (denoted by h in the Deal-Grove model [10]) is sufficiently large, the value of C_{O}^{S} is nearly equal to solubility limit of oxygen in SiO₂ (C^*). However, in the case that the emitted Si interstitials are exposed to the gas phase, a much larger concentration of oxygen than C^* should be given. For this reason, we gave a 10^4 times larger C_{O}^{S} than previous one and recalculated the growth rates at 0.02 atm on Si-face.

Figure 3 shows the calculated growth rates, F , F_{sur} , and F_{int} , for without and with $\times 10^4$ enhanced C_{O}^{S} (denoted by without and with prime, respectively). Note that the oxide growth rates inside the oxide (F_{ox} and F'_{ox}) are not shown here because their influences to the total growth rate are negligible and also the values of F and F_{int} are omitted because they overlap F'_{int} . The figure indicates that this modification is quite effective for a more accurate reproduction of the observed growth rate. Therefore, our assumption that the rapid growth rate reduction is attributed to the enhanced oxide growth on the oxide surface in the initial oxidation stage is thought to be reasonable. Moreover, the

factor of 10^4 roughly corresponds to the difference in oxygen flux between in SiO_2 and gas phase, evidencing the validity of the modification. Although the calculated growth rate curve is still deviated from the measured data, we consider that further refined parameters will make a better fit to the observed data.

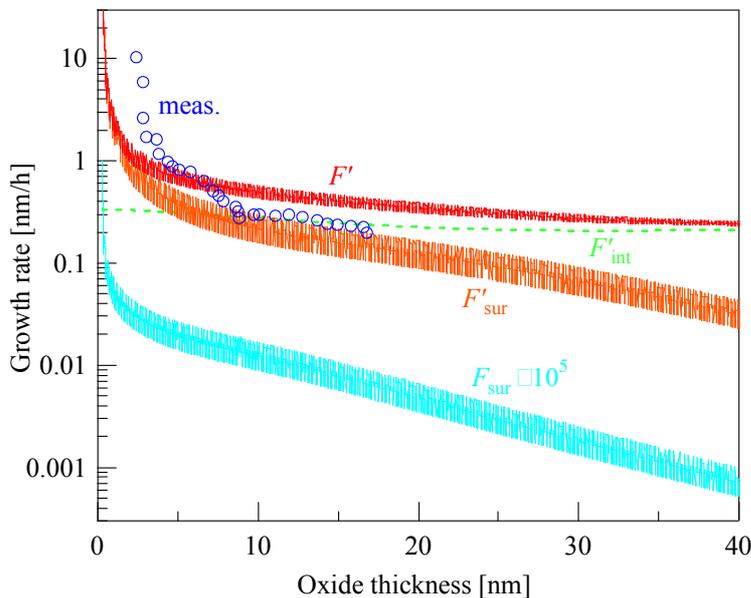


Fig. 3. Calculated oxide growth rates, that on the surface, and at the SiC– SiO_2 interface (F , F_{sur} , and F_{int} , respectively) at 0.02 atm on Si-face. The letter with prime means the case that the concentration of oxygen on the oxide surface C_{O}^{S} is multiplied by 10^4 .

Summary

We performed model calculations based on the Si and C emission model and tried to reproduce the oxide growth rates at various sub-atmospheric pressure. The calculation results exhibit that a rapid growth rate reduction in the initial oxidation stage eased as lower pressure, which is opposite tendency to the observed growth rates. To solve this discrepancy, we gave a much higher oxygen concentration on the oxide surface and showed that this modification is valid for the reproduction of oxide growth rate in the initial stage, especially for the case of low oxygen pressure, which may also be available for Si oxidation.

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References

- [1] For example, Y. Hijikata, H. Yaguchi, and S. Yoshida, Growth Rate Enhancement, in R. Gerhardt (Ed.), Properties and Applications of Silicon Carbide, InTech, Croatia, 2011, Chapter 4.
- [2] Y. Hijikata, H. Yaguchi, and S. Yoshida, Appl. Phys. Express 2 (2009) 021203.
- [3] H. Kageshima, K. Shiraishi, and M. Uematsu, Jpn. J. Appl. Phys. 38 (1999) L971-L974.
- [4] M. Uematsu, H. Kageshima, and K. Shiraishi, J. Appl. Phys. 89 (2001) 1948-1953.
- [5] K. Kouda, Y. Hijikata, S. Yagi, H. Yaguchi, and S. Yoshida, J. Appl. Phys. 112 (2012) 024502.
- [6] T. Iida, Y. Tomioka, K. Yoshimoto, M. Midorikawa, H. Tukada, Y. Hijikata, M. Orihara, H. Yaguchi, M. Yoshikawa, Y. Ishida, and S. Yoshida, Jpn. J. Appl. Phys. 41 (2002) 800.
- [7] H. Seki, Y. Hijikata, H. Yaguchi, and S. Yoshida, Mater. Sci. Forum 615-617 (2009) 505.
- [8] M. E. Thomas, Handbook of Optical Constants of Solids, 177 (Academic Press, 1991).
- [9] J. Farjas and P. Roura, J. Appl. Phys. 102 (2007) 054902.
- [10] B. E. Deal and A. S. Grove, J. Appl. Phys. 36 (1965) 3770.

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