

Oxygen-Partial-Pressure Dependence of SiC Oxidation Rate Studied by In-situ Spectroscopic Ellipsometry

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Abstract. Real time observations of SiC (000-1) C-face and (0001) Si-face oxidation were performed using an *in-situ* ellipsometer over the oxygen-partial-pressure range from 0.1 to 1.0 atm. We analyzed the relations between oxide growth rate and oxide thickness by applying an empirical relation proposed by Massoud *et al.* We found the occurrence of oxidation enhancement in the thin oxide regime also for Si-face as well as for C-face. We have discussed the oxygen-partial-pressure dependence of the oxidation rate constants between SiC C- and Si face, comparing with that of Si.

Introduction

Silicon carbide (SiC) has attractive properties, such as wide band gap, high thermal conductivity and high breakdown electric field, for electronic device applications including high-power and high-frequency devices whose specifications cannot be obtained using Si and GaAs [1]. In addition, SiC surfaces can be thermally oxidized and SiO₂ layers can be formed as the gate insulator for metal-oxide-semiconductor applications similarly to Si. SiC-metal-oxide-semiconductor field-effect-transistors (MOSFETs) are expected to have an on-resistance two orders of magnitude lower than those of Si-MOSFETs at the same breakdown voltage [2]. Therefore, SiC-MOSFETs have been ardently researched and developed.

However, SiC-MOSFETs have some problems to be solved before practical use, such as their higher on-resistance than that predicted from bulk properties. This poor electrical characteristic is attributed to high interface state density at the SiC/oxide interface. In order to elucidate the origin of the interface states, it is important to study the oxidation mechanism of SiC. In the previous study, we observed SiC oxidation in real time using an *in-situ* ellipsometry [3]. We have found that SiC oxidation can be generally represented by the Deal-Grove (D-G) model [4], which is originally proposed for Si oxidation. On the other hand, Massoud *et al.* [5] reported that growth rate enhancement, which cannot be explained by the D-G model, appears at the initial stage of Si oxidation. We have studied the initial oxidation stage of SiC (000-1) C-face using the *in-situ* spectroscopic ellipsometer, and have found that the growth rates in initial stage of oxidation are much larger than those predicted by the D-G model [6]. Also Massoud *et al.* [5] studied the oxygen-partial-pressure dependence of growth rate enhancement to make clear the oxidation mechanism of Si.

In this paper, we have measured the oxidation rates of SiC (000-1) C-face and (0001) Si-face at different oxygen-partial-pressures using *in-situ* spectroscopic ellipsometry and have discussed the oxygen-partial-pressure dependence of the oxidation rate constants between SiC C- and Si-faces, comparing with that of Si.

Experiment

Epitaxial wafers of 4H-SiC (9mm × 9mm) with 8° off-oriented (000-1) C-face and (0001) Si-face, *n*-type were used in this study. Immediately after RCA cleaning, the sample was put into a furnace and heated at 1215°C. First, to determine the optical constants of SiC at this temperature, polarization parameters (Ψ , Δ) were measured in the argon atmosphere. The parameters Ψ and Δ are defined by $r_p/r_s = \tan \Psi \exp(i\Delta)$, where r_p and r_s are the reflected amplitudes for *p*- and *s*-polarized light, respectively. Then, the parameters (Ψ , Δ) were measured during oxidation in a mixture of oxygen and Ar flow of 1 slm. The partial pressure of oxygen was varied between 0.1 and 1.0 atm. Oxidation time dependences of (Ψ , Δ) were measured in the wavelength range from 310 to 490 nm, at an angle of incidence of 75.8°. The oxidation for C-face was performed up to the oxide thickness around 100 nm. The oxidation time was 1.5 h under oxygen partial pressure of 1.0 atm and 5 h under 0.1 atm. The oxidation time for Si-face was 8 h to obtain the oxide thickness up to 20 nm at all the oxygen-partial-pressures. In the derivation of oxide thickness, we used a model of the three-layer structure, a SiO₂ layer, an interface layer and SiC substrate, and assumed the interface layer is ~1 nm in thickness and has high refractive indices. Details of the evaluation of oxide thickness were described elsewhere [6].

Results and discussion

Figures 1 and 2 show the oxidation rate dX/dt of SiC (000-1) C-face and (0001) Si-face, respectively, as a function of the oxide thickness, X , at various oxygen-partial-pressures.

In Fig. 1, it can be seen that the growth-rates in thin oxide regime are much larger than the values calculated from the D-G model at all the oxygen-partial-pressures. These growth-rate enhancements are seen for the oxide thickness below *ca.* 25 nm at any oxygen-partial-pressure.

As shown in Fig. 2, the growth-rate enhancements are also seen for Si-face in the oxide thickness below *ca.* 15 nm at any oxygen-partial-pressure, which means that the oxidation enhancement is not peculiar to SiC C-face.

The relation between oxidation rate dX/dt and oxide thickness X in the thermal oxidation of Si has been given by the D-G model [4],

$$\frac{dX}{dt} = \frac{B}{A + 2X} \quad (1)$$

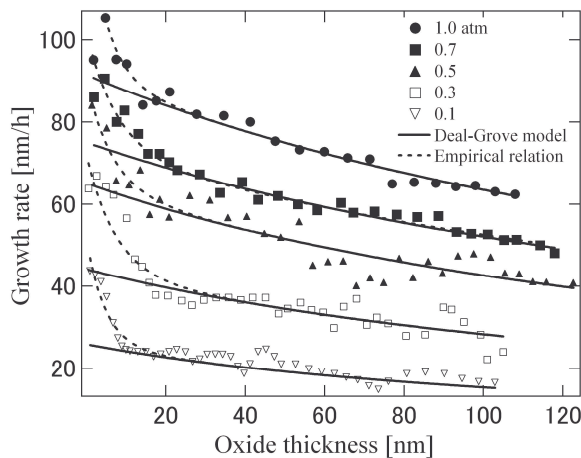


Fig. 1. Oxide thickness dependence of oxidation rate at various oxygen partial pressures for SiC (000-1) C-face. The solid and dashed lines denote the values derived from the Deal-Grove mode Eq. (1) and those from the empirical relation Eq. (2), respectively.

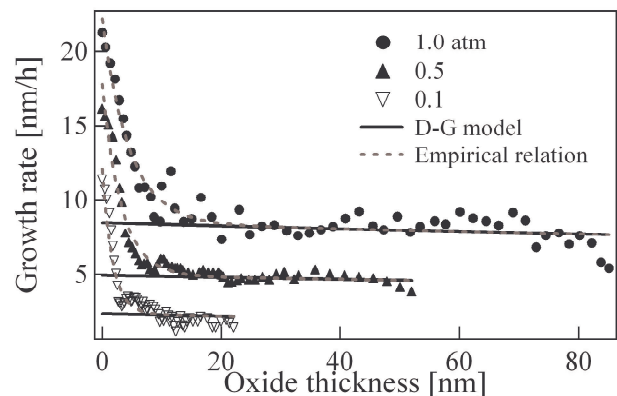


Fig. 2. Oxide thickness dependence of oxidation rate at various oxygen partial pressures for SiC (0001) Si-face. The solid and dashed lines denote the values derived from the Deal-Grove mode Eq. (1) and those from the empirical relation Eq. (2), respectively.

where B/A and B are denoted as the linear and parabolic rate constants of oxidation. To explain the growth rate enhancement of Si oxidation in thin oxide regime, Massoud *et al.* have added an exponential term $C\exp(-X/L)$ to the D-G equation as

$$\frac{dX}{dt} = \frac{B}{A + 2X} + C\exp\left(-\frac{X}{L}\right), \quad (2)$$

where C and L denote a pre-exponential constant and a characteristic length which the oxidation rate decays with the increase in the oxide thickness, respectively. We have applied this empirical equation (2) to the oxidation of SiC. The dotted lines shown in Figs. 1 and 2 are the values obtained by fitting the values calculated from Eq. (2) to the observed ones by adjusting 4 parameters B/A , B , C and L . The calculated values are well fitted to the observed ones in whole thickness range for all the oxygen-partial-pressure studied.

Figure 3 shows the parabolic rate constant B as a function of the oxygen-partial-pressure p for C-face and Si-face. The values of B are approximately proportional to p both for C- and Si-face, as in the case of for Si [5]. This result is reasonable considering that B corresponds to oxygen diffusivity through the oxide layer, though the value of B obtained for C-face is larger than that of Si-face.

On the contrary, the linear rate constant B/A for C-face and Si-face are proportional to $p^{0.58}$ and $p^{0.54}$, respectively. In the case of Si oxidation, the linear rate constant B/A is proportional to $p^{0.8}$ at low pressures [5], and $p^{0.7-0.8}$ at high pressures [7]. According to the D-G model [4], B/A is given as $B/A = k_s C^*/N$, where k_s , C^* and N are the chemical surface-reaction rate constant for the oxidation, the equilibrium concentration of oxidant in the oxide and the number of oxidant molecules incorporated into a unit volume of oxide, respectively. As C^* is given as $C^* = kp$, where k is Henry's law constant, B/A values should be proportional to p . However, B/A values for C and Si-face oxidation are not proportional to p as in the case of Si.

Figure 4 shows a pre-exponential constant C and the characteristic length L as a function of oxygen-partial-pressure p . The values of C for C-face are about three times larger than that for Si-face, i.e., around 30 and 12 nm/h on an average, respectively. As shown in this figure, the values of L for C-face are larger than that for Si-face, i.e., around 6 and 4 nm, respectively. Therefore, the growth-rate enhancement for C-face occurs up to the oxide thickness larger than that for Si-face. In comparison with Si, the values of L both for SiC C- and Si face oxidation are smaller than that for Si (~ 7 nm) [5]. The figure also shows that the values of C and L are weakly dependent on the oxygen-partial-pressure, i.e. nearly constant. These results suggest the existence of another oxidation-rate-limiting mechanism, which is independent of the quantity of oxygen supplied, other than the

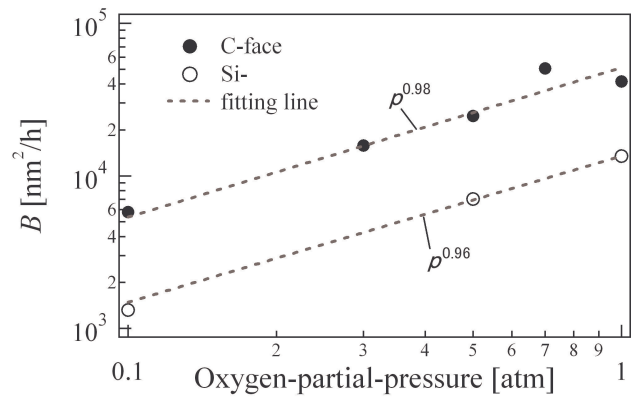


Fig. 3. Oxygen-partial-pressure dependence of the parabolic rate B for C-face and Si-face oxidation.

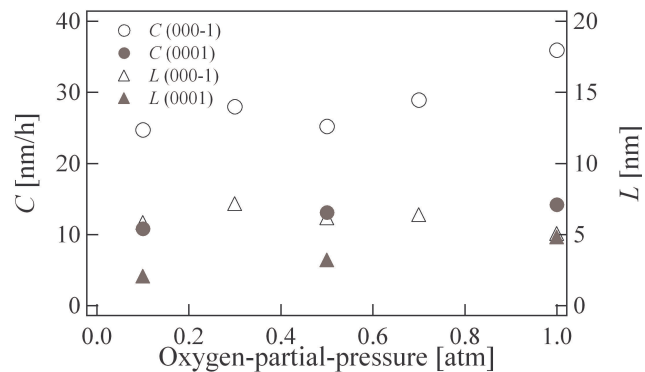


Fig. 4. Oxygen partial pressure dependence of a pre-exponential constant C and the characteristic length L for SiC C- and Si-face at the oxygen partial pressure of 0.1 – 1.0 atm.

interface reaction of oxygen with SiC and the diffusion of oxygen through SiO₂ layers.

In order to elucidate the enhancement of SiC oxidation both for Si- and C-faces in the thin oxide regime, including the oxygen-partial-pressure dependence of oxidation rate found in this study, at any rate, an atomistic model for SiC oxidation (e.g. Ref. [8]) should be established.

Summary

We have measured the SiC oxidation rate at different oxygen-partial-pressures using *in-situ* spectroscopic ellipsometry. It was found that growth-rate enhancements are seen for SiC (0001) Si-face as well as for (000-1) C-face at any oxygen-partial-pressure from 0.1 to 1.0 atm. We have fitted the Massoud empirical equation to the oxidation rate of SiC, and have obtained the oxygen-partial-pressure dependence of the four parameters, B , B/A , C and L . The parabolic rate constant B both for C- and Si-faces are proportional to the oxygen-partial-pressure. The linear rate constant B/A is proportional to $p^{0.5-0.6}$. A pre-exponential constants C for C- and Si-faces are around 30 and 12 nm/h on an average, respectively. The characteristic length of enhancement rate L for C-face is larger than that for Si-face, i.e., around 6 and 4 nm, respectively. The oxygen-partial-pressure dependence of the values of C and L is nearly constant.

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References

- [1] S. Yoshida: *Electric Refractory Materials*, ed. Y. Kumashiro (Marcel Dekker, New York, 2000), p. 437.
- [2] V. V. Afanas'ev, M. Bassler, G. Pensl and M. Schultz: *Phys. Stat. Sol. (a)* Vol. 162 (1997), p. 312.
- [3] K. Kakubari, R. Kuboki, Y. Hijikata, H. Yaguchi, and S. Yoshida: *Mater. Sci. Forum* Vol. 527-529 (2006), p. 1031.
- [4] B. E. Deal and A. S. Grove: *J. Appl. Phys.* Vol. 36 (1965), p. 3770.
- [5] H. Z. Massoud and J. D. Plummer, *J. Electrochem. Soc.* Vol. 132 (1985), p. 2685.
- [6] T. Yamamoto, Y. Hijikata, H. Yaguchi, and S. Yoshida: *Jpn. J. Appl. Phys.* Vol. 46 (2007), p. L770.
- [7] M. Uematsu, H. Kageshima, and K. Shiraishi: *Jpn. J. Appl. Phys.* Vol. 38 (1999), p. 971.
- [8] Y. Hijikata, T. Yamamoto, H. Yaguchi, and S. Yoshida: *Submitted to this conference.*