

Model calculations of SiC oxide growth rate at various oxidation temperatures based on the silicon and carbon emission model

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Abstract. We have tried to apply the oxidation model of SiC proposed previously, termed ‘Si-C emission model’, to the oxide growth rate at various oxidation temperatures. We have found that the model well reproduces the oxide thickness dependences of oxide growth rates for all of the temperatures measured for both of the SiC Si- and C-faces. We have estimated the temperature dependence of oxide depth profiles of Si and C interstitials by using the Si-C emission model, and discussed the structure at/near the SiC–oxide interface.

Introduction

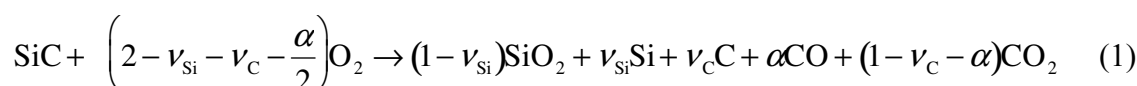
Silicon carbide (SiC) is an attractive material for applying to electronic devices because it can be thermally oxidized and SiO₂ layers, known as a superior insulator for metal-oxide-semiconductor (MOS) applications, can be formed on the surface. However, despite of many active researches, SiC MOSFETs still have serious problems, such as a higher on-resistance than those expected from the physical properties of SiC and a low long-term reliability of oxide layers. In comparison to Si, very little is known about the oxidation mechanism of SiC, which may bring about the difficulty in the solution of these problems.

We have proposed a kinetic model of SiC oxidation, termed ‘Si-C emission model’, taking into account the interfacial Si and C emission accompanied by the oxidation of SiC and the suppression in interfacial reaction rate caused by the accumulation of interstitials emitted, and showed that the model well reproduces the oxide thickness dependence of oxide growth rates of SiC at the entire oxide thickness range both for (0001)Si-face and (000-1)C-face [1,2]. We also showed that the cause for the low oxide growth rate for Si-face compared with that for C-face can be attributed to the low intrinsic interfacial reaction rate and the high Si emission rate for Si-face.

In this report, we try to apply the Si-C emission model to the oxide growth rates of SiC at various oxidation temperatures and discuss the oxidation mechanism of SiC more in details from the temperature dependence of parameter values deduced from the curve fits. We also discuss the SiC–oxide interface structures with the oxide depth profiles of Si and C interstitials estimated using the Si-C emission model.

Calculation Method

Considering Si and C atoms emitted from the interface during the oxidation, the reaction equation for SiC oxidation can be written as



where ν and α denote the interfacial emission rate and the production rate of CO, respectively, and the subscripts, Si and C, denote the values for the corresponding atoms. In our model, as the interfacial

reaction rate for SiC oxidation (k) is thought to be suppressed by the accumulation of Si atoms and C atoms emitted near the interface, we assumed that k is given by multiplying decreasing functions for Si and C:

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

where C^{I} and C^0 are the interfacial concentration of corresponding interstitials and the solubility limit of the corresponding interstitials in the oxide, respectively, and k_0 is the interfacial reaction rate when oxide thickness nearly equals zero, i.e., intrinsic interfacial reaction rate without the influence of the accumulation of emitted Si and C atoms. The details for the calculation have been described in elsewhere [1]. The parameters related to the properties of SiO_2 were set to the same values as obtained for Si oxidation [3]. The parameters concerning C interstitials as well as the values of ν_{Si} and k_0 were deduced by fitting the calculated oxide growth rates to the measured ones.

Results and Discussion

Figure 1 shows the oxide growth rates as a function of oxide thickness, observed for the dry oxidation of C-face at various oxidation temperatures [4] and those given by the Si-C emission model. The figure indicates that the Si-C emission model reproduces the oxide growth rate curves for all of the temperatures measured. Some articles [5,6] have suggested that the SiC oxidation can be described by using the Deal-Grove model [7]. However, there are several issues in the application of Deal-Grove model to SiC oxidation, in which unreasonable parameter values need to fit to the measured oxide growth rates. For example, the values of parabolic oxidation-rate constant (B) for SiC, corresponding to the diffusivity of oxidant in the oxide significantly different from that for Si [5] is required to fit the growth rate curve despite both of oxides on SiC and Si are SiO_2 . In accordance with Si-C emission model, on the contrary, the oxide growth rates of SiC for all of the temperatures measured can be derived using the same diffusivity values of oxidant as those for Si. This shows that the Si-C emission model is more adequate than Deal-Grove model to explain SiC oxidation process.

Figure 2 shows the temperature dependences of Si and C emission rates (ν_{Si} and ν_{C} , respectively) and intrinsic interfacial reaction rate (k_0) for C- and Si-face deduced from the curve fits. The figure indicates that the ν_{C} and ν_{Si} for Si-face are larger than those for C-face, in particular, the ν_{Si} for Si-face is remarkably large. These results suggest that, as we previously reported [2], the high Si emission rate is a cause for the low oxide growth rate for Si-face, as well as the low intrinsic interfacial reaction rate k_0 . The figure also indicates that the activation energy of k_0 for Si-face is larger than that for C-face. This means that the Si-face intrinsically needs higher energy to proceed the oxidation of SiC than C-face, which agrees with the result from *in-situ* photoemission spectroscopic study performed by Virojanadara and Johansson [8] and *ab-initio* studies performed by Gavrikov *et al.* [9] and by Ohnuma *et al.* [10].

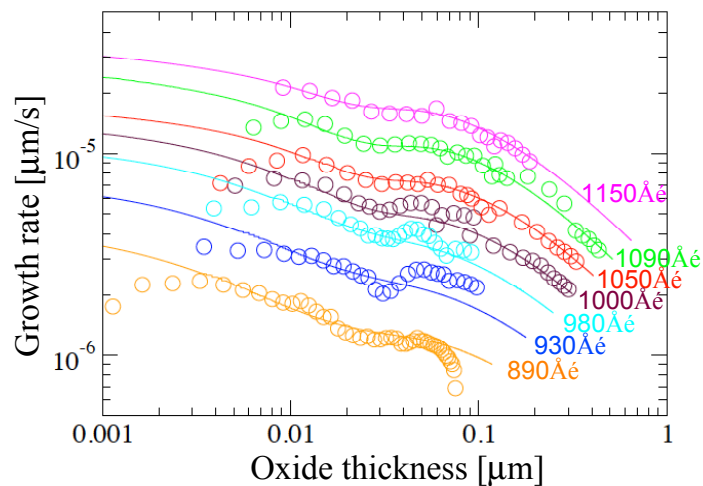


Fig. 1 Oxide thickness dependence of oxide growth rates at various oxidation temperatures for (000-1)C-face. The circles and the solid curves denote measured growth rates and calculated ones, respectively.

We have estimated the oxide depth profiles of Si and C interstitials emitted at oxidation temperatures of 1000, 1100 and 1200°C, oxide thickness of 50 nm for Si- and C-face. The parameters used in the calculations are obtained from the interpolations of Arrhenius plots of v_C , v_{Si} and k_0 (shown in Fig. 2), and the reference [3]. Figures 3 (a) and (b) show the estimated oxide depth profile of Si interstitials C_{Si} and that of C interstitials C_C , respectively. The figure 3(a) shows that the higher oxidation temperatures result in the higher areal densities of Si interstitials (*i.e.* the area below C_{Si} curve) regardless of Si- and C-face. The decay of C_{Si} with respect to the distance from the interface for Si-face is little dependent on oxidation temperature, in contrast, that for C-face decreases remarkably with decreasing oxidation temperature. In comparison of Si- and C-face, C_{Si} for Si-face is higher than that for C-face at any temperature. The figure 3(b) shows that, different from the case of Si interstitials,

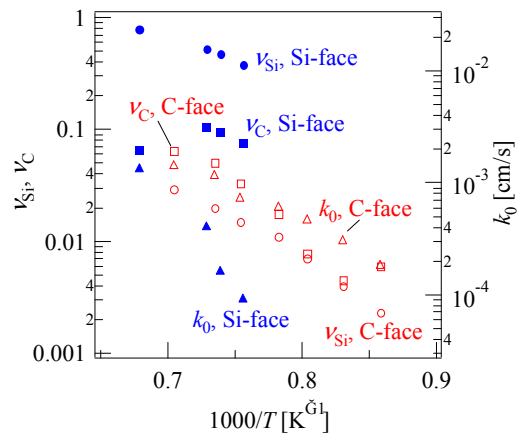


Fig. 2 Arrhenius plots of v_{Si} , v_C , and k_0 (circles, squares, and triangles, respectively) for Si- and C-face.

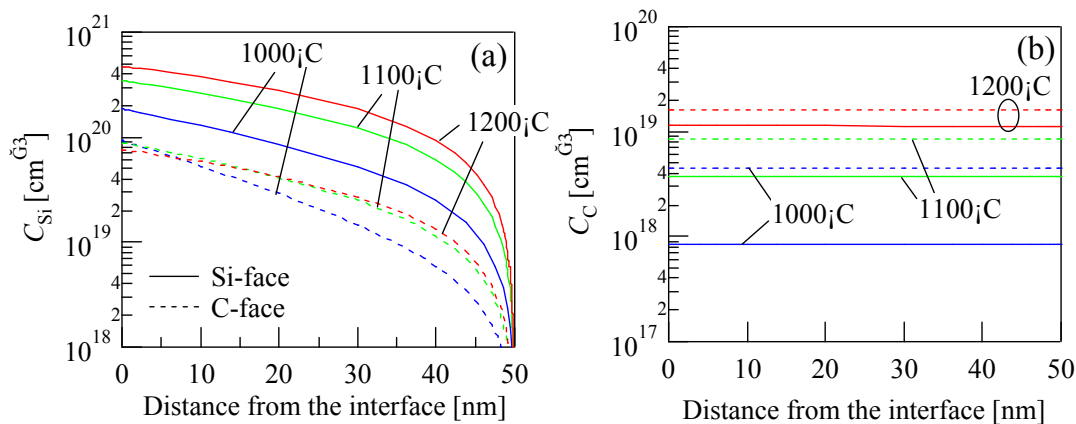


Fig. 3 Simulations of oxide depth profiles of interstitials at various oxidation temperatures for Si- and C-face (solid line and broken line, respectively): (a) Si interstitials, (b) C interstitials.

the concentration of C interstitials C_C is almost constant against the distance from the interface at any temperature for both of Si- and C-faces, indicating that C interstitials rapidly diffuse through the oxide. The figure also shows that, similarly to the case of Si interstitials, the higher oxidation temperatures bring about the higher concentrations of C interstitials regardless of Si- and C-face. In comparison of Si- and C-face, the C_C for Si-face is lower than that for C-face at any temperatures, which is opposite tendency to the case of Si interstitials. According to our recent work with deep-ultraviolet spectroscopic ellipsometry [11,12], the interface layer is considered to be a modified SiC layer, such as a strained SiC layer or a SiC layer with interstitials, based on the experimental results that the dispersion relation of refractive indices of the interface layer is similar to that of SiC but its absolute value is higher than that of SiC and the value of extinction coefficient is almost equal to that of SiC. In the case of Si oxidation, the Si atoms are emitted into Si as well as into oxide layer, resulting in the formation of Si layers containing Si interstitials near the Si-oxide interface [13,14]. On the analogy of Si oxidation, there should be an interface layer that includes Si and C interstitials at the SiC-side of SiC-oxide interface. These considerations for the origins of interface layers well

explain the results from *in-situ* ellipsometric observations of SiC oxidation in the ultra-thin oxide regime, in which the refractive index of the interface layer increases with oxide thickness and then saturates at around 1 nm in oxide thickness [15]. We have also reported that there is a good correspondence between interface state density (D_{it}) and refractive index of the interface layer [11], which is understood by assuming the interfacial Si and C atoms emitted relate to the generation of interface states. From these considerations, it is said that the SiC-oxide interface structure can be discussed on the basis of Si-C emission model, leading to the estimation of D_{it} .

Finally, we discuss the origins of D_{it} , assuming that the temperature dependences of Si and C interstitial concentration at the SiC-side are same as or similar to those for the oxide-side. In accordance with our recent work [11], D_{it} for Si-face is little dependent on oxidation temperature, while for C-face D_{it} depends on the temperature and the lower temperatures bring about the lower D_{it} values. As shown in Fig. 3, although none of temperature dependences of Si and C interstitial accounts for the temperature dependences of D_{it} for both of Si- and C-faces, a part of temperature dependences of interstitial agrees with that of D_{it} , such as a relation between C-face temperature dependence of C interstitial and that of D_{it} . These results suggest that the generation of the interface states might relate to the interfacial Si and C emission accompanied by the oxidation of SiC.

Summary

We tried to apply the Si-C emission model to the oxide growth rate data at various oxidation temperatures and found that the model reproduces the oxide growth rate curves for all of the temperatures measured for both of the Si- and C-faces. From the parameters deduced by the curve fits, we discussed the differences in oxidation process between Si- and C-face. We also discussed the interface structure and the origin of interface states in the light of temperature dependence of oxide depth profile of emitted Si and C interstitials estimated from the Si-C emission model.

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