Materials Science Forum Vols. 679-680 (2011) pp 429-432
Online available since 2011/Mar/28 at www.scientific.net
© (2011) Trans Tech Publications, Switzerland
doi:10.4028/www.scientific.net/MSF.679-680.429

Theoretical studies for Si and C emission into SiC layer during oxidation

Yasuto Hijikata[1, a], Hiroyuki Yaguchi[1,b], and Sadafumi Yoshida[2,c]

[1]Division of Mathematics Electronics and Informatics, Saitama University, 255 Shimo-Okubo, Sakura-ku, Saitama 338-8570, Japan

[2]Advanced Power Electronics Research Center, AIST, 1-1-1 Umezono, Tsukuba 305-8568, Japan

[a]yasuto@opt.ees.saitama-u.ac.jp, [b]yaguchi@opt.ees.saitama-u.ac.jp, [c]s.yoshida@aist.go.jp

Keywords: oxidation, MOS structure, SiC–oxide interface, Si and C emission, interstitial, diffusivity.

Abstract. To understand the structure of SiC–oxide interface more in detail, we propose a profiling theory of Si and C emission into SiC layer during oxidation. Simulations of the depth profiles of Si and C interstitials results in the structures analogous with those observed from a spectroscopic ellipsometry. To determine the diffusivities of Si and C interstitials, we performed capacitance–voltage measurements for examining the re-distribution profiles of nitrogen after oxidation and compared between observed and calculated profile. The calculated nitrogen profiles showed good fits to the observed ones in the case of self-diffusivity of C interstitials magnified by several 10 times for literature value. Finally, we discuss the validity of the proposed theory.

Introduction

Silicon carbide (SiC) is a unique wide-gap semiconductor material because SiO_2 known as superior insulating material can be grown by thermally oxidizing a SiC substrate, leading to an easy fabrication of metal-oxide-semiconductor (MOS) structures likely as Si. In addition, SiC has excellent physical properties as power electronics devices and, thus, the realization of a high-performance SiC-MOS field-effect-transistor (FET) that replaces the previous Si power devices (e.g. insulated gate bipolar transistor (IGBT)) is ardently expected. However, SiC-MOSFETs 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. It has been considered that the poor understanding on the oxidation mechanism compared with that of Si may lead to the difficulty in the solution of these problems.

To understand the oxidation mechanism of SiC, we have proposed a kinetic model of SiC oxidation termed ‘Si-C emission model’, taking the interfacial Si and C emission into the SiO_2 layer accompanied by the oxidation of SiC into account. We calculated the oxide growth-rates of SiC on the basis of Si-C emission model and showed that the model well reproduced the oxide growth rates of SiC at the entire oxide thickness range both for the (0001)Si-face and (000–1)C-face at various oxidation temperatures [1,2]. According to the Si-C emission model, the interfacial oxidizing reaction is restricted by the accumulation of Si and C interstitials emitted into the oxide. We have accordingly not taken the emission into SiC-side in the calculation into account. However, it has been well known from the studies such as on oxide-induced stacking faults [3] and isotope-tracing experiments [4] that interfacial Si atoms emit into the Si and the oxide layers during Si oxidation. Therefore, for SiC oxidation, it is probable that interfacial Si and C emission occurs not only into the oxide but also into the SiC substrate and, hence, it is very important to estimate the Si and C interstitial profile in SiC for understanding of the structure of SiC–oxide interface.

On the other hand, we found from the spectroscopic ellipsometry studies that the SiC–oxide interface layer has the same photon energy dispersions of optical constants as those of SiC but higher refractive indices at entire photon energy and its thickness is about 1 nm [5,6]. These results suggest that the interface layer cannot be explained with the compositional transition layer such as a silicon oxycarbide or suboxide but with a modified SiC layer such as a SiC layer including Si and/or C interstitials or a stressed SiC layer. The article also indicate that there is a good correspondence between the refractive index of the interface layer, which is related to the density, and the interface

All rights reserved. No part of contents of this paper may be reproduced or transmitted in any form or by any means without the written permission of TTP, www.ttp.net. (ID: 133.38.240.110-20/04/11,02:51:13)

consult
comment
contact
click for feedback

state density estimated from capacitance–voltage (*C*–*V*) measurements [5]. Therefore, it can be considered that to know the depth profiles of Si and C interstitials in SiC after oxidation is also very important to solve the reason for the poor electrical characteristic of MOS interfaces.

In this report, we try to establish a profiling theory of Si and C interstitials emitted into the SiC layer during oxidation and simulate SiC–oxide interface structures. However, for self-diffusivities of Si and C interstitials in SiC necessary for the calculations, two values differing by several orders have been reported [7,8]. Moreover, it is possible that the diffusivity during oxidation may become larger than that for annealing, known as oxidation-enhanced diffusion (OED) [9]. To determine the diffusivity and to verify our theory, we compared the calculated depth profiles of Si and C interstitials with the observed re-distribution profiles after oxidation. Since there was no available data for a Si and C interstitial profile reported and it has been reported that boron (B) diffuses via same way as Si and C interstitials [8], we conducted re-distribution profiling of nitrogen (N) instead of those of Si and C interstitials.

Calculation method

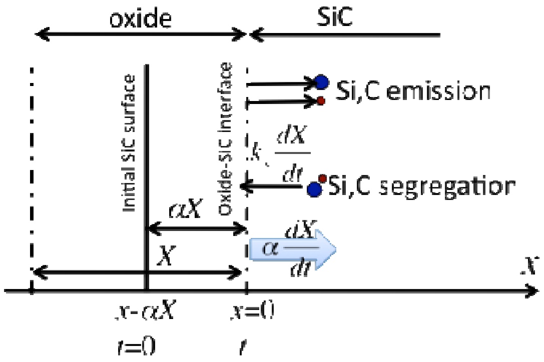

Fig. 1. Schema of calculation model.

Figure 1 shows the schema of calculation model, where *t*, α, *x*, *X*, and k_s denote oxidation time, the ratio of consumed SiC layer to SiO_2 thickness (0.44), distance from the oxide–SiC interface (the position $x = 0$ moves to SiC layer during oxidation), oxide thickness, and segregation coefficient, i.e. solubility limit in SiO_2 (C^0) / that in SiC (C^1), respectively. Since we did not obtain the C^1 for Si and C interstitials (C^1_{Si} and C^1_C), we gave the solubility limit of Si interstitials in Si [10] and assumed that $C^1_C = C^1_{Si}$. The values of C^0 for Si and C interstitials are referred from the references [1,2]. According to these references, C^0_{Si} is 10 times larger than C^0_C. The diffusion equation for Si and C interstitials in SiC can be written as [11]

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} + \alpha\frac{dX}{dt}\frac{\partial C}{\partial x} \qquad (1)$$

where *C* and *D* are concentration and diffusivity, respectively, of corresponding interstitials. The second term in the right-hand of eq. (1) means the moving interface accompanied with the oxidation. We obtain diffusivities from the relation $D=D^{SD}(N/C^1)$ and the self-diffusivities (D^{SD}) from the literatures [7,8], where *N* is molecular density of 4H-SiC (4.8×10^{22} cm^{-3}). The boundary conditions are written as:

$$C(\infty,t) = 0, \qquad (2\text{-}1)$$

$$D\left.\frac{\partial C}{\partial x}\right|_{x=0} = k_s\frac{dX}{dt}C(0,t) - \nu N\alpha\frac{dX}{dt}, \qquad (2\text{-}2)$$

where ν is emission ratio of corresponding interstitials. The first term and the second term in the right-hand of eq. (2-2) denote the segregation of interstitials from SiC layer to SiO_2 layer and the emission of interstitials into SiC layer, respectively. Here, we assumed that $\nu_{Si}=\nu_C=0.275$, which is the theoretical upper limit value for Si emission ratio for Si [3]. The values of *dX/dt* as a function of *X* are extracted from our previous works [12]. The equations (1)–(2) are numerically solved by a use of PDE solver [13].

consult
comment
contact
click for feedback

Experimental procedures

An *n*-type 4H-SiC bulk wafer with (0001)Si-face on-axis (nominal doping concentration N_d (=$|N_d–N_a|$)=2×10^{17} cm^{-3}) was employed for this study. To examine the concentration profile of doped nitrogen before and after oxidation, we used Schottky-contacts. For the samples with oxide, the oxide was removed in buffered HF solution before the formation of Schottky-contacts. Au was deposited as Schottky-contact pads with a diameter of 0.5 mm and Al was deposited as a backside ohmic-contact. Specimens were oxidized in dry oxygen flow of 1 slm at 1100°C for 3 h 40 min., resulting in oxide thicknesses of about 20 nm.

High-frequency (RF) *C*–*V* measurements were carried out at frequency of 1 MHz with small amplitude of 20 mV. To avoid detection of deep level states, a pulsed direct current (DC) bias voltage was applied with pulse width of 0.1 s and interval of 2 s.

Results and discussion

Figures 2 (a) and (b) show the concentration profiles of Si interstitials and C interstitials, respectively, in SiC substrate at *X*=10, 20, 40 nm, calculated for the case of oxidation temperature 1100°C for Si- and C-face. Here, we used the self-diffusivity values referred from Ref. [8]. The figures indicate that interstitials distribute in accordance with complementary error function, Si and C interstitials diffuse within the depth of about 1.5 nm for Si-face, 0.25 nm for C-face, and the depth is little dependent on oxide thickness. The order of depth as well as the thickness dependence agrees well with the experimental results from spectroscopic ellipsometry [5,6]. The difference in diffusion layer thickness between C-face and Si-face is due to that in oxidation rate. Namely, since the oxidation rate for C-face is faster, the diffusion layer is rapidly oxidized, resulting in the thin diffusion layer. Figure 2 also shows that interfacial concentration is not dependent on oxide thickness and interfacial concentration for Si interstitials is lower than that for C interstitials by a factor of 10, corresponding to the difference in solubility limit in SiO_2. Therefore, the concentration is surely inverse proportional to the segregation coefficient k_s.

In the calculations, we used the same k_s for Si interstitials as that of Si (6.9×10^7 [10]). Consequently, the interfacial concentration naturally results in the same value as that for Si oxidation (10^{13} cm^{-3} orders [10]), as shown in Fig. 2(a). However, according to our previous work [5,6], the interface layer has a higher refractive index than that of SiO_2 or SiC. If we assume that the interface layer is a SiC layer including Si and C interstitials, 10^{13} cm^{-3} orders inclusion of interstitials sounds like too small to explain the interface layer with such a high refractive index. Anyway, since the value of k_s (i.e. that of C^1) directly determine the concentration of interstitials in the SiC layer, it is important to know these values for SiC oxidation.

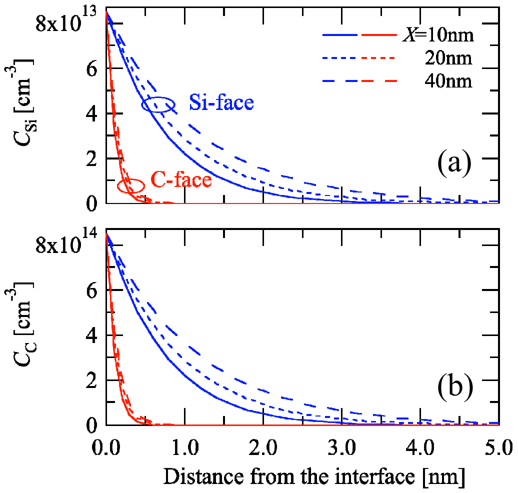

Fig. 2. Concentration profiles of (a) Si interstitials and (b) C interstitials in SiC substrate at *X*=10, 20, 40 nm for Si- and C-face.

We examined the effect of emission ratio *ν* on the interstitial re-distribution profile. As a result, we found that the interfacial concentration is proportional to the *ν* value. Therefore, the value of *ν* is also important factor to determine the interstitial concentration. Conversely, we can quantitatively predict re-distribution profiles of interstitials using the proposed theory if only the values of k_s and *ν* are obtained.

The symbols in Fig. 3 shows the observed N re-distribution profiles at *X* = 20 nm. As shown in the figure, nitrogen piles up near the oxidizing interface. However, such a large pile-up never bring about in the studied case that the diffusivity in oxidized substrate is smaller than that in oxide [14]. Although we are uncertain about the origin of this pile-up at the present, we regard it as some oxidation-induced donor-like traps in SiC layer. To calculate this donor concentration profile after oxidation, we have modified the eq. (2-1) to $C(\infty,t) = N_\mathrm{d}$ and vN in the eq. (2-2) to 5.5×10^{16} cm^{-3} (solubility limit of oxygen in SiO_2, i.e. oxygen concentration on the surface of SiC) and assumed that the diffusion of the donors proceeds via same process as the self-diffusion of C interstitial but the segregation coefficient k_s is changed to the value deduced from curve fits. Figure 3 also shows the calculated profiles using the self-diffusivity value of C interstitial ($D^{\mathrm{SD}}{}_\mathrm{C}$) referred from Ref. [7] (red long dashed line), and that from Ref. [8] (blue short dashed line), and that obtained from curve fit (green solid line) to the observed profile. The figure indicates that the $D^{\mathrm{SD}}{}_\mathrm{C}$ value from Ref. [7] is too large to reproduce the observed profile, as claimed by Rüschenschmidt *et al.* [8]. The fitted profile is obtained with the value larger than that of Ref. [8] by a factor of 36. Although further works are needed to clarify this discrepancy, it might be due to the OED [9].

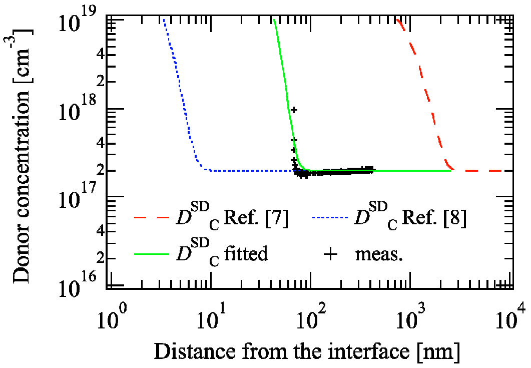

Fig. 3. Donor concentration profiles in SiC substrate.

Summary

We proposed a calculation theory giving Si and C interstitial profiles in SiC layer during oxidation by taking Si and C atom emission into SiC in the Si and C emission model into account. The theory indicated the presence of Si and C highly concentrated layer with thickness of a few nm and with weak dependence on oxide thickness, which are in agreement with those observed from spectroscopic ellipsometry. To determine the diffusivities of Si and C interstitials, we examined donor concentration profiles after oxidation and compared the depth profiles given by our calculation with observed ones. We found that the proposed theory reproduces the observed profiles when we gave a self-diffusivity of C interstitials reported by Rüschenschmidt *et al.*, which was used in the calculations of interstitial profiles. Therefore, it can be said that the calculated profiles strongly support the interpretation for the interface structure in spectroscopic ellipsometry studies, i.e., the interface layer consists of a SiC layer including Si and C interstitials with a thickness of a few nm.

References

[1] Y. Hijikata, H. Yaguchi, and S. Yoshida: Appl. Phys. Express Vol. 2 (2009), a.n. 021203
[2] Y. Hijikata, H. Yaguchi, and S. Yoshida: Mater. Sci. Forum Vols. 645-648 (2010), p. 809
[3] S. T. Dunham and J. D. Plummer: J. Appl. Phys. Vol. 59 (1986), p. 2541
[4] S. Hosoi *et al.*: Nucl. Instr. and Meth. in Phys. Res. B Vol. 249 (2006), p. 390
[5] H. Hashimoto *et al.*: Appl. Surf. Sci. Vol. 255(2009), p. 8648
[6] H. Seki *et al.*: Mater. Sci. Forum Vols. 615-617 (2009), p. 505
[7] J. D. Hong, R. F. Davis, and D. E. Newbury: J. Mater. Sci. Vol. 16 (1981), p.2485
[8] K. Rüschenschmidt *et al.*: J. Appl. Phys. Vol. 96 (2004), p. 1458
[9] K. Ibano, K. M. Itoh, and M. Uematsu: J. Appl. Phys. Vol. 103 (2008), a.n. 026101
[10] A. M. Agarwal and S. T. Dunham: J. Appl. Phys. Vol. 78 (1995), p. 5313
[11] T. Kato and Y. Nishi: Jpn. J. Appl. Phys. Vol. 3 (1964), p. 377
[12] T. Yamamoto *et al.*: Jpn. J. Appl. Phys. Vol. 47 (2008), p. 7803
[13] Information on http://www.pdesolutions.com/
[14] A. S. Grove, O. Leistiko, Jr., and C. T. Sah: J. Appl. Phys. Vol. 35 (1964), p. 2695

Silicon Carbide and Related Materials 2010
doi:10.4028/www.scientific.net/MSF.679-680

Theoretical Studies for Si and C Emission into SiC Layer during Oxidation
doi:10.4028/www.scientific.net/MSF.679-680.429

click for feedback
consult – comment – contact

consult
comment
contact
click for
feedback