Chemical phase transitions of a Si oxide film on SiC by MeV electron beam irradiation

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An ultrathin Si oxide film grown on a $6H$-SiC(0001) wafer was irradiated with 1 MeV electron beam to examine its effect on the chemical species of a Si oxide/SiC wafer, where the Si oxide film was composed of SiO_2, Si suboxides (Si^{3+}, Si^{2+}, and Si^{1+}), and Si oxycarbides (Si–C–O). Scanning photoelectron microscopy and Si $2p$ core-level spectroscopy show that e-beam irradiation induces chemical phase transitions from the Si suboxides and Si oxycarbides to SiO_2. This suggests that e-beam irradiation is an efficient and simple method of producing a chemically uniform SiO_2 film on SiC without thermal and chemical treatments. © *2007 American Institute of Physics.*
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The oxidation of a semiconductor wafer plays an important role in the fabrication of semiconductor devices. Recently, the oxide thickness has been reduced to less than a few nanometers. Therefore, it becomes increasingly important to prepare abrupt and defect-free oxide/semiconductor interfaces. Silicon has been chosen for semiconductor devices on account of the excellent properties of its native oxide (SiO_2) and the low defect density at the SiO_2/Si interface. For high-temperature, high-voltage, and high-frequency electronic devices, it is more efficient to adopt wide band gap semiconductors.[1] Among the wide band gap semiconductors, SiC has attracted interest partly because a stable native oxide (SiO_2) film can be grown only on SiC.[1] However, metal-oxide-semiconductor field effect transistors (MOSFETs) based on SiC have shown inferior electronic performance than expected from the properties of bulk SiC.[1] This poor electronic performance is the result of defects at the SiO_2/SiC interface which produces fixed charges and interface trap states.[2–5] Several experiments using x-ray photoemission spectroscopy have shown that these defects are related to nonstoichiometric oxidation products such as Si suboxides (Si^{3+}, Si^{2+}, and Si^{1+}) and Si oxycarbides (Si–C–O).[6–10]

The formation of a chemically uniform Si oxide/SiC interface is one of the crucial issues for device applications of the promising wide band gap SiC. A wide variety of methods such as preoxidation cleaning,[11] Si overlayer oxidation,[6] hydrogen annealing,[12] annealing in nitric oxides,[13–15] and Ar^+ ion irradiation during a thermal oxidation[16] have been applied in an attempt to achieve stoichiometrically uniform interfaces. However, it is inevitable that some of C–O bonds remain trapped at the Si oxide/SiC interface because carbon release in the form of a CO or a CO_2 molecule is limited during the oxidation processes.[17,18]

In this study, a Si oxide/SiC wafer was irradiated with 1 MeV electron beam (hereafter, e-beam) at room temperature and ambient conditions. The effects of the irradiation on the Si oxide/SiC wafer were investigated using synchrotron radiation scanning photoelectron microscopy (SPEM) with various photon energies ($h\nu$). The Si $2p$ core-level spectra of irradiated and nonirradiated regions were measured with a spatial resolution of 25 μm. The spatially resolved Si $2p$ spectra show that irradiation reduces remarkably the concentration of Si suboxides and Si oxycarbides in the Si oxide/SiC wafer leaving a chemically uniform SiO_2 film.

A Si oxide film with a thickness of about 1 nm was grown naturally on a $6H$-SiC(0001) wafer in air and irradiated without further chemical treatment. An electron beam accelerator at the Korea Atomic Energy Research Institute was used for the 1 MeV e-beam irradiation. The wafer was irradiated with a total fluence of 1×10^{16} cm^{-2} at room temperature and ambient conditions. In order to avoid thermal effects, the wafer temperature was kept below 50 °C during irradiation using repeated cycles of irradiation for 2 min with a sequent 2 min rest period. The chemical phase transition induced by the irradiation was examined by shielding half of the wafer with 600-μm-thick Ta foil.

The synchrotron radiation SPEM measurements were performed at the 8A1 beamline in the Pohang Accelerator Laboratory in Korea. The Si $2p$ and O $1s$ core-level spectra were measured with an incident angle of 0° and an emission angle of 55°, where the angle is 0° when the direction is perpendicular to the surface. The incident photon beam size on the sample, defined by a pinhole placed in front of the sample, was 50 μm.

Figure 1 shows the SPEM images and Si $2p$ and O $1s$ core-level spectra of the Si oxide/SiC wafer, where only half

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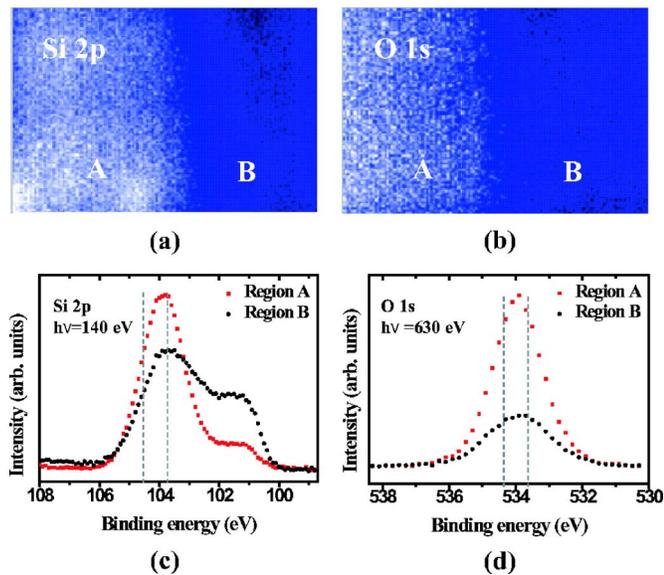[a] Electronic mail: cypark@skku.edu
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FIG. 1. (Color online) SPEM images of the Si oxide/SiC wafer for Si 2*p* (a) and O 1*s* (b) core-level spectra obtained at *hν*'s of 140 and 630 eV, respectively, after 1 MeV e-beam irradiation. Irradiated and nonirradiated regions are denoted by A and B, respectively. The intensity in the SPEM image is proportional to the number of photoelectrons within a defined BE window. The Si 2*p* (c) and O 1*s* (d) core-level spectra were measured from the two different regions. The dotted lines in (c) and (d) are the BE windows used to acquire the SPEM images (a) and (b), respectively.

FIG. 2. (Color online) Si 2*p* core-level spectra acquired at various photon energies (*hν*) from 140 to 630 eV of the nonirradiated and irradiated regions. The binding energy is relative to that of bulk SiC. The three component of the Si 2*p* core-level spectra are denoted by SiO_2 (light blue), D (pink), and SiC (dark blue).

of the wafer was irradiated. The SPEM images, shown in Figs. 1(a) and 1(b), were obtained using a binding energy (BE) window between 103.75 and 104.5 eV of the Si 2*p* core-level spectrum and a BE window between 533.6 and 534.35 eV of the O 1*s* core-level spectrum, respectively. The A and B regions indicate irradiated and nonirradiated regions, respectively. Figure 1(c) shows the Si 2*p* core-level spectra at the A and B regions. The peak with a BE of 104 eV is known to originate from SiO_2.[7,9,10] The brightness of the SPEM image in Fig. 1(a), which was acquired with a BE window between 103.75 and 104.5 eV, is thus proportional to the SiO_2 density. This indicates that e-beam irradiation induces the formation of SiO_2. The e-beam-induced oxidation was also observed in the O 1*s* core-level spectra [Fig. 1(d)] and its SPEM image [Fig. 1(b)], as shown by the higher O 1*s* intensity at the irradiated region than at the nonirradiated region.

The e-beam-induced oxidation was further analyzed by measuring the Si 2*p* core-level spectra of the irradiated and non-irradiated regions at different *hν*, as shown in Fig. 2. The Si 2*p* core-level spectra measured at *hν*=140 eV was the most surface sensitive one and became more bulk sensitive with increasing *hν*. The Si 2*p* core-level spectra were decomposed by a standard nonlinear-least-squares fitting procedure using Voigt functions and well fitted with three components, as shown in Fig. 2.[19] The component with the higher BE relative to that of bulk SiC [hereafter, core-level shift (CLS)] of 2.7 eV is known to originate from SiO_2, as denoted by SiO_2.[7,9,10] Another component with a CLS of 1.0 eV, which is denoted by D, is due to Si suboxides and Si oxycarbides.[6,7,10] The Si 2*p* core-level spectrum of the non-irradiated region at *hν*=140 eV [Fig. 2(a)] indicates that the density of Si suboxides and Si oxycarbides was almost half of the SiO_2 density. In contrast, irradiation reduces remarkably the D component enhancing the SiO_2 component, as
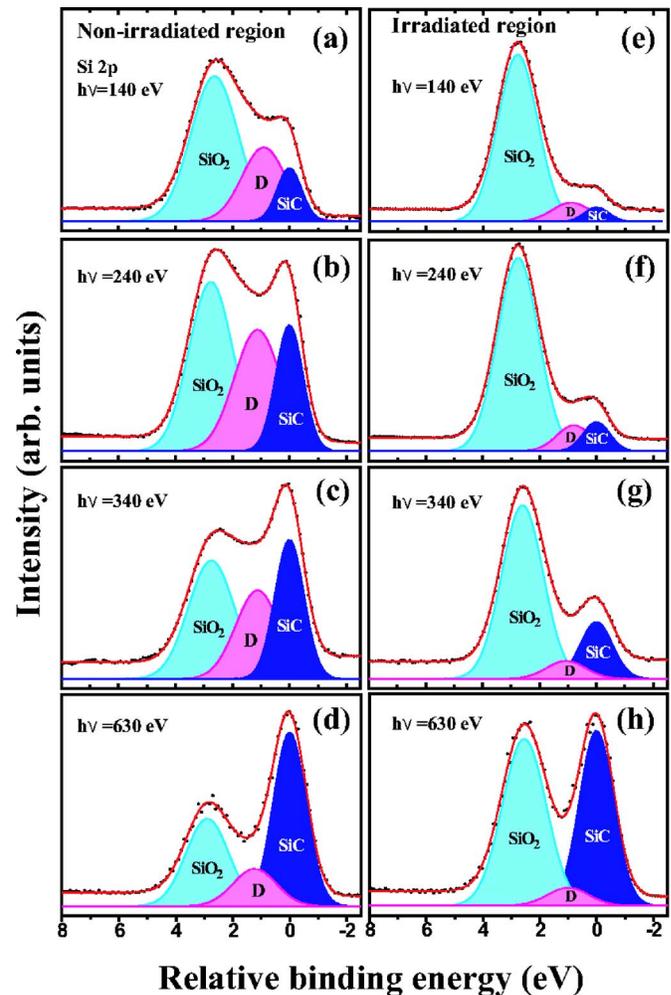
shown in Fig. 2(e). This suggests that most of the Si suboxides and Si oxycarbides changed to SiO_2 as a result of e-beam irradiation.

The depth dependence of the e-beam-induced chemical phase transitions was measured from the changes of the relative intensities in the three components as a function of *hν*, as shown in Fig. 3. The sampling depth at each *hν* is $\lambda \sin \theta$, where λ and θ are the inelastic mean free path and emission angle, respectively.[20] Note that 95% of photoelectrons come from the Si atoms located within the sampling depth and the energy resolution of *hν* was below 0.2 eV. At the nonirradiated region, the relative intensities of the SiC components at *hν*=140 and 240 eV were 0.11 and 0.21, respectively, and the sampling depths at *hν*=140 and 240 eV were 0.7 and 1.2 nm, respectively. This indicates that the thickness of the SiO_2 film is roughly below 1 nm because 95% of photoelectrons are emitted from the Si atoms located within the sampling depth.[20] The relative intensity of the D component at the nonirradiated region reached a maximum at *hν*=240 eV. This suggests that the density of the Si suboxides and Si oxycarbides increases at the Si oxide/SiC interface. Interestingly, at all photon energies, the D component at the irradiated region was dramatically reduced by irradiation compared with the nonirradiated region. This leads to the
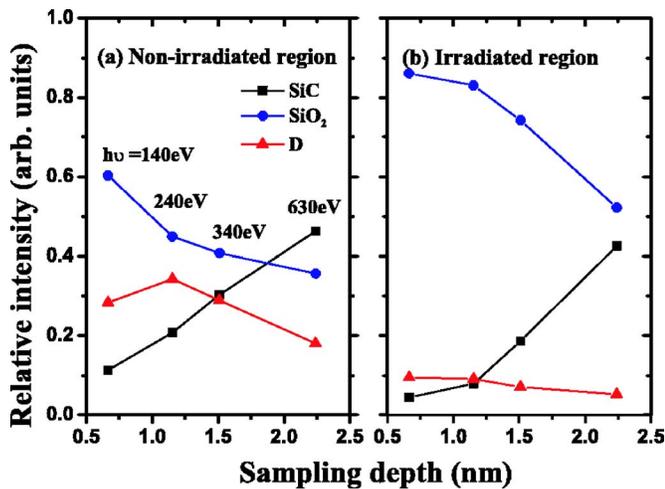
FIG. 3. (Color online) Plot of the relative intensities of the three components in the Si 2*p* spectra of the nonirradiated (a) and irradiated (b) regions. The three components, SiC, SiO_2, and D, are denoted by the black rectangle, blue circle, and red triangle, respectively.

conclusion that irradiation produces SiO_2 at the expense of the Si suboxides and Si oxycarbides, which occurs from the surface of the Si oxide film to the Si oxide/SiC interface. The carbon of the Si oxycarbides can be removed in the form of a CO or a CO_2 molecule during e-beam-induced reoxidation in air, as suggested theoretically.[18] The roughness of the Si oxide/SiC interface and the electronic performance of the MOSFETs based on Si oxide/SiC wafers will require further study.

In conclusion, we found that 1 MeV e-beam irradiation causes chemical phase transitions of the Si suboxides and Si oxycarbides of the Si oxide/SiC wafer to SiO_2 resulting in a chemically uniform SiO_2 film. The Si suboxides and Si oxycarbides were reduced from the surface of the Si oxide film to the Si oxide/SiC interface. Furthermore, e-beam-induced reoxidation can be performed at room temperature and ambient conditions. Therefore, MeV e-beam irradiation is a promising method for producing a high quality SiO_2 film on a SiC wafer.

[1]*Silicon Carbide, A Review of Fundamental Questions and Applications to Current Device Technology*, edited by W. J. Choyke, H. M. Matsunami, and G. Pensl (Akademie, Berlin, 1998), Vols. I and II, and references therein.

[2]Jayarama N. Shenoy, James A. Cooper, Jr., and Michael R. Melloch, Appl. Phys. Lett. **68**, 803 (1996).

[3]V. V. Afanas'ev and A. Stesmans, Appl. Phys. Lett. **69**, 2252 (1996).

[4]Vickram R. Vathulya, Dong Ning Wang, and Marvin H. White, Appl. Phys. Lett. **73**, 2161 (1998).

[5]V. V. Afanas'ev, A. Stesmans, M. Bassler, G. Pensl, M. J. Schulz, and C. I. Harris, J. Appl. Phys. **85**, 8292 (1999).

[6]F. Amy, P. Soukiassian, Y.-K. Hwu, and C. Brylinski, Appl. Phys. Lett. **75**, 3360 (1999).

[7]F. Amy, P. Soukiassian, Y. K. Hwu, and C. Brylinski, Phys. Rev. B **65**, 165323 (2002).

[8]C. Virojanadara and L. I. Johansson, Phys. Rev. B **71**, 195335 (2005).

[9]C. Önneby and C. G. Pantano, J. Vac. Sci. Technol. A **15**, 1597 (1997).

[10]C. Radtke, I. J. R. Baumvol, J. Morais, and F. C. Stedile, Appl. Phys. Lett. **78**, 3601 (2001).

[11]V. V. Afanas'ev, A. Stesmans, M. Bassler, G. Pensl, M. J. Schulz, and C. I. Harris, Appl. Phys. Lett. **68**, 2141 (1996).

[12]K. Fukuda, S. Suzuki, T. Tanaka, and K. Arai, Appl. Phys. Lett. **76**, 1585 (2000).

[13]Hui-feng Li, Sima Dimitrijev, H. Barry Harrison, and Denis Sweatman, Appl. Phys. Lett. **70**, 2028 (1997).

[14]G. Y. Chung, C. C. Tin, J. R. Williams, K. McDonald, M. Di Ventra, S. T. Pantelides, L. C. Feldman, and R. A. Weller, Appl. Phys. Lett. **76**, 1713 (2000).

[15]S. Hazra, S. Shakraborty, and P. T. Lai, Appl. Phys. Lett. **85**, 5580 (2004).

[16]C. Radtke, I. J. R. Baumvol, and F. C. Stedile, Phys. Rev. B **66**, 155437 (2002).

[17]Massimiliano Di Ventra and Sokrates T. Pantelides, Phys. Rev. Lett. **83**, 1624 (1999).

[18]Sanwu Wang, Massimiliano Di Ventra, S. G. Kim, and Sokrates T. Pantelides, Phys. Rev. Lett. **86**, 5946 (2001).

[19]H. W. Yeom, H. Hamamatsu, T. Ohta, and R. I. G. Uhrberg, Phys. Rev. B **59**, R10413 (1999).

[20]*Surface Analysis: The Principal Techniques*, edited by John C. Vickerman (Wiley, New York, 1997), Vol. I, p. 58.