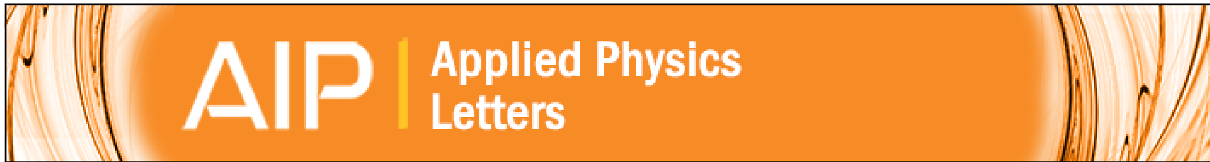

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Morphological and compositional changes in the SiO_2/SiC interface region induced by oxide thermal growth

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Changes in morphology and composition of interfacial regions of thermally grown SiO_2 films on SiC in dry O_2 induced by reoxidations were investigated using atomic force microscopy and oxygen profiling. The gradual oxygen profile near the interface in oxides grown at 1100 °C evidences a transition region between SiO_2 and SiC. Reoxidation at 950 °C leads to a decrease of the transition region thickness, while reoxidation at 1100 °C increases the transition region thickness. These results are discussed in terms of the role played by the reoxidation temperature on the formation and consumption of carbon compounds in the SiO_2/SiC interface region. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2167608]

Silicon carbide (SiC) is a suitable material for high-temperature, high-power, and high-frequency electronic devices due to its properties such as wide band gap, high breakdown electric field, high saturation electron drift velocity, and high thermal conductivity.[1] Besides, SiC is the only compound semiconductor on which an insulating film, namely SiO_2, can be thermally grown to form the gate dielectric in metal-oxide-semiconductor-based devices, taking advantage of the excellent electrical and thermochemical properties of SiO_2,[2] as well as of its already established processing technology. SiO_2 grown on SiC is similar to its counterpart grown on Si, at least in surface and bulk regions.[3] However, the SiO_2/SiC interface presents a higher density of interface electronic states[4,5] that prevents the broad use of SiC as a semiconductor material. Therefore, substantial efforts are currently been made in order to improve the electrical quality of this interface.[6–8]

The main difference between SiC and Si is the presence of carbon in the former. Carbon acts in the oxide thermal growth process by: (i) Changing the reactivity of O_2 with the semiconductor substrate, due to the stronger Si–C bond as compared to the Si–Si bond present in the Si substrate and (ii) forming carbonaceous species during oxide growth, by reaction of incoming O_2 molecules with the SiC substrate, which may be incorporated in the growing SiO_2 film. The consequence of such interaction is the formation of a C-rich region near the SiO_2/SiC interface, that was predicted theoretically[9,10] and observed experimentally[11–13] by different authors. This carbon accumulation is thought to be one of the major sources of the high density of interfacial states that degrade the electrical characteristics of the final device.[14,15]

A previous work[16] described a reduction of the interface states density when oxide films are nitrided in NO, which was attributed to passivation of electrically active defects, such as carbon clusters, silicon oxycarbides, and/or silicon suboxides.[12,13,17] Another route to reduce interface states density was wet reoxidation of the thermally grown SiO_2 film, performed at a lower temperature,[18] which reduced also the effective fixed oxide charge. Furthermore, it was shown recently[19] that during lower temperature dry reoxidation of SiO_2 films on SiC, oxygen from the gas phase is not only incorporated at the interface but also in the bulk of the previously grown SiO_2 layer, in striking contrast with SiO_2 films on Si.[3] This was explained by the reaction of O_2 with C clusters (produced in the SiO_2/SiC interface region during the first high-temperature dry oxidation step) leading to partial consumption of these clusters during the second lower temperature oxidation step.

The present letter reports on investigations of this complex transition layer between the bulk of the SiO_2 film thermally grown in dry oxygen and the SiC substrate. Relevant questions concerning the generation and evolution of this C-rich region during thermal oxidation are: How is carbon incorporated in the oxide film? Is this incorporation laterally homogeneous or somewhat nucleated? Which morphological and compositional changes are induced in the SiO_2/SiC interface region during thermal growth of the oxide films? These and other points deserve clarification, aiming at further improvements of SiC-based devices and are addressed. The abruptness of the interface region was accessed here performing oxygen profiling, whereas the topography of the formed interfaces was accessed by selectively etching the SiO_2 layer and analyzing the remaining surface.

Silicon-faced (0001) *n*-type on-axis 6H–SiC wafers manufactured by CREE Research Inc. were cleaned with the standard Radio Corporation of America process and etched in a 5% HF aqueous solution for 1 min. Immediately after cleaning they were loaded in a resistive quartz tube furnace. The first sample was obtained growing a SiO_2 film on SiC at 1100 °C for 1 h in 100 mbar of dry oxygen enriched to 97% in ^{18}O (termed $^{18}O_2$). This first sample is named "1100." By performing an identical growth step followed by reoxidation, again in 100 mbar of $^{18}O_2$, two other samples were pro-

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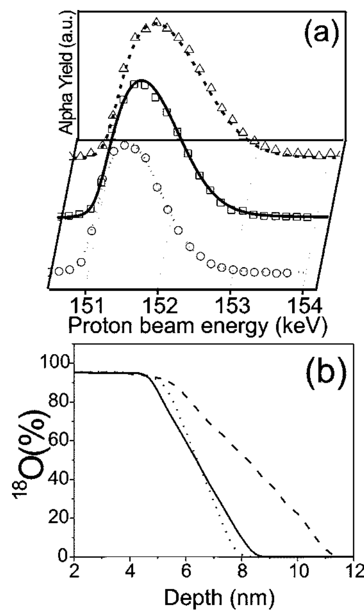

FIG. 1. (a) Experimental excitation curves (symbols) of the $^{18}O(p,\alpha)^{15}N$ nuclear reaction around the resonance energy $E_r = 151$ keV and the corresponding simulations (lines) for sample 1100 (open squares and solid line), sample 1100/950 (open circles and dotted line), and sample 1100/1100 (open triangles and dashed line). (b) ^{18}O profiles obtained from the simulation of the excitation curves presented in (a). Line types are the same as in (a). a.u. stands for arbitrary units. ^{18}O concentration is normalized to oxygen in stoichiometric SiO_2.

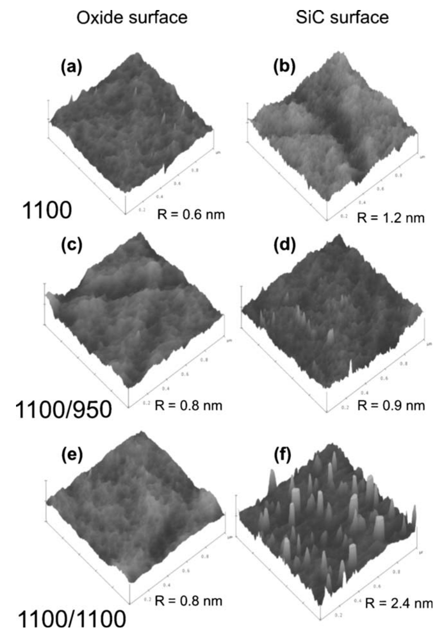

FIG. 2. AFM images of the surfaces of the oxides thermally grown on 6H–SiC (0001) and of the SiC surfaces after HF etching of the oxide film. The root-mean-square roughnesses (R) are indicated. (a) Oxide surface of sample 1100; (b) SiC surface of sample 1100 after HF etching; (c) Oxide surface of sample 1100/950; (d) SiC surface of sample 1100/950 after HF etching; (e) Oxide surface of sample 1100/1100; and (f) SiC surface of sample 1100/1100 after HF etching.

duced, namely "1100/1100" by reoxidation at 1100 °C for 1 h and "1100/950" by reoxidation at 950 °C for 3 h. ^{18}O profiles were determined by nuclear reaction profiling using the narrow resonance ($\Gamma = 100$ eV) in the cross section curve of the $^{18}O(p,\alpha)^{15}N$ nuclear reaction at 151 keV.[20] The proton beam has a diameter ~1.5 mm, averaging the information about the sample in a spot of this size. Atomic force microscopy (AFM) was performed with a Nanoscope IIIa instrument in tapping mode. Both the surface of the SiO_2 films and the surface of the SiC substrates after oxide removal were probed by AFM. A 5% HF aqueous solution was employed for oxide dissolution.

Excitation curves of the $^{18}O(p,\alpha)^{15}N$ nuclear reaction around the resonance at 151 keV (symbols) are shown in Fig. 1(a). The corresponding ^{18}O concentration versus depth curves are presented in Fig. 1(b), resulting in the simulated excitation curves (lines) in Fig. 1(a). Sample 1100 has a constant ^{18}O concentration in near surface and bulk regions of the oxide film [solid line in Fig. 1(b)]. This oxygen concentration, normalized to oxygen in stoichiometric SiO_2, is equal to the isotopic enrichment of the gas, evidencing the formation of a stoichiometric SiO_2 film in these regions. Nevertheless, in the interface region, the ^{18}O concentration decreases gradually to zero, within approximately 3 nm. The presence of residual carbon close to the SiO_2/SiC interface previously described[11–13,21] may justify this gradual lowering of the oxygen concentration. The ^{18}O profile in sample 1100/950 (dotted line) exhibits the same constant concentration of ^{18}O in near surface and bulk regions as sample 1100, evidencing once more[19] that stoichiometric SiO_2 is formed. However, near the interface, the ^{18}O profile exhibits a narrower transition region, about 2 nm thick. Finally, the ^{18}O profile in sample 1100/1100 (dashed line) shows the most gradual decrease of the ^{18}O concentration close to the interface. The transition region of this last sample is approximately 5 nm thick.

The AFM images and corresponding roughnesses of the above described samples are shown in Fig. 2, before (left-hand side) and after (right-hand side) etching the SiO_2 film. Concerning oxide film surfaces, the roughness of the 1100 sample slightly increases after reoxidations, with no observable difference between samples reoxidized at the two different temperatures. However, HF etching performed on both 1100/950 and 1100/1100 samples revealed remarkable differences close to the SiO_2/SiC interfaces. Sample 1100/950 presents a smoother surface after HF etching as compared to sample 1100, whereas a much higher roughness value is observed for sample 1100/1100. This latter surface evidences the formation of many nanoislands similar to others observed in the literature.[13,22]

These results can be explained by the formation and consumption of C clusters and/or silicon oxycarbides during oxidation. In this approach, two concurrent processes take place during reoxidation: (i) Consumption of existent C compounds by reaction with incoming oxygen and (ii) formation of new C compounds by reaction of carbonaceous by-products of SiC oxidation (mainly CO)[9] with the growing SiO_2 film. When performing a reoxidation at 1100 °C, mechanism (ii) prevails, while at a lower reoxidation temperature, namely 950 °C, the reaction between SiC and oxygen is strongly reduced, thus reducing the production of new C compounds. Indeed, the oxide growth rate on SiC (0001) at 950 °C is at least one order of magnitude lower than that at 1100 °C.[23] Thus, the lower temperature reoxidation acts mainly as an oxide "cleansing" step. This effect can also be observed when comparing the C contents of oxides grown on different faces of hexagonal SiC single crystals. Greater amounts of excess carbon were observed[21] in oxides thermally grown on 4H–SiC(000$\underline{1}$) (C face) as compared to

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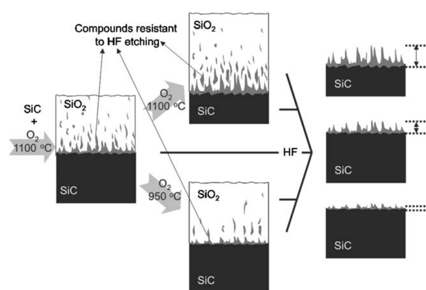

FIG. 3. Scheme of lateral cross section of SiC samples submitted to oxidation and reoxidations at the indicated temperatures. Cross-sectional profiles after HF etching of the oxide films are also represented. Different interface roughnesses result from different C contents incorporated in the oxide layer due to the effect of different reoxidation temperatures.

those grown on 4H–SiC(0001) (Si face), owing to the large difference in the oxide growth rates on these two polar faces. The oxide film growth on the (0001) face is much slower and therefore, in order to grow a comparable film thickness as that grown on the $(000\underline{1})$ face (at the same temperature and pressure), a larger exposure time to mobile O_2 incoming from the gas phase is required. In this way, the oxide layer grown on the (0001) face incorporates the same amount of C, although undergoing in parallel a much longer lasting, and hence more effective cleansing step.

In view of the above discussion, the largest roughness observed for sample 1100/1100 after HF etching seems to be due to the incorporation of extra C in a region close to the SiO_2/SiC interface. An interesting feature of this C incorporation is that it is not incorporated homogeneously at a given depth, but rather in the form of islands. At this point, it is worth mentioning that carbon species are not dissolved by HF etching.[24] Thus, the nanoislands observed on the AFM images of sample 1100/1100 after oxide removal consist in fact of remaining C compounds nucleated in the silicon oxide amorphous layer. The formation of C clusters in a much smaller scale (a few atoms) was already predicted theoretically.[9,10] The present experimental results support the idea that these agglomerations may occur in the nanoscopic scale. In a previous article,[25] we observed experimentally that the first oxidation products of SiC are silicon oxycarbides. Thus, these products of the incomplete oxidation of SiC seem to also contribute to a thicker transition region between SiO_2 and SiC observed in the present study. Another possibility for the determined roughness would be a SiO_2/SiC interface that, after oxide removal, would present SiC protuberances and consequently rough surfaces. Nevertheless, transmission electron microscopy investigations of this interface[11,26] discarded this hypothesis.

The findings of the present letter are summarized in Fig. 3. Owing essentially to the competition between removal of existent C compounds by reaction with incoming oxygen and formation of new C compounds by reaction of carbonaceous by-products of SiC oxidation with the growing SiO_2 film, the reoxidation temperature influences the remaining amount of C compounds in the oxide layer near the SiO_2/SiC interface. In the case considered here, the higher reoxidation temperature leads to higher C compounds concentration. This effect determines the thickness of the transition layers, which appear in the AFM images as islands of nonetched compounds and as roughness of samples surfaces after HF etching. Oxygen profiling confirms the picture: The oxygen depth distribution in the transition region between SiO_2 and SiC is more gradual in the sample reoxidized at a higher temperature, as compared to the more abrupt oxygen distribution for the sample reoxidized at the lower temperature. The interface roughness developed during oxidation, which appears also as a transition region between SiO_2 and SiC, reflect the formation of HF-resistant compounds in the SiO_2/SiC interface region. These compounds are most probably associated to silicon oxycarbides and/or silicon suboxides resulting from incomplete oxidation of SiC. Another possible mechanism that can lead to the same near-interface structure is the presence of silicon oxycarbides and/or carbon clusters in this region, formed due to reaction of carbonaceous gaseous species produced during SiC oxidation with SiO_2. Currently, different annealing conditions are being investigated, aiming at further reduction of the roughness and gradual composition of the SiO_2/SiC interface.

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