Nuclear Reaction Profiling unraveling the incorporation of water in SiO_2/SiC structures

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Silicon carbide (SiC) is a wide-band-gap semiconductor suitable for applications under extreme conditions. SiC-based metal-oxide-semiconductor field-effect transistors (MOSFETs) are expected to be a key component for next generation green electronics. However, to exploit its potential, reliable devices must be achieved. The presence of water-related species might be a source for instabilities during devices operation, as it was already reported for silicon-based devices. However, this is still a neglected factor for the technology based on SiC.

In this work, we report the use of ion beam analyses as an effective method to unravel the incorporation process of water vapor in silicon dioxide (SiO_2) films on SiC or Si substrates. To increase sensitivity and selectivity for quantification and profiling of hydrogen and oxygen, water isotopically enriched (termed heavy water) simultaneously in deuterium (^2H or D) and in ^{18}O was used, assuming that they mimic ^1H and ^{16}O, respectively, which are the most abundant of these nuclides in nature. The use of the rare isotopes ^{18}O and D (natural abundances of 0.205 and 0.015%, respectively) allows one to distinguish them from O and H incorporated during air exposure and/or from nuclides present in the isotopically natural SiO_2 film. SiO_2 films were deposited by RF sputtering on SiC or on Si wafers and/or thermally grown at 1100ºC in 100 mbar of dry natural O_2. Samples were afterwards submitted to annealings in 10 mbar of heavy water vapor for 1 h at temperatures ranging from 20 to 1000ºC. The water vapor pressure used in these annealings corresponds approximately to the water partial pressure in air with 30% relative humidity at 25ºC, typical of a clean room.

The incorporation of water in SiO_2 films was investigated using Narrow Nuclear Reaction Profiling (NNRP), Nuclear Reaction Analysis (NRA), and Rutherford Backscattering Spectrometry (RBS). ^{18}O profile and quantification were determined by using the narrow resonance ($\Gamma \sim 100$ eV) and the plateau in the cross section curve of the $^{18}O(p,\alpha)^{15}N$ nuclear reaction at 151 keV and at 730 keV, respectively. D quantification was accomplished by NRA, using and the $D(^3He,p)^4He$ nuclear reaction at 700 keV. The

areal density of ^{16}O was determined by RBS in channeling geometry (c-RBS). The profiling of D was obtained by combining step-by-step dissolution of the oxide film in a diluted HF aqueous solution with D and (^{18}O+^{16}O) quantifications by NRA and c-RBS.
In a first moment, SiO_2 films with thicknesses in the 6 to 50 nm range were thermally grown in dry natural O_2 on SiC or on Si wafers. ^{18}O profiling reveals that in all $D_2{}^{18}O$ annealing temperatures, ^{18}O is incorporated in the oxide films until reaching the SiO_2/SiC interface. In contrast, the incorporation in SiO_2/Si structures occurs only in the near surface region for water exposure temperatures between 20 and 600ºC. Annealing at 1000ºC allowed ^{18}O to reach the SiO_2/Si interface forming $Si^{18}O_2$ due to the reaction between oxidant species and the Si substrate [1]. Concerning D incorporation, results shown in Fig.1 evidence its presence in the surface, bulk, and interface regions of SiO_2/SiC structures, whereas in the case of SiO_2/Si, it is observed only in near-surface regions of the oxide film [2]. Besides, higher incorporation of D was observed in SiO_2/SiC structures as compared to those of SiO_2/Si at temperatures above 600ºC, which can lead to electrical instabilities in the formers, especially in devices that operate at high-temperatures.

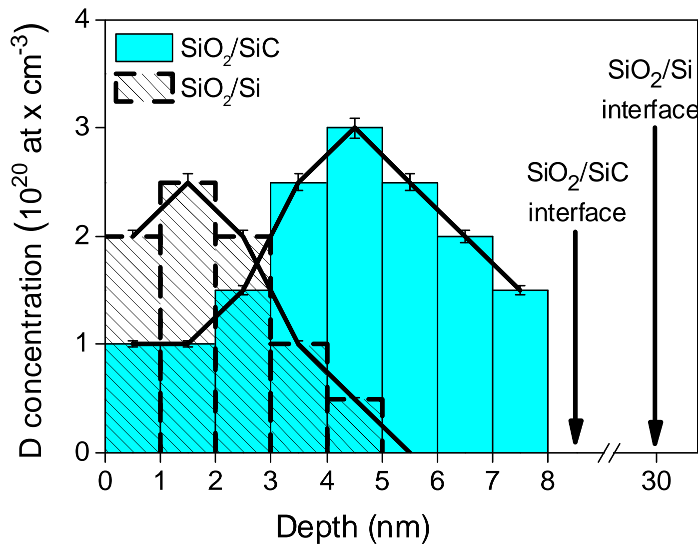

Figure 1: Deuterium profiles in natural SiO_2 films, initially 6 nm thick, thermally grown on SiC (cyan columns) and Si (dashed columns) after thermal treatment in $D_2{}^{18}O$ at 1000ºC. The positions of new film/substrate interfaces are indicated in both cases. Lines are only to guide the eyes.

The route employed to obtain SiO_2 films on SiC was observed to affect the electrical characteristics of the SiO_2/SiC interface, which is key for MOS devices [3]. Thus SiO_2 films were either deposited by RF sputtering or thermally grown on SiC wafers. The longer the thermal oxidation, the more degraded were the electrical properties of the SiO_2/SiC interfacial region. Additional samples were synthesized using short oxidation

times and then covered by a deposited SiO_2 film. In a following step, all samples were submitted to annealing in heavy water. Isotopic exchange between oxygen from the water vapor and oxygen from SiO_2 films deposited on SiC was observed in the whole depth of the films, differently from the behavior of SiO_2 films thermally grown on SiC, where it occurs mainly in the surface region of the film [4].

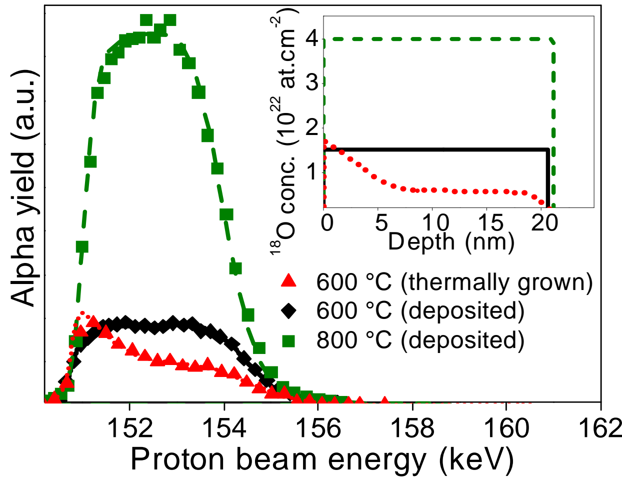

Figure 2: Experimental (symbols) excitation curves of the $^{18}O(p,\alpha)^{15}N$ nuclear reaction around the resonance at 151 keV and the corresponding simulations (lines) for a SiO_2 film 20 nm thick thermally grown on SiC submitted to $D_2{}^{18}O$ annealing at 600ºC and for SiO_2 films ~23 nm thick deposited by sputtering and submitted to $D_2{}^{18}O$ annealings at 600 or at 800ºC . **Inset:** ^{18}O profiles obtained in the simulations using the same line types. 4×10^{22} $^{18}O/cm^3$ corresponds to the oxygen concentration in stoichiometric SiO_2.

The incorporation of hydrogen from water vapor in SiO_2/SiC and SiO_2/Si structures, whose films were deposited by sputtering, occurred mainly in the SiO_2 film/substrate interfacial region. Longer thermal oxidations of the SiC prior to the deposition of the SiO_2 film led to larger amounts of D incorporated. The thermal growth of a very thin SiO_2 film followed by the deposition of SiO_2 led to the lowest amounts of D incorporated. These results were accompanied by the improvement in the electrical characteristics observed for SiO_2/SiC structures obtained by these routes, suggesting that the D incorporation occurs in defects in the structure that exist prior to the water vapor annealing. As a consequence of the annealing, a significant reduction in the negative effective charge in MOS capacitors and the removal of the SiO_2/SiC interfacial region was observed, which were assigned to the reduction of the amount of silicon oxycarbide (SiO_xC_y) compounds in the interfacial region.

As a general conclusion, our results indicate that strict control of water vapor contents in SiO_2/SiC is mandatory in order to achieve further improvements in the SiC-based device

technology.

References

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