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Structural defects in SiO_2/SiC interface probed by a slow positron beam

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Abstract

We studied structure of SiO_2/SiC interfaces grown by thermal oxidization using low energy positron beams. From the positron lifetime measurements, typical two lifetime components related to amorphous network and large open spaces are observed in SiO_2, while only bulk lifetime in SiC. The lifetime of positrons near the interface is similar to that of SiO_2 amorphous network and no lifetime components related to large open spaces are detected. From the Doppler broadening measurements, the momentum distribution, probably related to oxygen valence electrons, is enhanced near the interface. The above results imply that the interface region has less open spaces than SiO_2 involving many oxygen dangling bonds.
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1. Introduction

Silicon carbide (SiC) is a wideband gap semiconductor which is expected as high power device applications. Above all, 4H–SiC has an advantage to high power devices due to its wide bandgap (3.2 eV) [1]. One of the most attractive features of SiC is that the oxide layers needed for metal-oxide-semiconductor (MOS) devices can be grown by conventional thermal oxidation. However, it is reported that many interfacial defects remain near the SiO_2/SiC interface and these degrade performance of the MOS-based field effect transistor (MOSFET). Ordinarily produced SiO_2/SiC interface still remains in the range of 10^{11} to $10^{12}\ cm^{-2}$, which is about two orders of magnitude higher than those for SiO_2/Si interfaces [2–4]. The reduction of these centers is an important issue to realize of the high performance MOS device. In recent

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years, although the pyrogenic oxidation improve the electrical properties of interface as compared to dry oxidation [5], the detailed mechanism is not clarified. The structure of SiO_2/SiC interfaces should be revealed.

Positron annihilation spectroscopy (PAS) is a powerful tool to detect open volume defects in solids [6,7]. Using slow positron beam, the depth distribution of defects near subsurface region of several microns can be obtained. The PAS technique can be also used to characterize defects near SiO_2/SiC interfaces. Indeed, previous positron annihilation studies suggest the existence of open volume type defects at SiO_2/Si interfaces and their passivation with some specific treatments [8–10]. In this study, we investigate the characteristics of the SiO_2/SiC interface in SiC–MOS grown pyrogenic and dry oxidation methods using PAS.

2. Experimental

The samples used in this study (10 mm × 10 mm) were cut from CVD-grown n-type 4H–SiC epilayers on 8°-off oriented 4H–SiC(0 0 0 1) substrates purchased from CREE Research Inc. These were subjected to the pyrogenic oxidation at 1100 °C for 2 h or to the dry oxidation at 1200 °C for 3 h. The oxide thickness was approximately 40 nm. Slow positrons generated by a ^{22}Na source with the energies of 0.2–20 keV are injected into specimens. Implanted positrons annihilate with electrons to emit two gamma quanta (511 keV) per one positron–electron pair. The energy spectrum is Doppler broadened depending on electron momenta. The Doppler spectrum was measured by a high energy-resolution Ge detector. *S* and *W* parameters defined as the normalized peak and tail intensity of Doppler spectrum is determined [8]. In this study, the peak region for *S* parameter is $p = (0\text{–}2) \times 10^{-3} m_0c$ and the tail region for *W* parameter is $p = (10\text{–}15) \times 10^{-3} m_0c$. To obtain the chemical surroundings of positron annihilation sites, the Doppler spectrum with enhanced signal-to-noise ratio are measured using the coincidence Doppler broadening (CDB) technique [11]. In this study, p-type SiC was used as a reference because of negligible positron trapping centers inside it. Moreover, positron lifetime measurements were also carried out using the AIST pulsed positron beam. After subtraction of the background components, the lifetime spectra were analyzed using the PATFIT program.

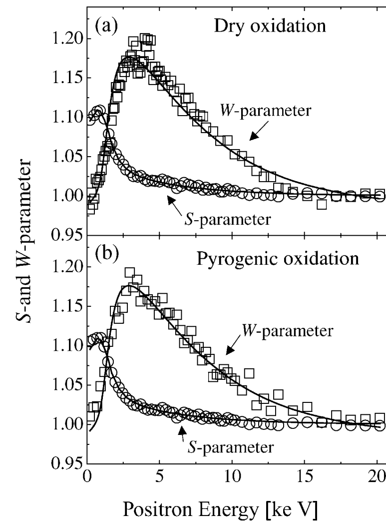

Fig. 1. *S* and *W* parameters as a function of incident positron energy for SiO_2/SiC structures fabricated by dry oxidation (a) and pyrogenic oxidation (b). Open circles denote *S* parameters and open rectangular are *W* parameters. These parameters are normalized to the bulk values. Lines are fitting result obtained from VEPFIT code.

3. Results and discussion

Fig. 1 shows *S* and *W* parameters as a function of incident positron energy obtained after dry and pyrogenic oxidation process. In order that *S* and *W* parameter is influenced by the annihilation ratio with valence and core electrons respectively, change of these parameters is usually contrary to each other. *S* and *W* parameters remain constant at $E > 15$ keV. This reflects the annihilation of positrons in the SiC epitaxial layers. At $E < 1$ keV, most positrons stop in the SiO_2 layers. The enhanced *S* parameter is caused by the small energy distribution of positronium formed in the SiO_2 amorphous network. The small *W* parameter in this region is also reflecting positronium annihilation. A little reduction of *S* parameter at $E = 0.2$ keV indicates the positron annihilation at the surface. The energy range corresponding to the SiO_2/SiC interface is $E = 3$–6 keV. Here, no significant change of *S* parameter is found. On the contrary, *W* parameter dramatically

changes in the same energy range. This is a remarkable phenomenon. Under an assumption that positrons annihilate in the ideal interface of SiC and SiO_2, S parameter is expressed with the linear combination of S parameters of each layer by giving weight with an annihilation ratio x, like $S = xS_{SiO_2} + (1 - x)S_{SiC}$. However, in this region, change of S and W parameter cannot be expressed with the same change of x because W parameter changes with an extremum although S parameter changes in monotone. This suggests that the existence of a transition region that is not a simple mixture of SiO_2 and SiC but another chemical state with different electron momentum distribution is detected. For the above two types of SiO_2/SiC samples, both S–E and W–E plots are nearly the same.

To determine the electron momentum distribution more in detail, CDB measurements were performed. Ratio curves to the SiC bulk are shown in Fig. 2. The intensity for SiO_2 region is enhanced at $p < 3 \times 10^{-3} m_0c$. This corresponds to the high S parameter in Fig. 1 because of the positronium formation. A large bump also appears at $p = (10\text{–}20) \times 10^{-3} m_0c$. In the case of SiO_2/SiC transition region, the intensity at $p < 3 \times 10^{-3} m_0c$ is rather reduced, while that at $p = 10\sim20 \times 10^{-3} m_0c$ is fairly pronounced. This enhancement is not simply explained as a relative increase due to the balance for the decrease at $p < 3 \times 10^{-3} m_0c$. Indeed, Fig. 1 shows no significant decrease in S parameter where W parameter increases ($E \sim 3$ keV). The bump at $p = (10\text{–}20) \times 10^{-3} m_0c$ may be explained as (i) the missing of the neck for the second Brillouin zone which clearly appears in the case of crystalline structure, i.e., in SiC region, or (ii) the chemical environment of positron annihilation sites is different from that in SiC matrix. However, since the neck of the second Brillouin zone of SiC is located at $p = (8\text{–}15) \times 10^{-3}$ [12], the former possibility is not favored. It is known that positrons are attracted to oxygen atoms rather strongly [13–16]. Thus, as for the second possibility, we may consider that positrons preferentially annihilate with valence electrons of oxygen atoms.

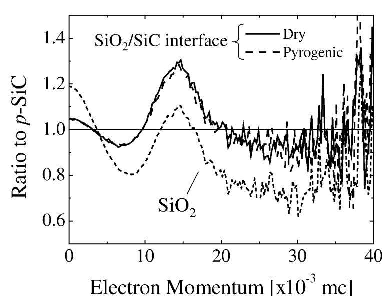

Fig. 2. Ratio curves of electron momentum distribution for the SiO_2 and interface to the SiC bulk observed by coincidence Doppler broadening measurement.

Table 1
Parameters obtained by fitting the positron lifetime spectrum of SiO_2 and interface layer

	SiO_2 ($E = 0.8$ keV)		Interface ($E = 3.7$ keV)
	τ_1 (ns)	τ_2 (ns)	τ_1 (ns)
Dry	0.408 (39.3%)	1.63 (60.7%)	0.451 (100%)
Pyrogenic	0.419 (41.0%)	1.58 (59%)	0.470 (100%)

Table 1 shows the results of positron lifetime measurements for SiO_2 layer and SiO_2/SiC interface. In the SiO_2 layer, two lifetime components were determined; one is about 400 ps attributed to free annihilation in SiO_2 amorphous network and the other 1.6 ns to pick-off annihilation of ortho-positronium. This means that in the SiO_2 layer there are large voids to allow the positronium formation. In the interface region, only a single positron lifetime component of about 450 ps is resolved. This result shows that the structure of interface layer is rather porous but the positronium formation is forbidden. Probably, this is explained as the reduced concentration of large voids at the interface. Alternatively, though the interface is resembles with SiO_2, a large amount of defects exists to reduce the positronium formation as competitive trapping centers.

From the above results, the structure of the interface transition region is not simple admixture between SiO_2 and SiC. By the way, there are almost no differences of PAS result between specimens obtained by dry and pyrogenic oxidation. However, from the C–V measurements the net number of interface traps per unit area (N_{it}) obtained for SiO_2/SiC structure by the dry oxidation is one order of magnitude higher than that made by the pyrogenic oxidation [17]. This is considered that electrically active centers may be terminated by steam (moisture existing oxidation ambient). On the contrary, the oxygen related defects

are observed in PAS measurements. Those may be attributed to the imperfect oxides generated during oxidation process because interface structure is not simple transition layer from SiO_2 to SiC. This shows that the moisture existing oxidation ambient works the reduction of the interface state density, but have little effect on the formation of the imperfects oxides. Such defects are formed due to the lack of oxygen in oxidization. It is suggested that a reoxidation process is valid for the improvement of the interface properties. For the clarification of interface properties more in detail, it is necessary to measure SiO_2/SiC interfaces fabricated with the technique of reducing interface state density, such as post-oxidation annealing.

4. Summary

We studied structural defects at SiO_2/SiC interface grown by dry and pyrogenic oxidization using slow positron beams. From the Doppler broadening measurement, W parameter dramatically increases in the energy range corresponding to the SiO_2/SiC interface. The CDB measurements show that the chemical environment of positron annihilation sites in transition layer is different from that in SiC matrix, and show that positrons annihilate with valence electrons of oxygen atoms due to its strong affinity for positrons. From the positron lifetime measurements, the structure of interface layer is porous without large voids to allow the positronium formation. As a result, oxygen related defects exist in the interface transition layer. Those defects are probably concerned with the imperfect oxides because of its SiO_2-like porous structure. There are almost no differences of PAS result between specimens obtained by dry and pyrogenic oxidation. This shows that no significant contributions of the moisture in oxidization ambient to the formation of such defects.

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