Distribution and Chemical bonding of N at NO Nitrided SiC/SiO₂ Interface

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Abstract—This paper presents results of the physical characterization of NO nitrided SiC/SiO₂ interfaces by XPS analysis. The results show different interface chemistries between NO nitrided and Ar annealed SiC/SiO₂ interfaces. After NO nitridation, N builds up at the SiC/SiO₂ interface forming Si₃N bonds. The NO nitrided SiC/SiO₂ interface is free of the complex interface oxide/carbon compounds which are suggested to be the reason for the inferiority of the SiC/SiO₂ interface compared to the Si/SiO₂ interface

I. INTRODUCTION

Silicon carbide (SiC) is an attractive semiconductor material because of its wide bandgap, high thermal conductivity, high breakdown electrical field, and high electron mobility[1]. The unique property of SiC wide bandgap semiconductors is their ability to be thermally oxidized in a similar way to Si to grow a layer of SiO₂ on SiC. This implies the possibility of creating MOSFETs on SiC. Although it has been reported by many investigators that there are a lot of similarities between the SiC/SiO₂ and Si/SiO₂ interfaces [2,3], it has also been revealed that significant differences exist between these two structures[4]. The main difference[4] is the existence of complex interfacial oxide/carbon compounds which is believed to be the main cause of defects at the SiC/SiO₂ interface. This is in contrast to the Si/SiO₂ interface where the main defects are due to interfacial Si dangling bonds. Interfacial dangling bonds can be passivated by hydrogen, which is accomplished by either annealing the Si/SiO₂ structure in

hydrogen or by post metal annealing (PMA) in forming gas. It has been shown, however, that either annealing in hydrogen or PMA at high temperature have little effect on the SiC/SiO₂ interface.

We have previously shown[5~7] that NO nitridation can reduce SiC/SiO₂ interface trap densities significantly in both n-type SiC and p-type SiC. We have also shown[8] that NO nitridation improves the reliability of the SiC/SiO₂ interface. In this paper we present the physical analysis of NO nitrided SiC/SiO₂ interface by XPS.

II. EXPERIMENTAL DETAILS

The Si-faced 4H-SiC wafers, purchased from CREE Research, were used in this experiment. The wafers were first cleaned in a mixture of H₂SO₄/H₂O₂ followed by a standard RCA clean. Immediately prior to oxidation, the wafer was dipped in 1%HF for 1 minute and then oxidized in ultrahigh purity O₂ at 1150°C for 3 hours. After oxidation, the samples were annealed in NO (99%) at 1130°C for 1.5 hours. As a comparison, the samples were also annealed in Ar at the exactly the same conditions.

XPS analysis was performed using a Perkin Elmer PHI 560 multitechnique surface analysis system. An Ar beam was used to remove the SiO₂ layer gradually. The XPS spectra were recorded by performing multiple scans in each energy concerned with a 25eV pass energy.

III. RESULTS AND DISCUSSIONS

Fig.1 shows the depth profiles of the atomic concentration of Si, O, C, and N of an NO nitrided sample of SiO₂/SiC measured by XPS. It can be seen that there is a nitrogen peak at the

SiC/SiO₂ interface. The nitrogen peak value is about 1.6 at.% situated at the interface. This is similar to the case of NO nitrided Si/SiO₂ structures [9]. However, NO nitridation in

Fig.1 Depth profiles for an NO nitrided SiC MOS capacitor

SiC appears to be much more complicated than in Si because it takes much longer to perform NO nitridation on SiC than on Si. It can also be seen that nitrogen has a uniform distribution of around 0.7 at.% throughout the oxide dielectric.

Fig.2 Deconvolution of N 1s spectrum at the interface of the NO nitrided SiC MOS capacitor

The nitrogen N 1s core level spectrum of NO nitrided SiC/SiO₂ structure at the interface is a symmetrical line and only consists of a single peak, as shown in Fig.2. The peak has a binding energy of 397.8eV with the full width at half maximum (FWHM) of 2.16eV. The binding energy of 397.8eV is very close to the binding energy for N 1s in silicon nitride which is 397.7eV, indicating the formation of Si≡N bonds at the interface of SiC/SiO₂. This is the

Fig.3 Deconvolution of Si 2p spectrum at the interface of NO nitrided SiC MOS capacitor

Fig.4 Deconvolution of Si 2p spectrum at the interface of Ar annealed SiC MOS capacitor

same as NO nitrided Si/SiO₂ interface where it has been demonstrated that NO oxynitride exhibits Si≡N bonds at the Si/SiO₂ interface[10].

Fig.3 shows the deconvolution of the Si 2p core level spectrum of NO nitrided SiC/SiO₂ structure at the interface. As a comparison, the spectrum of Si 2p core level of the Ar annealed SiC/SiO₂ structure at the interface is shown in Fig.4. It is evident that the Si 2p spectrum of the Ar annealed sample is much wider than that of the NO nitrided sample. The Si 2p spectrum of the NO nitrided sample can be fitted with two Gaussian peaks labelled as Si-1 (100.1eV, FWHM=2.16eV) and Si-3 (101.9eV, FWHM=2.16eV) while there are three fitted gaussian peaks in the Si 2p spectrum of Ar annealed sample labelled as Si-1, Si-2 (101.4eV, FWHM=2.16eV), and Si-4 (103.5eV, FWHM=2.16eV). Both Si 2p spectra of the NO nitrided and Ar annealed sample have Si-1 species which describe SiC from the substrate. Si-4 represents SiO₂ formed during oxidation. Onneby *et al*[11] investigated the SiO₂/SiC system and claimed the formation of silicon oxycarbide at the interface. They identified the silicon oxycarbide as SiO₃C (binding energy 102.1-102.2eV) and SiO₂C₂ (binding energy 101.2-101.6eV). Hornetz *et al*[12] studied the SiO₂/SiC interface with angle resolved XPS (ARXPS) and revealed the interface oxide Si₄C_{4-x}O₂ (x≤2) with binding energy of 101.25eV. Therefore, we regard Si-2 as the complex interface oxide/carbon compound. The Si-3 peak in the NO nitrided sample, however, indicating the formation of silicon oxynitride with oxygen partly replaced by nitrogen in Si-O₄ structure of SiO₂ (binding energy 103.3eV) by considering the pile-up of N at the SiC/SiO₂ interface. The shift of binding energy to lower energy is caused by the replacement of some oxygen with N because N has smaller electronegativity than O.

IV. Conclusions

The physical characteristics of NO nitrided SiC/SiO₂ MOS capacitors have been examined by XPS analysis. A nitrogen peak has been observed at the NO nitrided SiC/SiO₂ interface similar to the nitrided Si/SiO₂ interface. The Si≡N bonds have been demonstrated at the

SiC/SiO₂ interface. The XPS spectra show that the NO nitrided SiC/SiO₂ MOS capacitors are free of the complex interface oxide/carbon compounds, as opposite to the Ar annealed SiC/SiO₂ MOS capacitors.

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