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Profiling of the SiO_2 - SiC Interface Using X-ray Photoelectron Spectroscopy

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ABSTRACT

The implementation of SiC based sensors and electronics for operation in chemically harsh, high temperature environments depends on understanding the SiO_2/SiC interface in field effect devices. We have developed a technique to fabricate wedge polished samples (angle ~ $1x10^{-4}$ rad) that provides access to the SiO_2/SiC interface via a surface sensitive probe such as x-ray photoelectron spectroscopy (XPS). Lateral scanning along the wedge is equivalent to depth profiling. Spatially resolved XPS images of the O 1s and Si 2p core levels were obtained of the interfacial region. Samples consist of device-quality thermally grown oxides on 4H-SiC single crystal substrates. The C 1s spectrum suggests the presence of a graphitic layer on the nominally bare SiC surface following thermal oxidation.

INTRODUCTION

Recent advances in silicon carbide device technology have enabled the implementation of SiC based sensors and electronics for operation in chemically harsh, high temperature environments that are beyond the reach of Si based technology. Despite their initial promise, the performance of SiC field effect devices is limited by the low mobility, compared to the bulk, of electrons in a two dimensional electron gas at the SiO_2/SiC interface. There are a number of mechanisms responsible for short range non-uniformities in the electrostatic potential at the SiO_2/SiC interface that contribute to additional scattering of the confined electrons. These may include:

a) interface roughness, i. e., spatial inhomogeneities of the SiO_2/SiC interface
b) random distribution of excess charge in the oxide or close to the interface
c) structural disorder of the SiC lattice at the interface, which may create a transitional layer in both the oxide and the silicon carbide.

Both theoretical and experimental studies of the of the oxidation of SiC [1, 2] suggest the presence of carbon dangling bonds at the interface and/or small carbon precipitates remaining in the SiC following oxidation.

Our interest is the chemical disorder of the SiO_2/SiC system and how it results in electron scattering by fluctuations in the electrostatic potential at the interface between the two materials. A number of different experimental techniques have been utilized to study this problem. Atomic resolution Z-contrast microscopy, combined with spatially resolved electron energy loss spectroscopy, have revealed a 1.5-6 nm thick layer with a monotonically decaying C concentration at the interface [3, 4]. X-ray photoelectron spectroscopy (XPS) together with sputter depth profiling has indicated a transitional layer containing Si-Si bonds [5]. Our approach is to utilize spatially resolved XPS of the SiO_2/SiC interface, which has been exposed and magnified a thousand-fold via wedge polishing (see Fig. 1). XPS is a surface sensitive tool that enables both the detection of a particular chemical species and its local electronic environment. We therefore probe the local chemical environment at the interface to investigate: a) the differences in the Si bonding environment in the carbide versus that of the oxide, b) the presence of C in the oxide and c) the presence of a SiCO "amalgam" at the interface.

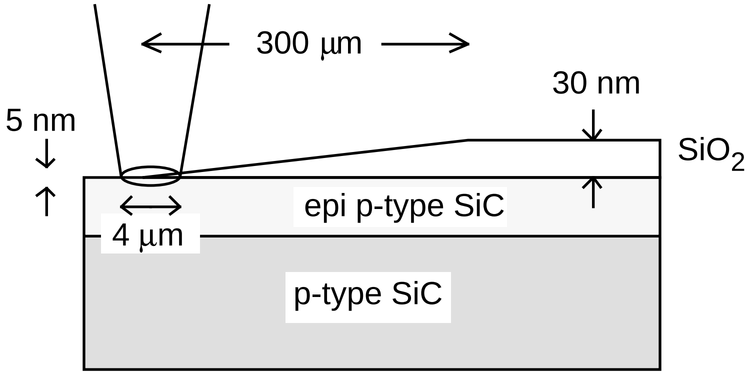


Figure 1. *Idealized cross sectional view of the SiO_2/SiC wedge polished sample.*

EXPERIMENTAL DETAILS

An Axis Ultra scanning XPS system was used to obtain both photoelectron spectra of the sample and spatially resolved photoelectron images of the wedge polished region. The measurements were performed using monochromatised Al x-rays (hν = 1428 eV). The photoelectrons passing through the magnetic immersion lens were collected with a spherical mirror analyzer resulting in an overall instrument resolution of 0.5 eV. An example of the spectra obtained from the oxide is shown in Fig. 2, where the O 1s, Si 2s and Si 2p peaks are

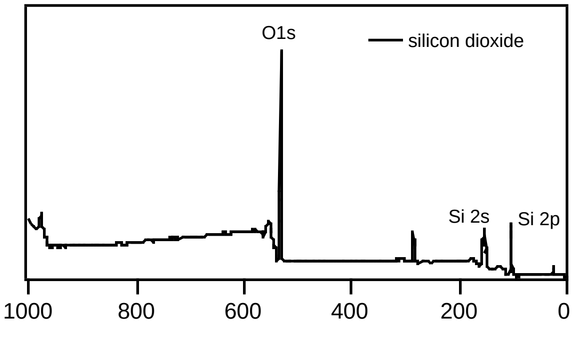


Figure 2. *X-ray photoelectron spectrum of the oxide away from the SiO_2/SiC interface.*

clearly resolved. The binding energies have been referenced to the Ag 4d peak. From the observed chemical shifts we can determine the ionic state of a particular species. Although the incident x-rays penetrate deep into the sample, only electrons emitted from a thin surface layer are detected. The electron escape depth for Si, C and O ranges from 2.0 to 2.5 nm [6]. We will exploit the surface sensitivity of XPS on a wedge polished sample to obtain chemical state data as a function of position away from the SiO_2/SiC interface.

Fig. 1 shows an idealized cross sectional view of the wedge geometry of our samples. The starting material is a gate quality oxide grown on a p-type SiC epitaxial layer on top of a p-type 4H-SiC 8° degree miscut single crystal substrate. The electrically measured interface state densities near mid gap and fixed oxide charge densities are $1x10^{11}/eV/cm^2$ and $1x10^{12}/cm^2$, respectively [7]. A very shallow angle (~ $1x10^{-4}$ rad) was mechanically polished on the top surface using a cerium oxide aqueous slurry. A lateral translation of 1 μm corresponds to 0.1 nm in the vertical direction. The spatial resolution of the electron detection system was determined to be 4 μm by measuring the 20 to 80 % edge profile of patterned Au lines. Since we are using a monochromatised Al x-ray source, the electron escape depth limits our resolution in the vertical direction. We estimate our spatial resolution in this dimension to be ~5 nm. Therefore, obtaining a series of spectra along the wedge is equivalent to depth profiling.

DISCUSSION

A scanning electron micrograph of the wedge polished sample is shown in Fig. 3. In this image the oxide is bright, the carbide is dark and the oxide/carbide interface runs horizontally. The XPS images were taken over a $(800\ \mu m)^2$ region, as indicated by the square box. The 300 μm wide sloped region of the wedge is indicated by the dotted lines.

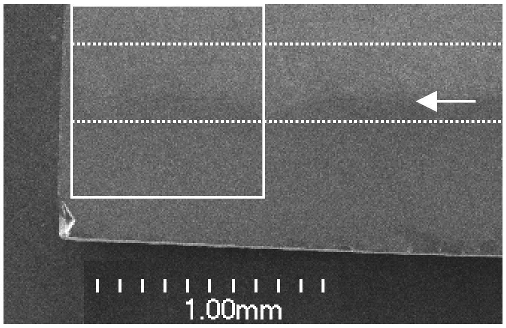
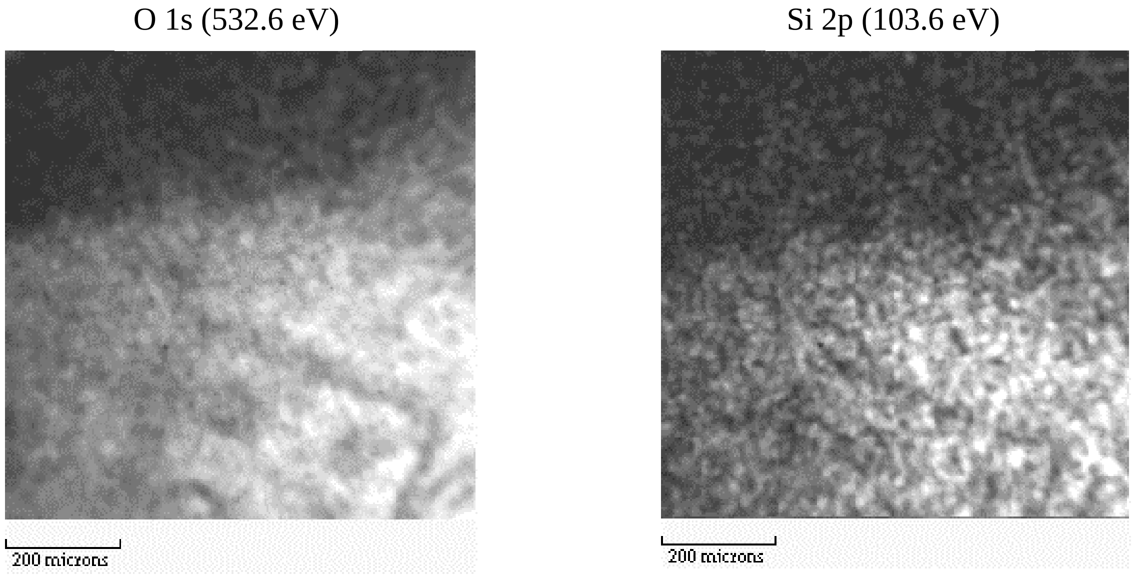


Figure 3. *Scanning electron micrograph of the wedge polished SiO_2/SiC sample. The bright region corresponds to the oxide and the dark region corresponds to the carbide, the interface is indicated by the arrow.*

Fig. 4 shows the XPS images of the SiO_2/SiC interface as obtained using (a) the O 1s peak and (b) the Si 2p peak. Before discussing the images in detail we consider the Si 2p spectra shown in Fig. 5. The line labeled "SiC" is the Si 2p spectrum of the SiC, in a region far from the interface, after removal of the gate oxide. The line labeled "SiO_2" is the Si 2p spectrum from the full oxide, again far from the interface. We observe two distinct peaks from these regions with the oxide Si 2p peak shifted by 3.4 eV to higher energy from the carbide Si 2p peak. This peak shift is due to the difference in oxidation state of the Si atoms. Since SiC is a covalently bonded semiconductor, Si is expected to be in the charge neutral oxidation state, whereas in the oxide the Si is in the 4+ valence state. A higher oxidation state corresponds to less screening by the valence electrons, resulting in a higher core level binding energy. A similar shift in binding energy was observed earlier [5]. In Fig. 4, the Si 2p XPS image was obtained using the higher energy oxide peak. As expected there is a one to one correspondence between the O 1s image and the Si 2p image of the SiO_2/SiC interface. Note that the square structures observed in the oxide are depressions that have been transferred to the oxide during the chemical etching performed to remove the top polysilicon gate.


O 1s (532.6 eV)

Si 2p (103.6 eV)

Figure 4. *Spatially resolved XPS images of the SiO_2/SiC interface. The bright regions correspond to the oxide and the dark regions correspond to the carbide. The interface runs from left to right across the images.*

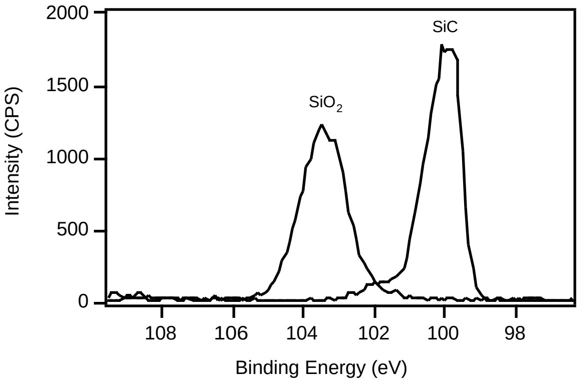


Figure 5. *Si 2p XPS spectra of the carbide and oxide regions away from the interface.*

Additional information on the interface was obtained from the C 1s photoelectron spectrum of the nominally bare SiC, far from the interface as shown in Fig. 6. The narrow high energy peak is the expected C 1s signal from bulk SiC [8]. At about 3 eV above the C 1s peak is a broad additional feature. Others have noted the appearance of a similar feature from single crystal SiC wafers that have been subjected to high temperature anneals above 1100K and attribute the feature to graphite formation on top of the SiC [8]. We therefore suggest that the high energy feature observed in the C 1s spectrum is due to the formation of a SiCO “amalgam” following oxidation of the SiC surface.

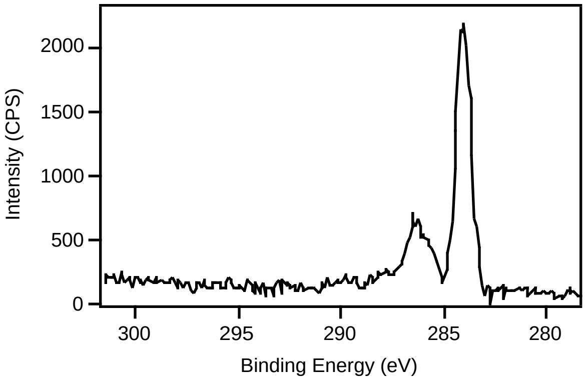


Figure 6. *C 1s XPS spectrum of the bare SiC following thermal oxidation.*

CONCLUSIONS

We have developed a technique to fabricate wedge polished samples (angle ~ $1x10^{-4}$ rad) that provides access to the SiO_2/SiC interface via a surface sensitive probe such as x-ray photoelectron spectroscopy. Lateral scanning along the wedge is therefore equivalent to depth profiling. Spatially resolved XPS images of the O 1s and Si 2p core levels were obtained of the interfacial region. The observed shift in the Si 2p peak between the oxide and the carbide is consistent with the expected change in oxidation state. Experiments are in progress to obtain spatially resolved C spectra of the interface to investigate both the possible presence of C in the oxide and the formation of graphite on the SiC surface following thermal oxidation.

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