The oxidation of silicon carbide and structure-defects-mobility relations

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Background

Oxidation of materials is a ubiquitous process, but the effects of oxidation on the substrate have not been investigated thoroughly on the atomic scale. Oxidation of silicon is an essential step in microelectronics. For high-power applications, however, Si-based microelectronics requires continuous cooling. Microelectronics based on semiconductors with a wider energy gap would significantly improve efficiency of energy utilization and management. For high-temperature applications, a wide-gap semiconductor is an absolute necessity. One of the most promising wide-gap semiconductors is SiC, in large part because its native oxide is also SiO2. The properties of SiC/SiO2 interfaces, however, remain the key limiting factor that has held back the commercial development of SiC-based electronics. A measure of merit is the electron mobility in SiC metal-oxide-semiconductor structures, which is endemically poor. Research that leads to better understanding of the oxidation process and its detrimental effect on the substrate would impact the development of better high-power, high-temperature electronics for energy-related applications.
Proposed Research

We propose a systematic study of the oxidation process of SiC to elucidate the structure-mobility relationship in the SiC layers adjacent to the SiC-SiO2 interface and to expand knowledge on the nature of interfacial defects in this system. A key feature of the proposed research is that we will simultaneously pursue extensive physical and electrical characterization of SiC-SiO2 structures (MOS capacitors and MOSFETs) and combine the experimental data with pertinent first-principles calculations. The objective will be a thorough understanding of structure-defects-mobility relations and optimization of mobilities for electronic device applications. The concomitant broader understanding of the oxidation process will impact other applications entailing oxidation.
Experimental Results
An atomic resolution Z-contrast image of the SiC / SiO2 interface. The SiC is Al implanted by Cree to produce a large transition layer which is visible as a dark region near the interface.
A Z-contrast image of a 4 degree miscut SiC /SiO2 interface of a non-processed (blanket) wafer from Cree. No substantial transition layer is detectable in the image.
Result of a spectrum image data set, with the new correction scheme. Top left shows the Z-contrast image of the interface, where the investigated area is indicated by the green rectangle. Top right shows the Z-contrast image that is acquired. The % atom concentrations found are an improvement of a factor ~100 compared to the previous work. The line profile shows a C excess of only ~1% at the interface as well a decreasing C content in the oxide.
Interface trap densities near the conduction band edge for different growth / passivation processes for SiO2/4H-SiC including NO passivation, PSG (phosphorous glass) annealing and O2/HCl annealing.
On the left, the $D_{IT}$ (at 0.2eV~0.6eV below $E_C$) of oxides subjected to the different processes are shown. Interestingly, the sodium enhanced oxide which results in high mobility also has high $D_{IT}$ which is explained within the impurity band model discussed below. For Rb implanted devices, the MOS capacitance is observed for various annealing. Importantly, the C-V curve is stable during bias and temperature stress. The field effect mobility for Rb implanted devices is currently being performed. Measurements performed at Auburn University.
At Auburn University, MOS capacitor and MOSFET samples were passivated using a small planar diffusion source (PDS) furnace instead of a POCl₃ bubbler to produce P₂O₅ passivating ambient as shown at top. For various processing steps, the drain-source current is measured and the field effect mobility is extracted. Phosphorous enhanced mobility but degrades threshold voltage effects.
Upgraded microwave plasma system for the introduction of nitrogen without oxidation. We hope to introduce significantly more nitrogen and reduce the time for our post-oxidation plasma anneal from 20hr to around 4hr.
Here we report the formation of a stable Si-O-N structure after exposing (0001) n-type SiC to N$_2$ gas at 1 atmosphere pressure at 1600$^\circ$C. The samples are prepared by Dr. Weijie Lu at Air Force Research Lab, and they are characterized at Rutgers University. Above is the XPS spectrum of N 1s peak from the sample subjected to the high temperature N$_2$ anneal. The spectrum indicates that the same nitrogen species at the interface as the NO anneal. The estimated interfacial nitrogen content is higher compared to NO, at $\sim$1.5×10$^{15}$cm$^{-2}$. 
Theoretical Results
At Vanderbilt, the properties of C rich Si-C were investigated theoretically. Above shows an aggregation of C interstitial clusters after a 24 ps quantum molecular dynamics simulation. grey = C, orange = Si (after annealing), red = Si (ideal crystalline) atoms
The lowest unoccupied state of a \((\text{C}_i)_2\) defect in two different SiC bulk samples. The Si and C atoms are shown in yellow and blue, respectively. The defect state in 4H-SiC on the left is localized around the di-interstitial whereas the defect state on the right in 3C-SiC is de-localized. This latter fact explains why 3C-SiC MOSFETs are insensitive to defect concentration. Comparing defect level calculations to recent experiments, we show that carbon di-interstitials are a dominant electrically active defect complex in 4H-SiC MOSFETs.
On the left, we report midgap voltage shift ($\Delta V_{mg}$) for n- and p-substrate 4H-SiC MOS capacitors stressed at 150 °C with alternating positive and negative bias stress. The midgap voltage shift is a measure of charge buildup in the oxide. Interestingly, the p-substrate devices show a significant shift under negative stress without any recovery under positive stress. This phenomena is explained in the diagrams on the right. Under negative stress, holes tunnel to oxide vacancies which undergo structural changes which raise the defect level. Under positive bias, the hole in the higher defect level is unable to recombine at the interface.
At Vanderbilt, we performed a comprehensive theoretical analysis of the effects of phosphorus in the 4H-SiC/SiO$_2$ system using density functional calculations in the context of new data by our group at Auburn university. On the left above, we show the structure and the defect level of an interfacial three fold carbon defect. In the middle, the carbon defect is replaced by phosphorous. On the right, complete passivation is found for carbon defect replaced by oxygen bonded phosphorous.
Investigated the role of sodium ions in SiC-MOSFETS. Above is a ball-and-stick model of SiC/SiO2 (left) and gate oxide model (middle) along with the calculated energy barrier (right) for sodium in the oxide:

grey = Si, blue = C, red = O atoms and white = sodium
At Cree, we have measured enhanced field-effect mobilities due to Na ions in the gate oxide of SiC MOSFETs as shown above. Field-effect mobility of lateral MOSFETs as-processed (labelled ‘initial’) and sodium ions drifted to the SiO2/SiC interface (labelled ‘Sodium IN’).

The mobilities at the top left are explained by the impurity band model we developed. At the top right, we show that near interface sodium ions cause shallow defect levels in the SiC channel. High concentration of sodium ions are represented in the bottom right interface density of states figure. The Fermi level is within the impurity band causing high mobility and the negative threshold voltage observed experimentally.
Journal Publications:

Zhu, XG; Lee, HD; Feng, TA; Ahyi, AC; Mastrogiovanni, D; Wan, A; Garfunkel, E; Williams, JR; Gustafsson, T; Feldman, LC, "Structure and stoichiometry of (0001) 4H-SiC/oxide interface", APPLIED PHYSICS LETTERS, vol. 97, (2010), p. ., "10.1063/1.348167 " Published


Shen, X; Oxley, MP; Puzyrev, Y; Tuttle, BR; Duscher, G; Pantelides, ST, "Excess carbon in silicon carbide", JOURNAL OF APPLIED PHYSICS, vol. 108, (2010), p. ., "10.1063/1.351714 " Published


Tuttle, BR; Dhar, S; Ryu, SH; Zhu, X; Williams, JR; Feldman, LC; Pantelides, ST, "High electron mobility due to sodium ions in the gate oxide of SiC-metal-oxide-semiconductor field-effect transistors", JOURNAL OF APPLIED PHYSICS, vol. 109, (2011), p. ., "10.1063/1.353376 " Published

Shen, XA; Zhang, EX; Zhang, CX; Fleetwood, DM; Schrimpf, RD; Dhar, S; Ryu, SH; Pantelides, ST, "Atomic-scale origins of bias-temperature instabilities in SiC-SiO2 structures", APPLIED PHYSICS LETTERS, vol. 98, (2011), p. ., "10.1063/1.355442 " Published

Outreach & Education
Funded students including undergraduates such as Josiah Oduor shown above in front of his poster at the undergraduate conference at UTK
Delivered Teacher Workshop including a day of lectures and activities:
(top left) Group photo including Prof. Tuttle at left-front, (top right) Marshmallow model of Si(100) surface, (bottom right) three teachers working on structural model
Delivered Teacher Workshop including a day of lectures and activities: (top left) Group photo including Prof. Tuttle in the center. The focus this year was on Energy and Materials.
One of the co-Pis, Dr. Weijie Lu has been a professor at Fisk University in Nashville, a historically black university. An African-American master’s student is funded by the grant and is getting trained in experimental research on SiC, co-supervised by Professors Lu, Feldman, and Pantelides.