The primary objective of this NSF-GOALI project was to use a combination of experimental and theoretical methods to investigate the effect of oxidation on the structural and electronic properties of the substrate and the quality of the oxide-substrate interface. Silicon carbide (SiC) was selected as a prototype material because it is a semiconductor with a large energy gap, a feature that is needed for the fabrication of electronic devices that are suitable for applications involving high power (power grid controls, all-electric ships) or high temperatures (automobile controls). Though the large energy gap, compared with the energy gap of Si, is a big advantage for high-power, high-temperature applications, other conditions need to be met. In particular, electrons in the substrate, SiC in this case, need to have a high mobility. The mobility is generally limited by scattering from defects at the interface with the oxide or by oxidation-induced defects in the substrate itself.

The main findings were as follows: (i) Theoretical and experimental work conducted under this project has conclusively determined that the interfacial region is chemically stoichiometric, and that the effects that have been attributed to a transition layer are in fact caused by interfacial roughness (**Figure 1**). (ii) Following reports of high mobility produced by incorporating sodium in SiC-SiO2 structures, we provided theoretical understanding of the phenomenon and confirmed it experimentally (**Figure 2**). Sodium, however, is highly mobile and devices are unstable and unsuitable for applications. (iii) A comprehensive theoretical study of the oxidation mechanisms of the different SiC surfaces and comparison with the corresponding oxidation mechanisms of different Si surfaces was carried out and the results explained and reconciled diverse experimental data (**Figure 3**). (iii) Following a report that using phosphosilicate glass (PSG) as the gate dielectric of MOSFETs results in higher performance, we established that, while the performance is high, the stability of the device is extremely poor as a result of polarization of the dielectric. A new approach was developed using a stacked gate oxide that consists of a thin (~100 A) PSG layer at the interface which results in better stability while maintaining the high performance. (**Figure 4**) (iv) High channel mobility has been obtained using antimony as a surface counter-dopant. This process is very promising for future SiC MOSFET technology (**Figure 5**). It can also serve as an experimental platform for independently studying the effects of trap passivation and counter-doping on 4H-SiC MOSFET channel mobility. All these results provide very valuable information that benefits the processing methodology of commercial SiC power devices by industrial partner Cree Inc. as well as others.

On the outreach and educational front, the project funded a Masters student (Sorrie Ceesay) at nearby historically black Fisk University. Mr. Ceesay gave an oral presentation based on his Master's thesis at the 2012 Spring meeting of the Materials Research Society in San Francisco, CA (Figure 6). Upon graduation, he entered Dayton University in Dayton, OH, as a Ph.D. graduate student in Materials Science and worked on this project for the first year, mentored by his former Fisk advisor Prof. Weijie Lu who had moved to the Air Force Laboratory near Dayton.

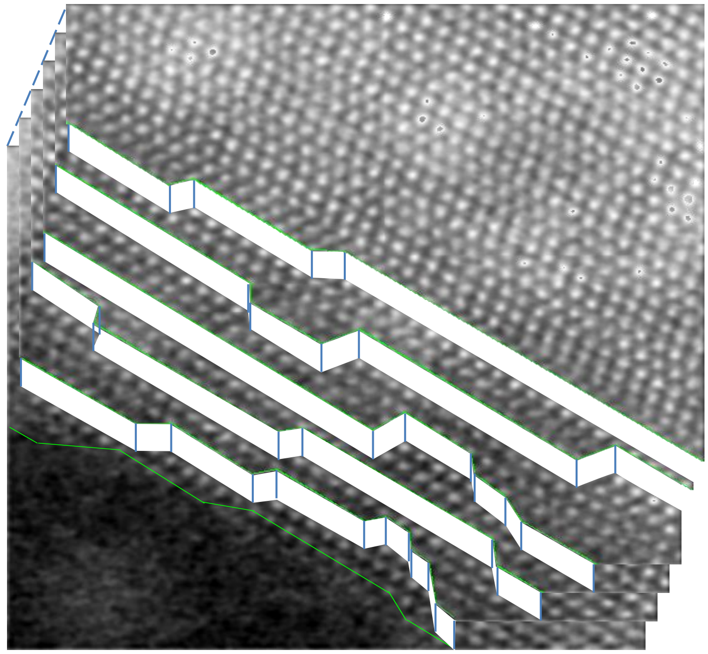

Figure 1. Extensive investigations using atomic-resolution scanning transmission electron microscopy and electron energy loss spectroscopy determined that roughness of about 1 nm (the atomic steps shown above) is intrinsic to the SiC-SiO_2 interface. This roughness cause mobility degradation and the effects that have been attributed to a transition layer in the SiC substrate. From P. Liu, G. Li, Y. K. Sharma, A. C. Ahyi, T. Isaacs-Smith, S. Dhar, J. R. Williams, and G. Duscher, "Roughness of the SiC/SiO_2 vicinal Interface and atomic structure of the transition layers", *Journal of Vacuum Science and Technology*, in press (2014).

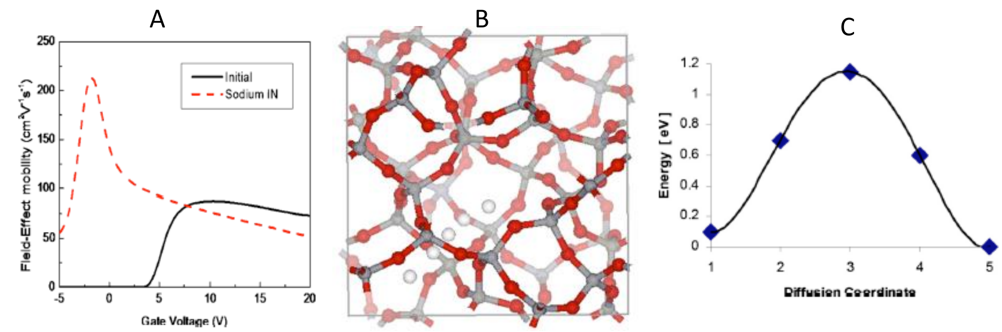

Figure 2. A) Electron mobility of a SiC-SiO_2 structure prior to and after sodium incorporation. B) Schematic diagram of a SiO_2 structure (Si atoms are grey, oxygen atoms are red) with sodium ions (white balls) diffusing through the rings. C) Calculated activation energy for the sodium ion diffusion. From B. R. Tuttle, S. Dhar, S.-H. Ryu, X. Zhu, J. R. Williams, L. C. Feldman and S. T. Pantelides, “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, article # 023702 (2011).

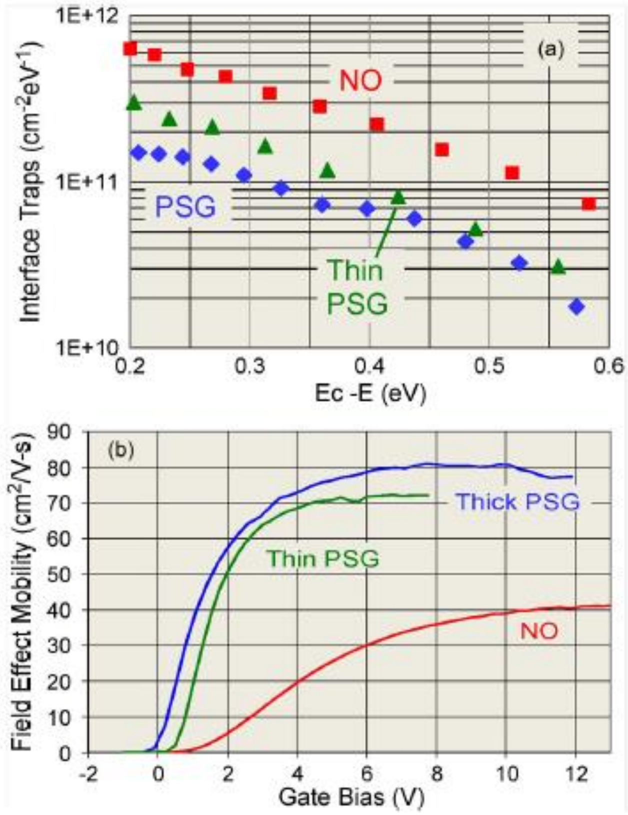

Figure 3. (a) Interface trap densities of SiC-SiO_2 capacitors with only the standard NO treatment and with additional treatment with P_2O_5, which converts the SiO_2 into phsphosilicate glass (PSG). (b) The corresponding electron mobilities. From Y. K. Sharma, A.C. Ahyi, T. Isaacs-Smith, A. Modic, M. Park, Y. Xu, E.L. Garfunkel, L.C. Feldman, S. Dhar, and J.R. Williams, "High Mobility Stable 4H-SiC MOSFETs Using Phosphorus Passivation", *IEEE Electron Device Letters*, vol. 34, p. 175 (2013)

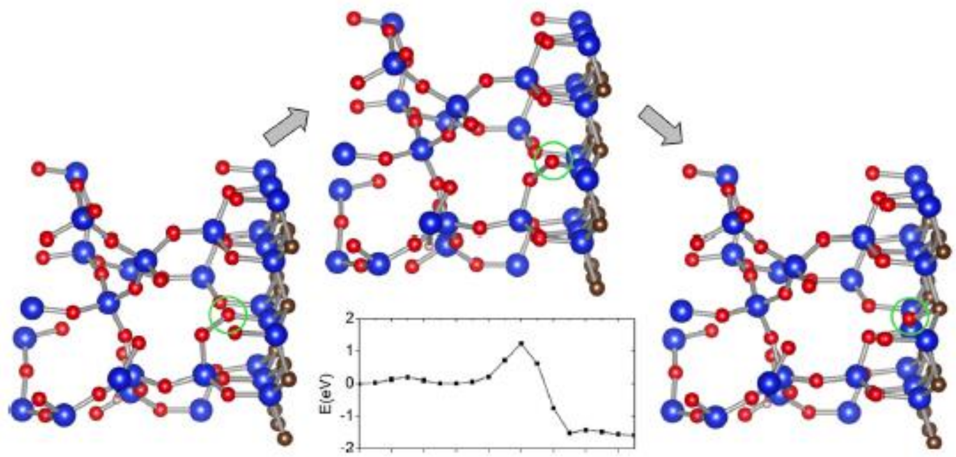

Figure 4. The initial, transition, and final states of an interstitial O arriving at the Si-face of SiC. Blue balls denote Si atoms, red balls denote O atoms and brown ball denote carbon atoms. The extra interstitial O is highlighted by a green circle. Only one layer of the SiC carbide substrate in each panel. The energy profile along the reaction path is also shown. Similar results were obtained for the other faces of SiC and for all Si faces as well. From X. Shen, B. R. Tuttle, and S. T. Pantelides, “Competing atomic and molecular mechanisms of thermal oxidation – SiC versus Si”, *Journal of Applied Physics*, vol. 114, article # 033522 (2013).

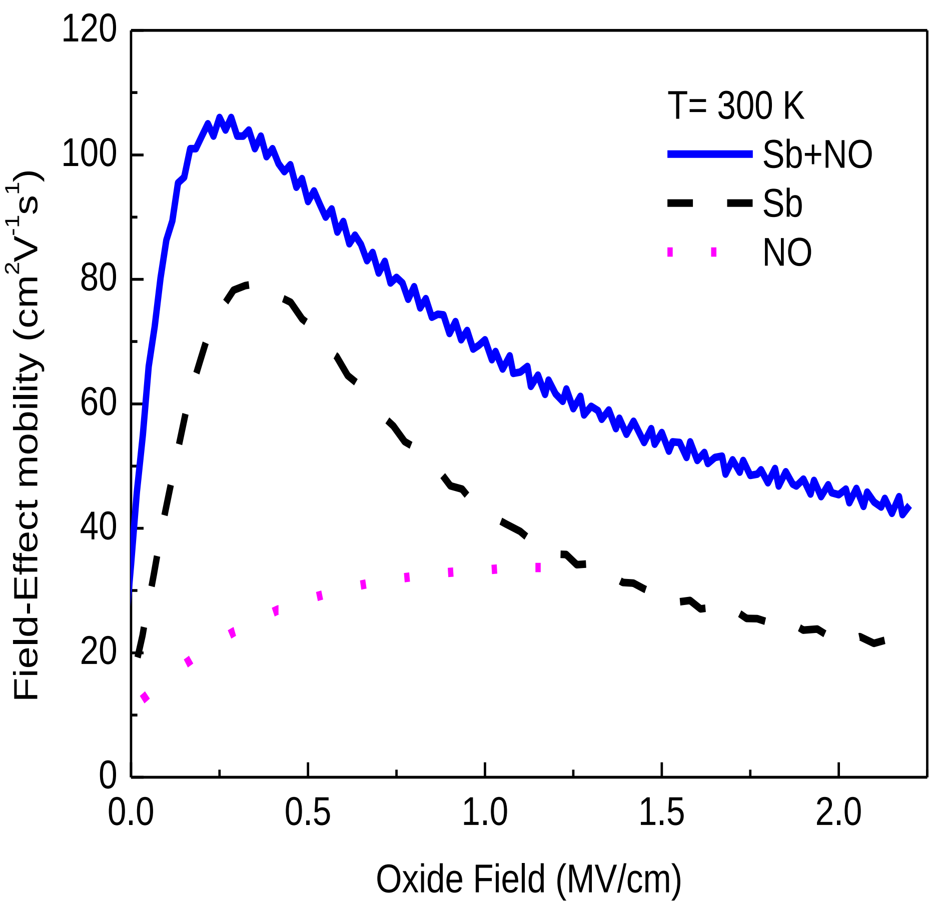

Figure 5. Field-effect mobility of 4H-SiC MOSFETs fabricated with three processes (i) NO: The standard method (ii) Sb: Antimony Counter-doping method (iii) Sb+NO: Combination of the two methods. Adapted from A. Modic, A.C. Ahyi, Y. Xu, P. Xu, M. Hamilton, Y. Zhou, L. C. Feldman, J. R. Williams and S. Dhar "High channel Mobility 4H-SiC MOSFETs by Antimony counter-doping", *IEEE Electron Device Letters*, vol. 35, p. 894-896 (2014)

Figure 6. Mr. Sorrie Cesay giving a presentation based on his Master's thesis at the Spring 2012 meeting of the Materials Research Society in San Francisco, CA.