

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Structure and defects at the SiC:SiO₂ interface¹ BLAIR TUTTLE,
Penn State Behrend, SOKRATES PANTELIDES, Vanderbilt University — The
pervasion of defects at the SiC:SiO₂ interface has limited the performance and com-
mercializing of SiC based transistors. While the defects are believed to be related
to excess carbon in the interfacial region, no compelling microscopic models exists.
Here we report the generation of microscopic interfaces models for the SiC:SiO₂
interface. These models include a 1 nm amorphous oxide and several layers of crys-
talline SiC. Defect and defect reactions are explored. For instance, the 3-fold bonded
carbon defect is calculated to have an acceptor level at $E_v + 1.4$ eV close to the
value found experimentally and encouraging confidence in the methods employed.
The recently discovered beneficial effect of sodium ions motivates our examination of
the basic electrochemistry of the sodium ion interactions with the ideal and defected
interfaces. A comparison between microscopic defect results and experiment will be
presented.

¹Work supported by the NSF grant DMR-0907385

Blair Tuttle
Penn State Behrend

Date submitted: 20 Nov 2009

Electronic form version 1.4