Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A theoretical study on the thermal oxidation of silicon carbide: Chemical species at the SiO_2/SiC interface[1] NOBUO TAJIMA, The University of Tokyo, TOMOAKI KANEKO, JUN NARA, TAKAHIRO YAMASAKI, TATSUO SCHIMIZU, National Institute for Materials Science, KOICHI KATO, The University of Tokyo, TAKAHISA OHNO, National Institute for Materials Science
— Silicon carbide (SiC) is potentially a suitable candidate of the channel materials of power devices since it has wide bandgap, high electron mobility, and thermal conductivity. Furthermore, it is favorable for device fabrication as it can be thermally oxidized to create insulating silicon oxide (SiO_2) layer. However, the SiC devices of current technology do not show acceptable performance because of a defective nature of the created SiO_2/SiC stacking structure, which causes problems such as channel mobility degradation, threshold voltage increase, and leakage current. The origins of the defective nature are not understood so far, though it is presumed that they are rather concentrated at the interface. In the present study, we have performed first principles calculations to know the chemical species possibly produced at the oxide interface of thermally oxidized SiC. The First principles simulation code PHASE/0 (http://www.ciss.iis.u-tokyo.ac.jp/riss/english/project/device/) was used in the theoretical calculations.

[1]A portion of this research was supported by the grant from MEXTs project and carried out in partnership with the University of Tokyo

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Date submitted: 02 Nov 2015 Electronic form version 1.4