Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

First-principles calculation of oxidation process of SiC substrate TOMOYA ONO, Osaka University & JST-PRESTO, SHOICHIRO SAITO, Osaka University — The atomic structure of 4H-SiC(0001)/SiO_2 interface is still under discussion since the conclusion derived by HRTEM is different from that by SIMS and XPS. The oxidation processes as well as the CO desorption of a SiC substrate are investigated by first-principles calculations. We employ SiC surface and SiC/SiO_2 interface models to imitate initial and middle stages of oxidation, respectively. O atoms are inserted between Si-C bond sequentially and the energy gain of the CO desorption is calculated by removing a C atom as a form of CO molecule. We found that the CO desorption becomes preferable when the number of inserted O atoms is three because the perfect SiO_2 network remains after the CO desorption and the stress is relaxed by removing the CO molecule from the SiC/SiO_2 interface. When C atoms are not removed as CO molecules at the interface, the unoxized Si-C bond remains in SiO_2. We also investigate the CO desorption from SiO_2. The energy gain of the CO desorption indicates that the CO desorption is unfavorable because the rearrangement of Si-O bonds costs more energy than the CO desorption. Thus, C atoms are immediately emitted from the interface as CO molecules and not kicked out from SiO_2. Our results support the conclusion obtained by SIMS and XPS.

Tomoya Ono
Osaka University

Date submitted: 14 Nov 2013 Electronic form version 1.4