Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Diffusion of carbon oxides in SiO_2 during SiC oxidation[1] TORU AKIYAMA, KOHJI NAKAMURA, TOMONORI ITO, Department of Physics Engineering, Mie University, HIROYUKI KAGESHIMA, NTT Basic Research Laboratories, NTT Corporation, MASASHI UEMATSU, Faculty of Science and Technology, Keio University — SiC is a wide-band-gap semiconductor and has an advantage to fabricate electronic devices such as MOSFETs due to the ability to thermally oxidize to SiO_2. Despite many studies conducted on the oxidation of SiC, the kinetics such as diffusion and interface reaction is not fully understood. Here, we focus on the diffusion process during SiC oxidation, and clarify the diffusion mechanism of carbon oxides (CO and CO_2) in SiO_2 by means of density functional calculations. Our calculations demonstrate that the CO without any chemical bonds with host SiO_2 is stabilized while the CO_2 is incorporated between Si-O bonds of SiO_2 to form a carbonate group. The energy of CO_2 is found to be lower than that of CO by 3.7 eV, indicating that the most stable form of carbon oxides in SiO_2 is CO_2. Furthermore, the calculated energy barriers for diffusion of CO and CO_2 are found to be 0.1 and 1.8 eV, respectively. These results thus imply that CO molecules easily react with oxidant such as O_2 to form CO_2 and the outward diffusion of resultant CO_2 is rate-limiting. Indeed, the estimated activation energy for CO_2 diffusion (3.5 eV) reasonably agrees with that for Si-face SiC (3.1 eV) obtained by Deal-Grove model considering product gas out-diffusion.

[1]This work was supported in part by Grant-in-Aid for Scientific Research (No. 24560025) from the Japan Society for the Promotion of Science.

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Date submitted: 02 Nov 2012 Electronic form version 1.4