Thermal oxidation simulation of silicon carbide (SiC) semiconductor

Background

Power electronics apparatus using SiC power devices can achieve large reduction in power consumption by low-loss operation and in size of apparatus by high-voltage blocking capability in comparison with Si-based devices. Silicon carbide (SiC) is particularly attractive for metal-oxide-semiconductor (MOS) applications (Fig.1) because among compound semiconductors, only SiC has a thermal oxide SiO_2, which is a good insulator. However, it is known that SiO_2/SiC interfaces have a higher density of interface traps than SiO_2/Si interfaces and the channel mobility of MOS devices is two orders lower than theoretically expected values. In order to improve the characteristic of MOS devices, it is important to clarify the generation mechanism of interface traps in the SiC thermal oxidation process.

Objective

In order to clarify the origin of the interface trap of SiO_2/SiC interface, we elucidate the thermal oxidation process of SiC semiconductor using first-principle molecular dynamics *1.

Principal results

We performed dynamic simulation in the course of the oxidation process of the SiO_2/4H-SiC *2 interface at the temperature 2500K for the first time using the Earth simulator, which is one of the fastest supercomputers in the world.

1. Dissociation reaction of oxygen molecule at the SiO_2/SiC interface

In the SiC thermal oxidation process, it is considered that oxygen molecules diffuse in the form of oxygen molecules, and oxidation occurs at the interface. We assume that the oxygen diffuses to the interface as the O_2 molecule during thermal oxidation of the SiO_2/SiC interface. We introduce the carbon vacancy into the SiC layer near the interface in order to trigger the oxidation process. The O_2 molecule bonds to the Si atom in the SiO_2 layer and dissociates through the transition state (Fig.2). Although it was considered the O_2 molecule directly reacts to SiC layer, we found that the O_2 molecule reacts to the Si atom in the SiO_2 layer

2. Formation of CO, C_2O molecules, and carbon clusters

In the oxidation process simulation, we observed the formation of the CO and C_2O molecules. We also observed the carbon clusters *3, which are one of the candidate of the interface traps, formed in the oxidation process (Fig.3).

*This work is the joint research of Japan Atom Energy Agency

Future Developments

We will systemically clarify the thermal oxidation process of SiO_2/SiC interface using first-principle molecular dynamics.

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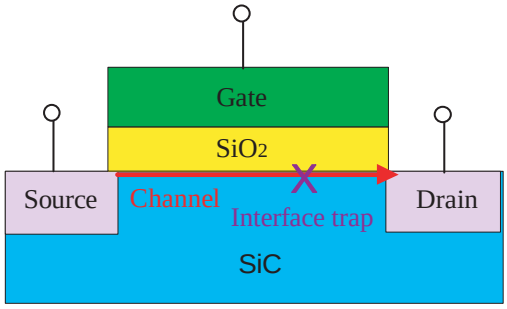
Reference

"Dynamical simulation of SiO_2/4H-SiC(0001) interface oxidation process: from first-principles," Materials Science Forum 556-557 (2007) 615-620 (Invited Paper)

*1：First-principle molecular dynamics is one of the atomistic simulation methods. Interatomic forces are calculated based on quantum mechanics. It is applicable for the chemical reaction. Demerit is the huge computational cost.

*2：SiC has various crystal structures, such as 3C, 4H and 6H, etc. by the symmetry. 4H-SiC is the most widely studied as a power electronics device

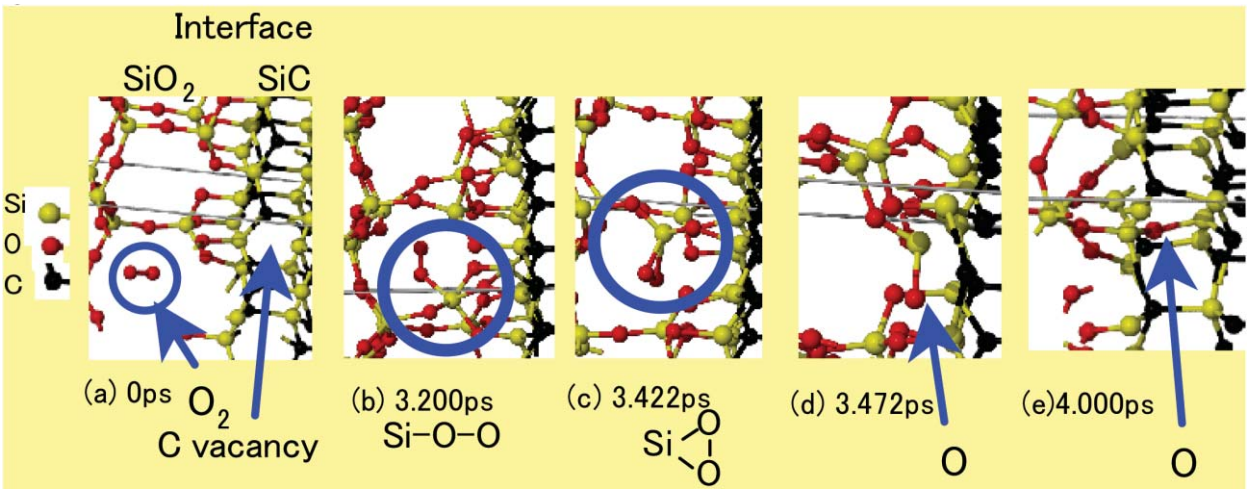
*3：Carbon atoms are clustered at the SiO_2/SiC interface



MOS (Metal Oxide Semiconductor) device

The MOS structure is produced by attaching the electrode, after the thermal oxidation of SiC.
The channel where the electron is easy to move between semiconductor and insulating layer appears, when the voltage is applied between gate electrode and semiconductor (SiC). However, the electron becomes difficult to move, when the interface trap exists.

Fig.1 Structure of the MOS (Metal Oxide Semiconductor) device



(a) 0 ps (ps: 10^{-12} Second) O_2 molecule is added. (b) 3.200 ps: O_2 molecule bonds to the Si atom in the SiO_2 layer. (c) 3.422 ps: Si-O-O complex forms triangle configuration. (d) 3.472 ps: The O atom moves to the SiC layer. (e) 4.000 ps: O atom enters C vacancy position. Dissociation process of O_2 molecule is ended.

Fig.2 Dissociation process of O_2 molecule in the SiC thermal oxidation.

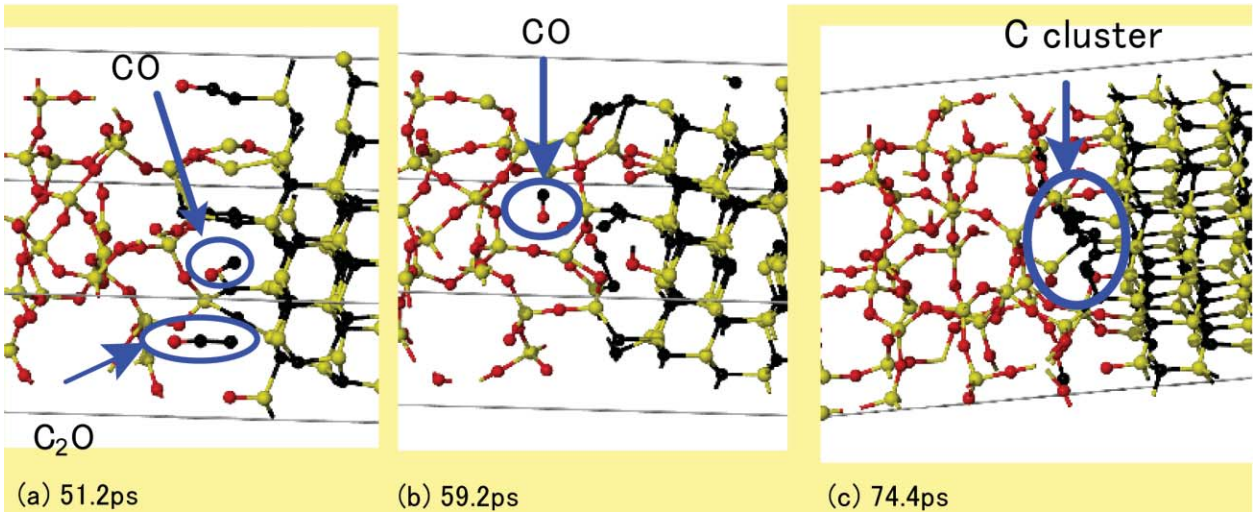


Fig.3 Formation of CO, C_2O molecules, and C cluster.

(a) 51.2 ps: Formation of CO and C_2O molecules. (b) 59.2 ps: Formation of CO molecule. (c) 74.4 ps: Oxidation of interface Si layer and formation of C cluster.