博士論文（要約）

Kinetic study of interfacial SiO_2 scavenging in HfO_2 gate stack on Si substrate

（**Si** 基板上 **HfO_2** ゲートスタックにおける **SiO_2** 界面層のスカベンジング現象に関する速度論的研究）

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"Scavenging" of SiO_2 interface layer (SiO_2-IL) in high-k gate stacks is a significant issue for interface materials science as well as for further scaling of equivalent oxide thickness (EOT) in high-*k* gate stacks. The mechanism in this process has not been fully understood so far. The objective of this study is to clarify what really occurs in SiO_2-IL scavenging in $HfO_2/SiO_2/Si$ stacks experimentally and physically.

First, the SiO_2-IL scavenging has been achieved by ultra-high vacuum annealing (UHV-PDA) in place of metal incorporating used in the literature so far reported. Because the UHV enable us to study what happen in this process more deeply and controllably through bare HfO_2 surface. The specific condition of for SiO_2-IL scavenging in UHV-PDA of $HfO_2/SiO_2/Si$ stack has been clarified and optimized. The effect of other reaction involved in UHV-PDA of $HfO_2/SiO_2/Si$ stacks on SiO_2-IL scavenging was also investigated.

Then the key issue, SiO_2-IL scavenging kinetics in $HfO_2/SiO_2/Si$ stack, has been experimentally investigated. Through studying the effect of V_O in HfO_2 and tracing the oxygen in SiO_2 by ^{18}O

isotope, it was found that oxygen atom in SiO_2 diffuses into Vo HfO_2 in SiO_2-IL scavenging. This provides the direct evidence for the model proposed in the literatures. More importantly, the substrate-Si has been found to be significant for SiO_2-IL scavenging for the first time by changing Si substrate to SiC, Ge and sapphire ones. It seemed Si in substrate is necessary for SiO_2-IL scavenging, but it was observed that Si substrate was not changed during scavenging. Furthermore, up-diffusion of Si atom in SiO_2 has been demonstrated for the first time by using ^{29}Si isotope. Thus the diffusion species and reaction system in SiO_2-IL scavenging has been clarified experimentally.

Based on the experimental results, the SiO_2-IL scavenging has been understood theoretically by taking account of both effects of V_O in HfO_2 and Si in substrate. It was described that substrate induced Si chemical potential gradient in SiO_2 together with V_O injection from HfO_2 drives the SiO_2-IL scavenging reaction at SiO_2/Si interface. A kinetic model where down-diffusion of V_O converts to up-diffusion of Si at SiO_2/Si interface has been proposed for SiO_2-IL scavenging in HfO_2/SiO_2/Si stacks. After that, the kinetic model has been formulated analytically. A formula looks like Deal-Grove model was obtained and discussed in detail.

In addition, considering the practical application of SiO_2-IL scavenging, the interface property in SiO_2-IL scavenging has been considered by capacitance-voltage characterization. Although a flat band voltage is observed in SiO_2-IL scavenging, the interface was not degraded. And the metal effect in SiO_2-IL scavenging has been discussed. It was considered that the thermodynamics and kinetics should be the same with that in our model.