

# Kinetic study of interfacial SiO<sub>2</sub> scavenging in HfO<sub>2</sub> gate stack on Si substrate

その他のタイトル	Si基板上HfO <sub>2</sub> ゲートスタックにおけるSiO <sub>2</sub> 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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論文の内容の要旨

**Kinetic study of interfacial SiO<sub>2</sub> scavenging in HfO<sub>2</sub>  
gate stack on Si substrate**

(Si 基板上 HfO<sub>2</sub> ゲートスタックにおける SiO<sub>2</sub> 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<sub>2</sub> interface layer (SiO<sub>2</sub>-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<sub>2</sub>-IL scavenging in HfO<sub>2</sub>/SiO<sub>2</sub>/Si stacks experimentally and physically.

First, the SiO<sub>2</sub>-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<sub>2</sub> surface. The specific condition of for SiO<sub>2</sub>-IL scavenging in UHV-PDA of HfO<sub>2</sub>/SiO<sub>2</sub>/Si stack has been clarified and optimized. The effect of other reaction involved in UHV-PDA of HfO<sub>2</sub>/SiO<sub>2</sub>/Si stacks on SiO<sub>2</sub>-IL scavenging was also investigated.

Then the key issue, SiO<sub>2</sub>-IL scavenging kinetics in HfO<sub>2</sub>/SiO<sub>2</sub>/Si stack, has been experimentally investigated. Through studying the effect of V<sub>O</sub> in HfO<sub>2</sub> and tracing the oxygen in SiO<sub>2</sub> by <sup>18</sup>O

isotope, it was found that oxygen atom in  $\text{SiO}_2$  diffuses into  $\text{V}_\text{O}$   $\text{HfO}_2$  in  $\text{SiO}_2$ -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  $\text{SiO}_2$ -IL scavenging for the first time by changing Si substrate to SiC, Ge and sapphire ones. It seemed Si in substrate is necessary for  $\text{SiO}_2$ -IL scavenging, but it was observed that Si substrate was not changed during scavenging. Furthermore, up-diffusion of Si atom in  $\text{SiO}_2$  has been demonstrated for the first time by using  $^{29}\text{Si}$  isotope. Thus the diffusion species and reaction system in  $\text{SiO}_2$ -IL scavenging has been clarified experimentally.

Based on the experimental results, the  $\text{SiO}_2$ -IL scavenging has been understood theoretically by taking account of both effects of  $\text{V}_\text{O}$  in  $\text{HfO}_2$  and Si in substrate. It was described that substrate induced Si chemical potential gradient in  $\text{SiO}_2$  together with  $\text{V}_\text{O}$  injection from  $\text{HfO}_2$  drives the  $\text{SiO}_2$ -IL scavenging reaction at  $\text{SiO}_2/\text{Si}$  interface. A kinetic model where down-diffusion of  $\text{V}_\text{O}$  converts to up-diffusion of Si at  $\text{SiO}_2/\text{Si}$  interface has been proposed for  $\text{SiO}_2$ -IL scavenging in  $\text{HfO}_2/\text{SiO}_2/\text{Si}$  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  $\text{SiO}_2$ -IL scavenging, the interface property in  $\text{SiO}_2$ -IL scavenging has been considered by capacitance-voltage characterization. Although a flat band voltage is observed in  $\text{SiO}_2$ -IL scavenging, the interface was not degraded. And the metal effect in  $\text{SiO}_2$ -IL scavenging has been discussed. It was considered that the thermodynamics and kinetics should be the same with that in our model.