

## Mobility Degradation and Interface Dipole Formation in Direct-Contact HfO<sub>2</sub>/Si MOSFETs

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### 1. Introduction

Controlling interface dipoles in the high- $k$  gate stack is a key issue for accurate  $V_{th}$  control of the advanced MOSFETs. However, disordered dipoles in gate stack structures degrade the carrier mobility due to the fluctuated Coulomb potential [1]. The so-called direct-contact HfO<sub>2</sub>/Si interface at which only about one monolayer Si oxide exists has a strong dipole layer ( $>0.5$  V) [2], although this structure has an advantage in scaling EOT down to sub 1 nm [3].  $V_{th}$  and mobility characteristics for the direct-contact HfO<sub>2</sub>/Si structure have not been investigated in detail. In this paper, we first describe electrical characteristics of n-channel MOSFET with a direct-contact HfO<sub>2</sub>/Si interface, and then discuss the effect of interface dipoles on the electron mobility.

### 2. Experimental

The n-MOSFETs were fabricated using a gate last process. To examine the dependence on the interface SiO<sub>2</sub> thickness in detail, a HfO<sub>2</sub>/Gradually etched (GE) SiO<sub>2</sub>/Si gate stack structure was integrated into the devices (Fig. 1). About 10-nm-thick SiO<sub>2</sub> layer was first thermally grown on the Si surface. The SiO<sub>2</sub> layer was then gradually etched by a diluted HF solution. A 2.6-nm-thick HfO<sub>2</sub> film was deposited on this surface by an ultra-high vacuum electron-beam evaporation method [3]. The postdeposition annealing (PDA) was performed at 400°C in  $2 \times 10^{-6}$  Torr O<sub>2</sub> pressure. Finally, a metal gate layer of iridium was deposited on the HfO<sub>2</sub> surface.

### 3. Results and Discussion

Well-behaved  $I_d$ - $V_d$  characteristics were obtained from the direct-contact-HfO<sub>2</sub>/Si MOSFETs as shown in Fig. 2. The  $I_d$ - $V_g$  characteristics in Fig. 3 show an on/off ratio of about 10<sup>7</sup> and a subthreshold slope (S) of 72mV/decade. These data are quite normal, so we considered that our HfO<sub>2</sub> film works well as a gate dielectric, even though the direct-contact interface was employed. However, large negative  $V_{th}$  shift can be observed for the direct-contact structure; the direct-contact and stack structures have  $V_{th}$  of 0.16 V and 0.62 V, respectively. The split  $C$ - $V$  curves shown in Fig. 4 show similar voltage shift. These  $C$ - $V$  curves also show that the larger inversion capacitance can be obtained for the direct-contact structure. The EOT value was estimated to be 0.62 nm. Here, we assume that the thickness of interface SiO<sub>2</sub> layer ( $t_{IL}$ ) in the HfO<sub>2</sub>/SiO<sub>2</sub>/Si stack structure corresponds to the EOT difference between the stack and direct-contact structures. The  $t_{IL}$  dependence of  $V_{th}$  shown in Fig. 5 indicates that negative  $V_{th}$  shift is

effectively suppressed by insertion of a monolayer thick Si oxide ( $<1$  nm) into the HfO<sub>2</sub>/Si interface. Similar behavior has been observed for  $V_{fb}$  of MOS capacitors, as previously reported [2]. It was suggested from detailed analysis of the  $V_{fb}$  behavior that a strong dipole layer ( $>0.5$  V) exists at the direct-contact HfO<sub>2</sub>/Si interface, and it disappears with several monolayer thick Si oxides. Consequently, we concluded that similar dipole formation and annihilation take place at the HfO<sub>2</sub>/Si interfaces in the present MOSFETs.

Electron mobility curves estimated for three types of interfaces are shown in Fig. 6. The mobility decreases with decreasing interface SiO<sub>2</sub> layer in the whole effective field range. In general, such  $t_{IL}$ -dependent degradation was explained by remote scattering mechanisms, e.g., remote Coulomb scattering by fixed charges in high- $k$  layer and high- $k$  phonon scattering [4-6]. To extract this additional mobility component ( $\mu_{add}$ ), the other scattering factors should be subtracted from measured mobility ( $\mu_{mea}$ ). In this study, mobility curve measured for the HfO<sub>2</sub>/SiO<sub>2</sub>/Si-stack MOSFET with thick  $t_{IL}$  ( $\sim 5.4$  nm) was used as a reference curve ( $\mu_{ref}$ ), and  $\mu_{add}$  was estimated by Matthiessen's rule;  $1/\mu_{add} = 1/\mu_{mea} - 1/\mu_{ref}$ . The estimated  $\mu_{add}$  curves are shown in Fig. 7. Typical bulk Coulomb and phonon scattering curves are also plotted, since it is expected that the remote scattering also have similar field dependence. This result suggests that at least both Coulomb and phonon scattering contributes to the  $t_{IL}$ -dependent degradation.

In general, remote scattering shows an exponential decay with decreasing interface SiO<sub>2</sub> layer [1,4,6];  $1/\mu_{add} \propto \exp(-2k_F t_{IL})$ , where  $k_F$  is the Fermi wavenumber of channel electron and  $t_{IL}$  is the thickness of interface SiO<sub>2</sub> layer. Figure 8 shows the dependence of  $\mu_{add}$  at 0.35 MV/cm on  $t_{IL}$ .  $\mu_{add}$  decreases exponentially, and this tendency can be explained with the remote scattering process (solid line). If the dipoles induced at direct-contact interfaces largely degrade the mobility, it is expected to find some deviation from the remote scattering tendency. Figure 8 obviously indicates that the dominant degradation mechanism is remote scattering even for the direct-contact structures. It was proposed that Si-O chemical bonds at the HfO<sub>2</sub>/Si interface are mainly responsible for the dipole formation [7]. It seems that such uniformly arrayed dipoles do not produce large Coulomb potential fluctuation which induces serious mobility degradation. Consequently, suppressing remote phonon scattering and eliminating fixed charges are important for improving electron mobility for direct-contact structures as well as for conventional stack structures.

#### 4. Conclusion

The effect of dipole layer on the HfO<sub>2</sub>/Si MOSFTE characteristics was investigated by using HfO<sub>2</sub>/GE-SiO<sub>2</sub>/Si structures. The direct-contact HfO<sub>2</sub>/Si MOSFTEs showed serious electron mobility degradation. Its origin was ascribed to remote Coulomb and phonon scattering rather than the dipole scattering.

#### References

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#### Process flow

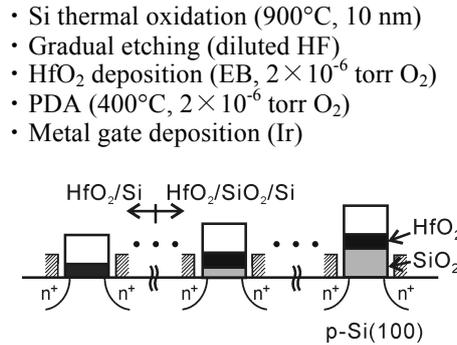


Fig. 1 Process flow of gate stack and fabricated HfO<sub>2</sub>/GE-SiO<sub>2</sub>/Si MOSFET structure.

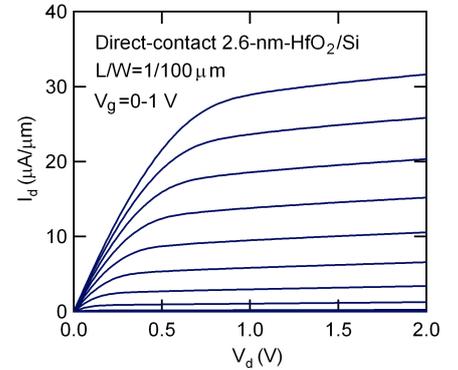


Fig. 2  $I_d$ - $V_d$  characteristics of direct-contact HfO<sub>2</sub>/Si MOSFET.  $V_g$  was increased from 0 to 1.0 V in 0.1-V steps.

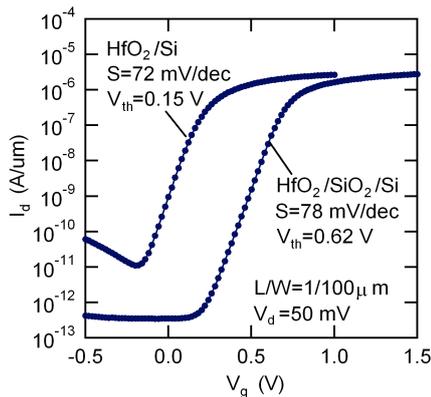


Fig. 3  $I_d$ - $V_g$  characteristics of direct-contact-HfO<sub>2</sub>/Si and HfO<sub>2</sub>/SiO<sub>2</sub>/Si-stack MOSFETs.  $V_d$  was 50 mV.

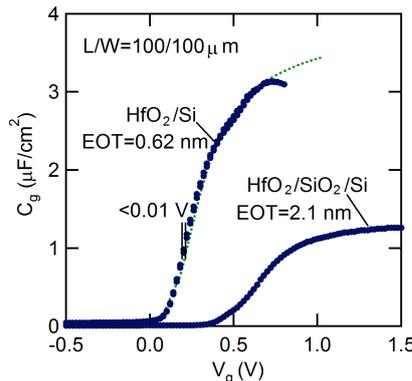


Fig. 4  $C$ - $V$  characteristics for direct-contact-HfO<sub>2</sub>/Si and HfO<sub>2</sub>/SiO<sub>2</sub>/Si-stack MOSFETs.

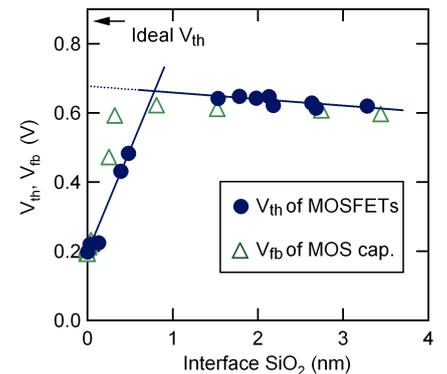


Fig. 5 Dependence of  $V_{th}$  on thickness of interface SiO<sub>2</sub> layer.  $V_{fb}$  of 2.5-nm-HfO<sub>2</sub>/GE-SiO<sub>2</sub>/n-Si MOS capacitors were also plotted as a reference.

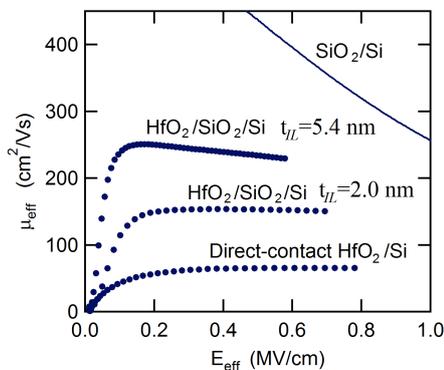


Fig. 6 Electron mobility characteristics of direct-contact HfO<sub>2</sub>/Si and HfO<sub>2</sub>/SiO<sub>2</sub>/Si-stack MOSFETs.

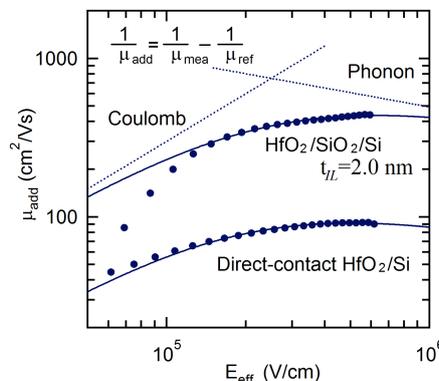


Fig. 7 Additional electron mobility ( $\mu_{add}$ ) caused by thinning of interface SiO<sub>2</sub> layer.

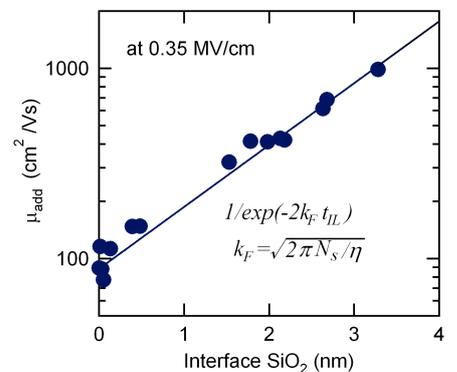


Fig. 8 Dependence of  $\mu_{add}$  on thickness of interface SiO<sub>2</sub> layer ( $t_{IL}$ ).