

# Surface-sensitive chemical analysis of ultrathin Hf/Si(557) film by photoelectron - Auger-electron coincidence spectroscopy

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## 1 Introduction

Drastic downsizing of the ultrathin SiO<sub>2</sub> gate dielectric film (< 10 Å) for the metal-oxide-semiconductor field effect transistor (MOSFET) has caused a critical leakage current [1]. Therefore, the identification of an alternative SiO<sub>2</sub> dielectric was an immediate issue to keep the development of semiconductor industry by following Moore's law. Hafnium dioxide (HfO<sub>2</sub>, Hafnia) is a promising candidate for the alternative gate dielectric due to (1) a high dielectric constant ( $k$ , ~25), (2) a stability in contact with silicon, (3) a large bandgap (> 4-5 eV), (4) a low density of defects at the interface between HfO<sub>2</sub> and silicon, (5) an equivalent physical thickness to SiO<sub>2</sub> layer less than 10 Å, and so on [1-3].

In addition, an idea of the 3-dimensional structure of the MOSFET is attracting to increase the number of devices in an integrated circuit. This indicates that the behaviors of hafnium (Hf) species on various facets of silicon substrate become to be meaningful to control the stable operation.

In this study, we prepared ultrathin Hf film on a clean Si(557)-7×7 surface. After annealing at 1073 K, we investigated the chemical states at interface and surface by using a conventional photoelectron spectroscopy and a Si 2*p* photoelectron - Si L<sub>23</sub>VV Auger-electron coincidence spectroscopy (Si-2*p*-Si-L<sub>23</sub>VV PEACS).

## 2 Experiment

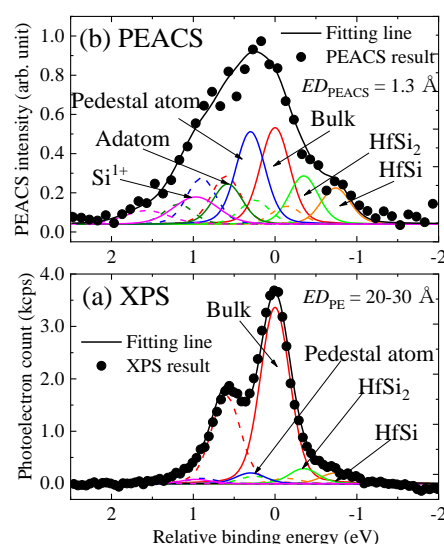
A clean Si(557)-7×7 with single domain (SD) structure was prepared by direct current heating at 1520 K in ultrahigh vacuum (UHV) achieved at  $4.0 \times 10^{-8}$  Pa. An ultrathin Hf film with a thickness of ~2.0 layers (1 layer = 2.4 Å [4]) was deposited on a clean Si(557)-7×7 surface.

Si 2*p* photoelectron spectrum and Si-L<sub>23</sub>VV-Si-2*p* APECS spectrum were measured with a handmade electron-electron-ion coincidence analyzer at BL-11D in PF, KEK. The photon energies ( $h\nu$ ) at 112 and 130 eV were irradiated to sample for ionization of Si 2*p* core level. The escape depth ( $ED$ ) of Si 2*p* photoelectron ( $ED_{PE}$ ) was estimated to be 20-30 Å at  $h\nu = 112$  eV. In addition, the escape depth of Si-2*p*-Si-L<sub>23</sub>VV PEACS ( $ED_{PEACS}$ ) can be obtained by  $1/ED_{PEACS} = 1/(ED_{PE} \cdot \cos\theta_{PE}) + 1/(ED_{AE} \cdot \cos\theta_{AE})$  [5]. Here, the  $ED_{AE}$  is the  $ED$  of Si L<sub>23</sub>VV Auger-electron, and the  $\theta_{PE}$  ( $\theta_{AE}$ ) is the detection angle of photoelectron (Auger-electron). In this study, the  $ED_{PEACS}$  was estimated to be 1.3 Å at  $h\nu = 130$  eV.

## 3 Results and Discussions

Figure 1 shows (a) the conventional Si 2*p* photoelectron spectrum measured at  $h\nu = 112$  eV and (b)

the Si-L<sub>23</sub>VV-Si-2*p* APECS spectrum measured at  $h\nu = 130$  eV, respectively. These are drawn by solid circles. Some fitting curves are drawn by solid lines (2*p*<sub>3/2</sub>) and dashed lines (2*p*<sub>1/2</sub>). The spectrum in Fig.1 (a) is mainly composed of bulk Si component, on the other hand, the spectrum in Fig. 1 (b) is composed of some surface components of Si(557)-7×7 and segregation components of Hf silicides (HfSi and HfSi<sub>2</sub>). These results indicate that islands of Hf silicides were formed on bare Si(557)-7×7 substrate after annealing over 1073 K. Our consideration is consistent with the observation in scanning electron microscope.



**Fig. 1:** Si 2*p* photoelectron peaks obtained by (a) a conventional Si 2*p* photoelectron spectroscopy and (b) a Si-2*p*-Si-L<sub>23</sub>VV PEACS.

## Acknowledgement

This work was supported by a Grant-in-Aid for Scientific Research (No. 17K06030) from the Japanese Ministry of Education, Culture, Sports, Science and Technology. We thank the PF staff for supporting our experiment.

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