2C/2002S2-002

Interfacial reaction of polycrystalline-Si /HfO_2/Si gate stacks with annealing studied by photoemission spectroscopy

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Introduction

For continuous improvements in ultra-large-scale integrated (ULSI) device performance, the device size has been shrinking following Moore's law. In the sub-nm scale of the gate dielectrics, the current processes using SiO_2 reach the limitation due to the direct tunneling leakage current. Recently, the alternative high dielectric constant (high-*k*) materials such as Al_2O_3, ZrO_2, Y_2O_3, and HfO_2 have been widely investigated. HfO_2 is one of the most promising materials because of its thermal stability, wide band gap, and high dielectric constant. In the current Si technology, polycrystalline-Si (poly-Si) is used as a gate electrode. One of the current problems for HfO_2 application is a thermal stability at the interface between poly-Si electrodes and high-*k* dielectrics during activation annealing of dopants. In order to improve device performances, chemical reactions at the interface have to be clarified explicitly.

Experimental

The HfO_2 layer was deposited on clean *p*-type Si (001) substrates by reactive magnetron sputtering using a Hf metal. The thickness was estimated by the elipsometry to be 2 nm for the HfO_2 layer and 0.5 nm for the interfacial Hf-silicate layer on Si substrates. Poly-Si electrodes of 3 nm were deposited on HfO_2 gate stacks at room temperature by magnetron sputtering. Photoemission spectroscopy was carried out at an undulator beam line BL-2C of the Photon Factory in High-Energy Accelerator Research Organization (KEK). Annealing was performed in ultra high vacuum (UHV) by a direct-current-flowing method through the samples for 10 min at each temperature before the photoemission measurements.

Results and Discussion

Hf 4*f* photoemission spectra are shown in Fig. 1. Angular dependence to increase the surface sensitivity is also investigated by changing the emission angle from surface normal to 60 °. The components appearing at the binding energy of 18 eV with spin-orbit splitting are derived from HfO_2. By the annealing at 700 °C, a new component appears at the binding energy of 14.5 eV, which can be assigned as the Hf-silicide component. The intensity ratio of the Hf-silicide component to the HfO_2 component increases by the surface-sensitive measurements in the emission angle of 60 °, suggesting that the Hf silicide is formed at the "upper interface" between poly-Si and HfO_2. On the contrary, the intensity ratio decreases in the surface-sensitive measurements by the annealing at 750 °C. This is because the silicidation promotes into the lower interface. Peak shifts in the HfO_2 component by 750 °C annealing are explained by the change of the interface component from Hf silicate to Hf silicide and the band offsets are also changed. By the annealing at 800 °C, the HfO_2 component completely disappears and only the Hf-silicide components remain. In the case without the poly-Si electrodes, the Hf-silicide formation occurred by the annealing at as high temperature as 900 °C in previous reports[1,2]. These results indicate that the poly-Si electrodes drastically influence the silicidation temperature at the "lower interface" between HfO_2 and Si substrate.

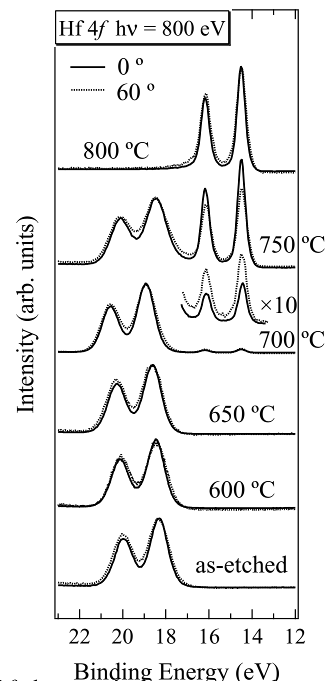

Fig. 1. Hf 4*f* photoemission spectra depending on the annealing temperature. Solid curves show the spectra taken at the emission angle of 0 °. Dashed curves show those of 60 °.

References

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