Characterization of ALD (HfO2)x(SiO2)1-x dielectrics on p-Si(100)

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Due to thecontinuous decrease in device size toward atomic dimensions, Si devices are closely approaching fundamental limits. To avoid quantum tunneling, high-*k*(high dielectric constant) gate dielectric layer is required to replace SiO_2. Hf-based transition metal dielectrics have received considerable attention. In particular the silicates, $(HfO_2)_x(SiO_2)_{1-x}$, which can be regarded as an alloy between a metal oxide and SiO_2, are proposed as promising high-*k* gate dielectrics. We characterize the chemical states and band gap for ultrathin 6 nm $(HfO_2)_x(SiO_2)_{1-x}$ deposited by atomic layer deposition with x equal to 0.75 and 0.25. We studied the silicates by using XPS and reflection electron energy loss spectroscopy (REELS). XPS measurement confirms the formation of silicate structure, and it shows the peak energy shifts with various Hf concentrations, which is due to the change in charge transfer amounts and change in Si second-nearest-neighbors. AES depth profiling analysis was obtained using a PHI 700 SAM system. As shown in depth profile, the Hf:O ratio is approximately 3:1 and 1:3 near the surface region. The band gap (E_g) was estimated from REELS. It was found that the band gap slightly increase from 5.52 eV for $(HfO_2)_{0.75}(SiO_2)_{0.25}$ dielectric thin film to 6.61 eV for $(HfO_2)_{0.25}(SiO_2)_{0.75}$ dielectric thin film. For Hf silicate dielectrics, the E_g is mainly determined by Hf *5d* conduction band state and O *2p* valence band state for Hf silicate with higher Hf concentration. Finally, a quantitative analysis of REELS spectra was completed. It provides a straightforward way to evaluate the dielectric function of a solid and to determine the inelastic scattering properties. The results of the quantitative analysis successfully reproduced the trend that has been found in the experimental measurements.