A Comprehensive Study of Thermal Stability on Microstructure and Residual Stress for ALD $HfZrO_2$ Dielectric Films at 28nm HKMG CMOS Applications

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The gate leakage current and reliability concern become more serious due to the aggressive scaling-down of the gate oxide thickness. High-k/metal gate is needed for highly scaled CMOS [1,2]. Adding ZrO_2 into HfO_2 has recently been highlighted with regard to improving high-k reliability [3]. The influence of thermal stability on microstructure, surface morphology and residual stress for gate stack structure of $HfZrO_2$ dielectrics grown by atomic layer deposition (ALD) were investigated. For many applications of Hf-based dielectric films , excessive residual stress can limit the reliability and function of thin films-based structures due to peeling, cracking and curling. Thus control of residual stress is crucial.

In this letter, we report the impact of thermal annealing treatment for ALD $HfZrO_2$ on microstructure, surface morphology. The influences of different annealing temperature with N_2 or O_2 ambient on the residual stress of ALD $HfZrO_2$ films are studied. The difference of spectra, residual stress, and structures for $HfZrO_2$ films are obtained by the changed thermal energy. A tetragonal to monoclinic phase transformation is observed during high temperature annealing for $HfZrO_2$ films. The variations of spectra can be attributed to the different residual stress of ALD $HfZrO_2$ films induced by the annealing temperature. The tensile residual stress of $HfZrO_2$ films were increased when increasing annealing temperature either for N_2 or O_2 annealing. ALD $HfZrO_2$ is one of the leading candidates for future gate dielectric material of advanced HKMG at 28nm CMOS applications.

$HfZrO_2$ films ranging from 20 to 200 Å thick were deposited on blanket 300 mm p-type Si (100) wafers in a commercially available ALD tool. ALD $HfZrO_2$ films were performed at 300 °C by using $HfCl_4$, $ZrCl_4$, and H_2O precursors. All films were annealed at different temperature in a nitrogen (or oxygen) ambient are compared. In order to study the microstructure of ALD $HfZrO_2$, film roughness was measured by atomic force microscopy (AFM) operated in tapping mode. SEMVision (SEMV) tool was used to detect the wafer surface image. X-ray diffraction (XRD) in powder mode was used to determine the preferred orientation of the films. Instrumentation consisted of a Rigaku Rotaflex RU-200BH with CuK α rotating anode and Dmax-Bgoniometer. High resolution transmission electron microscopy (HR-TEM) observations of the $HfZrO_2/SiO_2$ gate stack structure are presented. The substrate radius of curvature was measured by ZYGO interferometer. The residual stress σ in the dielectric film is then given by Stoney's equation. By convention, tensile stress was indicated to be positive, while compressive to be negative.

The SEMV micrographs of as deposited $HfZrO_2$ and annealed samples are compared in Fig. 1. The results of SEMV investigations of as deposition $HfZrO_2$ film (Fig. 1(a)~1(d)) with different $HfZrO_2$ thickness. After high temperature annealing (Fig. 1(e)~1(h)). The surface of annealed $HfZrO_2$ samples show significant difference due to dielectric films phase were changed when $HfZrO_2$ dielectric film thickness increased. Fig. 2 shows the surface roughness of $HfZrO_2$ film after PDA with N_2 or O_2 ambient under different temperature. This thermal effect on the surface roughness were more significant for thicker $HfZrO_2$ film which compared with the as deposition $HfZrO_2$ condition. Data collection was from KLA Surface Scan SP2.

Fig. 3 shows the residual stress of ALD $HfZrO_2$ thin films annealed at different temperature, the N_2 PDA and O_2 PDA are compared. The as deposited $HfZrO_2$ films exhibit tensile residual stress with a value of 208 MPa. We can find that annealing at lower temperatures has little influence on the residual stress of ALD $HfZrO_2$ films. After annealing at higher temperatures, the residual stress increases with the increasing annealing temperature either for N_2 or O_2 PDA. The O_2 PDA for $HfZrO_2$ films can have higher residual stress than N_2 PDA treatment . Fig. 4 shows XRD sepctra of samples for ALD $HfZrO_2$ after different annealing temperature with N_2 ambient. When the annealing temperature is lower, the thermal energy provide by annealing is mainly consumed to recover the film initial structure and not enough to make the grain growth. The dielectric grain would grow significantly when enough thermal energy is offered at higher annealing temperature. The ratio of tetragonal peak intensity height to the sum of tetragonal and monoclinic peak intensity heights of ALD $HfZrO_2$ samples after N_2 PDA with various annealing temperature is shown in the insert of Fig. 4. The percentage of tetragonal peak of ALD $HfZrO_2$ samples is decreased when increasing annealing temperature for $HfZrO_2$ samples.

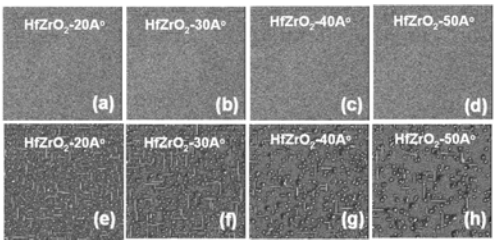

Figure 1. SEMV micrographs of different thickness $HfZrO_2$. The as deposited $HfZrO_2$ and N_2 annealed samples are compared. Image size: 400×400 nm.

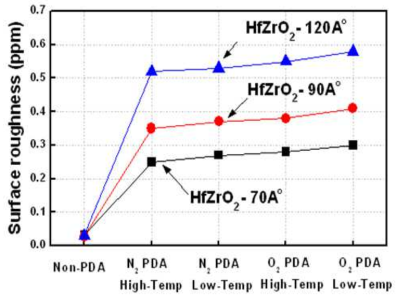

Figure 2. Surface roughness of $HfZrO_2$ film after different thermal treatment with N_2 or O_2 ambient under high/low temperature.

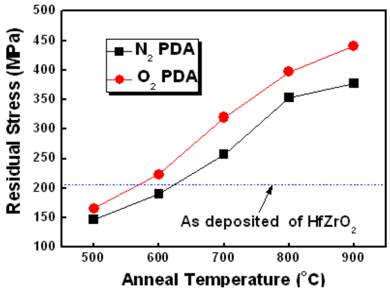

Figure 3. Residual stress of ALD $HfZrO_2$ samples after different annealing temperature with N_2 or O_2 ambient.

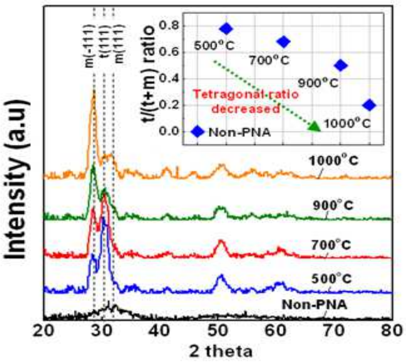

Figure 4. XRD spectra of samples for ALD $HfZrO_2$ after different annealing temperature with N_2 ambient. The insert of Fig. 4. shows the ratio of tetragonal peak intensity height to the sum of tetragonal and monoclinic peak intensity heights of the studied $HfZrO_2$ samples.

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