A Study on the Microstructures and Electric Properties of ZrO₂ Thin Films

SeokWoo Nam 1,2, JungHo Yoo 1, HaeYoung Kim 1, DaeHong Ko 1 and CheolWoong Yang 1
1Department of Ceramic Engineering, Yonsei University, 134 Shinchon-Dong, Sudaemoon-Ku, Seoul 120-749, Korea
Phone: +82-2-361-2854 Fax: +82-2-365-5882 e-mail: sswnam@unist.ac.kr
INTRODUCTION
Because of high gate leakage currents, a sub-20Å SiO₂ cannot be used as the gate dielectric of CMOS devices [1]. Gate dielectric materials having high dielectric constant, large bandgap, good thermal stability are required for replacing SiO₂. Materials such as Si₃N₄, Si₁₋ₓNₓOₓ, SiO₂, Si₃N₄/SiO₂ stack, Y₂O₃ and Al₂O₃ do not have enough dielectric constant [2]. And materials having higher dielectric constant such as Ta₂O₅, TiO₂, STO and BST are thermodynamically unstable when directly contacted with silicon [3]. Among the alternative materials as the gate dielectric, ZrO₂ has a dielectric constant of ~25 and good thermal stability. In this study, we investigated the microstructures and electrical properties of ZrO₂ thin films deposited by reactive dc magnetron sputtering method.

EXPERIMENTALS
ZrO₂ films were deposited on p-type (100) Si wafers by reactive dc magnetron sputtering method from Zr target with 99.9% purity in Ar+O₂ gas ambient. The sputtering was done at different conditions (substrate temperatures of RT~300°C, powers of 100W~400W) and followed by a high temperature anneal (450°C~850°C) in O₂ or N₂ ambient. Aluminium was used as the top electrode for MOSCAP. Microstructures were analyzed by XRD, RBS, XPS, AFM, TEM and electrical properties were performed using an HP4284A and HP4145B.

RESULT AND DISCUSSION
Fig.1 shows the deposition rate and the refractive index of as-deposited ZrO₂ thin films with powers. ZrO₂ films have a higher deposition rate and a higher refractive index with the increase of power. It is well known that the dense films have a higher refractive index. In Fig.2, the RBS spectra show that the composition of thin film deposited at room temperature at power of 300W on Si substrate is stoichiometrically ZrO₂. The ZrO₂ thin film deposited at RT is amorphous and the films deposited at higher temperatures have a crystalline structure with monoclinic (Fig.3). The ZrO₂ films deposited at a higher power also have monoclinic phases (fig.4). The AFM images show the RMS roughness of ZrO₂ thin film as-deposited at the temperature of 300°C at the power of 100W and 300W, respectively. The film deposited at 300W has a higher rms value of surface roughness than that of the film deposited at 100W (Fig.5). Fig.6 shows a cross-sectional TEM micrograph of ZrO₂ thin film deposited at room temperature at the power of 200W after furnace annealing at 750°C for 30 minute in N₂ and O₂ ambient, respectively. The as-deposited ZrO₂ film is amorphous. After annealing the film becomes polycrystalline with (111) monoclinic phases. In the case of annealing in N₂ ambient, the interfacial oxide layer between the ZrO₂ and Si substrate has a 15-20Å thickness. This amorphous oxide layer of interface is formed by rapid oxidation in Ar+O₂ ambient before sputtering. After the ZrO₂ thin film was annealed in O₂ ambient at 750°C for 30min, an interfacial oxide layer of ~30Å was observed. The final film consists of polycrystalline with (111) monoclinic phases. The leakage current decreases with the densification by N₂ annealing and the effect by O₂ annealing. The effect of O₂ annealing can be explained by the additional oxide of ~13 Å in the interface oxide layer. The thickness of the interfacial oxide layer as a conduction barrier depends upon the time and temperature of oxygen annealing.

CONCLUSION
The ZrO₂ film is stoichiometrically deposited by dc magnetron sputtering method. When the ZrO₂ thin films were deposited at the room temperature, they were amorphous, but were polycrystalline with monoclinic phases at the higher temperature and power. The film deposited at higher power has a higher Cmax. Also by annealing, the decreases of the leakage current were observed.

REFERENCE