

Title	Investigation of Ferroelectricity in Sputtered Y-doped HfO ₂ Thin Films
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Abstract

Usually HfO_2 is a dielectric material with high static dielectric constant (K) around 25. But, recently it has been found that HfO_2 thin films show ferroelectricity when they are doped with suitable amount of certain materials (Si, Y, Al etc.). Study shows that at room temperature HfO_2 crystallizes into the monoclinic phase ($P2_1/c$), but at higher or elevated temperatures it is transformed into tetragonal and then cubic phases. Doping HfO_2 thin films with suitable amount of dopant can cause the films to crystallize and stabilize in these other phases at significantly lower annealing temperatures. The previous study also shows that the origin of this ferroelectricity HfO_2 thin films was attributed to a non-centrosymmetric orthorhombic phase transition of space group $Pbc2_1$. There are various methods for fabricating ferroelectric HfO_2 thin films such as solution process, atomic layer deposition (ALD), pulsed laser deposition (PLD) etc. But sputtering method for fabricating ferroelectric HfO_2 is not investigated deeply yet. It is thought that sputtering would be the most suitable method for fabricating ferroelectric HfO_2 as sputtering is the most adopted method in the industries. Therefore, main purpose this study was to find the suitable condition for fabricating ferroelectric HfO_2 thin films and effect of changing the deposition conditions on the ferroelectric properties.

The complete metal insulator metal (MIM) structures with Y-doped HfO_2 (2 and 7 percent doping concentration) as the insulating material were fabricated by ac magnetron sputtering method on SiO_2 substrates. As the material of bottom and top electrodes of the MIM structures, Mo, Pt and TiN were tested. Also, the deposition conditions (Oxygen content, Substrate heating temperature) of Y-doped HfO_2 thin films were changed during the experiment. The change in the polarization vs electrical characteristics with the change in the above parameters are mainly investigated in this study.

The P-E Characteristics of the Samples with the structure Mo/ HfO_2 /Pt or Mo/ HfO_2 /TiN/ SiO_2 could not be measured. It is because the Mo oxidized when they were annealed in the air. After that the samples with more stable material (TiN/ HfO_2 /Pt) was also tested. But the mentioned material show remnant polarization, P_r around $8 \mu\text{C}/\text{cm}^2$ at lower temperatures (without annealing) and show P_r around $30 \mu\text{C}/\text{cm}^2$ at little bit elevated annealed temperature (around 400°C). In this case if the annealing temperature is increased further the

samples were destroyed. It is to mention that the P-E characteristics of those materials were asymmetric. The symmetric P-E characteristics with moderate remnant polarization was obtained when MIM structure was TiN/HfO₂/TiN/SiO₂/Si. But the study shows that the higher remnant polarization with lower leakage current was obtained when the leakage current of as deposited samples was lower (as the leakage current depends on crystalline quality). Therefore, we can conclude from our experiment that we might obtain a ferroelectric HfO₂ thin films with higher remnant polarization if we chose symmetric electrode with suitable thermal expansion co-efficient, with better thermal stability (can avoid oxidation during and after annealing) and lower surface roughness.