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Metal Electrode-induced Phase Uniformity on $Hf_{0.5}Zr_{0.5}O_2$ Thin Film

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Abstract

High-*k* gate oxides like $Hf_xZr_{1-x}O_2$ (HZO) have been the workhorse for the semiconductor industry in the last decades. The compatible fabrication process to MOSFET and room temperature ferroelectricity make HZO a long-time candidate for the high-*k* dielectric in NCFET. In the course of HZO development, it was found that for thin layers in the range of several nano-meters the ferroelectric phase becomes delicate. Phase determination in HZO used to rely on cross-comparison between x-ray diffraction (XRD) and polarization-electric (*P*-*E*) measurements. In this work, we develop a methodology for determining phase homogeneity and quantification based on X-ray absorption fine structure (XAFS). We established theoretical XAFS spectra of possible phases separately. By choosing different incident energy and scanning, the fluorescence on each spatial point can be detected. Through modified linear combination fitting, the phase composition can be obtained. Based on XAS mapping result, the ferroelectric property can be tuned by capping electrodes, TiN/TaN/Mo. The scanning phase composition shows good match to the P-E loops and XRD results. In conclusion, this method served a powerful way for probing phase homogeneity of HZO. Spatial mapping of the phase distribution would facilitate the device optimization as it establishes a bridge correlating HZO's microscopic and macroscopic properties.