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Electronic and Optical Properties of amorphous and crystalline Zirconium Oxide Thin Films on Si (100)

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ZrO_2 thin films as gate dielectrics have been proposed to overcome the problems of tunneling current and mobility degradation in achieving a thin equivalent oxide thickness.

The atomic structure of amorphous and crystalline zirconium oxide (ZrO_2) gate dielectrics thin films grown on Si (100) by mean of atomic layer deposition method was examined by using *Zr-K* edge X-ray absorption spectroscopy. EXAFS spectra show the ordered bonding of Zr–Zr for c-ZrO_2, but not for a-ZrO_2 thin film.

The electronic and optical properties were obtained by using X-ray photoelectron spectroscopy and reflection electron energy loss spectroscopy (REELS). The band gap of ZrO_2 thin films was 3.50±0.1 eV, which does not depend on atomic structure. The optical properties of ZrO_2 thin films were obtained from the experimental inelastic scattering cross section of REELS spectra. The optical properties, represented by the index of refraction (n), extinction coefficient (k) and dielectric function (ε), were obtained from REELS spectra by using QUEELS-$\varepsilon(k, \omega)$-REELS software package. The energy- dependent behaviors of reflection, absorption or transparency in ZrO_2 thin films were also determined from the optical properties. The difference between amorphous and crystalline ZrO_2thin films in optical property could not be observed.

Keywords: REELS; optical properties, EXAFS, and XPS