Band alignment and optical properties of $(\text{ZrO}_2)_{0.66}(\text{HfO}_2)_{0.34}$ gate dielectrics thin films on $p$-Si (100)


S. Heo, J. G. Chung, and J. C. Lee

1Department of Physics, Chungbuk National University, Cheongju, 361-763 Korea.
2Analytical Engineering Center, Samsung Advanced Institute of Technology, Suwon, 440-600, Korea

$(\text{ZrO}_2)_{0.66}(\text{HfO}_2)_{0.34}$ thin films as gate dielectrics have been proposed to overcome the problems of tunneling current and degradation mobility in achieving a thin equivalent oxide thickness. An extremely thin SiO$_2$ layer is used in order to separate the carrier in MOSFET channel from the dielectric field fluctuation caused by phonons in the dielectric which decreases the carrier mobility. The electronic and optical properties influenced the device performance to a great extent. $(\text{ZrO}_2)_{0.66}(\text{HfO}_2)_{0.34}$ dielectric films on $p$-Si (100) were grown by atomic layer deposition method, for which the conduction band offsets, valence band offsets and band gaps were obtained by using X-ray photoelectron spectroscopy and reflection electron energy loss spectroscopy. The band gap, valence and conduction band offset values for $(\text{ZrO}_2)_{0.66}(\text{HfO}_2)_{0.34}$ dielectric thin film, grown on Si substrate were about 5.34, 2.35 and 1.87 eV respectively. This band alignment was similar to that of ZrO$_2$. In addition, The dielectric function $\varepsilon(k,\omega)$, index of refraction $n$ and the extinction coefficient $k$ for the $(\text{ZrO}_2)_{0.66}(\text{HfO}_2)_{0.34}$ thin films were obtained from a quantitative analysis of REELS data by comparison to detailed dielectric response model calculations using the QUEELS-$\varepsilon(k,\omega)$-REELS software package. These optical properties are similar with ZrO$_2$ dielectric thin films.

Keywords: REELS; optical properties, and XPS