

Crystal Phases and Electro-Optic Properties of ZrO₂ and HfO₂ Ferroelectric Thin Films

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Abstract :

The ferroelectricity in ZrO₂ and HfO₂ oxides was discovered in 2011 in ultrathin layers and has garnered significant attention for its potential applications in microelectronics. These materials offer the advantage of maintaining ferroelectric properties even at thicknesses below 10 nm, which is considerably thinner than perovskite ferroelectrics. Additionally, they are compatible with silicon and can be readily integrated into silicon foundries. As non-centrosymmetric crystals, ZrO₂ and HfO₂ ferroelectrics are expected to exhibit an even nonlinear response, characterized by nonlinear susceptibility terms such as $\chi^{(2)}$. Based on this effect, these materials can also be explored for electro-optic applications in silicon photonics. However, the low thickness that is advantageous for microelectronic applications becomes a drawback for photonic ones. Therefore, the initial challenge is to increase the thickness of ZrO₂/HfO₂ ferroelectric thin films to approximately 50 nm to make them suitable for photonic devices. Our research demonstrates that pure ZrO₂ can maintain a ferroelectric state at a higher thickness compared to HfO₂, reaching approximately 40 nm (versus 10 nm in HfO₂). Moreover, through first-principle calculations, we demonstrate that ZrO₂ exhibits higher electro-optic (EO) coefficients compared to HfO₂, making ZrO₂-based ferroelectrics an attractive candidate for further research to optimize them for electro-optic applications.

