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Interfacial Characterization and Transport Conduction Mechanisms in Al|HfO_2|p-Ge Structures: Energy Band Diagram

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Ge-based metal-oxide semiconductor structures exhibiting thin ALD-grown high-k dielectric HfO_2 films were fabricated and characterized chemically, structurally, and electrically. X-ray photoelectron (XP) spectroscopy confirms the good stoichiometry of the ALD-grown HfO_2 films. Furthermore, through the analysis of the XP spectra, the conduction and valence band offsets of $HfO_2|p$-Ge were calculated to be equal to 1.8 ± 0.2 eV and 2.8 ± 0.2 eV, respectively. $C(V)$ and $G(V)$ analysis reveals structures with a well-defined MOS behavior with D_{it} values in the range of $10^{11}\,eV^{-1}cm^{-2}$ and a dielectric constant of HfO_2 films of 20. The dominant carrier transport conduction mechanisms were studied through $J(V)$ analysis, performed at both substrate and gate electron injection. Specifically, in the low voltage region ($V < 0.2$ V), the prevailing conduction mechanism is Ohmic, with an activation energy of 0.28 eV for both substrate and gate electron injection. In the voltage range $0.4-1.5$ V, the dominant conduction mechanism is Frenkel–Poole, through which the trap energy level into HfO_2 films (φ_t) is calculated to be $\varphi_t = 0.36$ eV. Schottky conduction mechanism is the prevailing one, for high applied bias voltages ($V > 3.0$ V) and high temperatures (> 450 K). Applying Schottky's emission model the energy barrier heights of $HfO_2|p$-Ge and Al|HfO_2 interfaces were evaluated equal to 1.7 ± 0.2 eV and 1.3 ± 0.2 eV, respectively. Combining the XPS and $J(V)$ analysis results, the energy band diagram of Al|HfO_2|p-Ge structures is constructed. The calculated values of conduction and valence band offsets via XPS and $J(V)$ measurements are in very good agreement.

Keywords: ALD HfO_2, p-Ge, XPS, conductivity mechanisms, energy band diagram.

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