Atomic, electronic structure and charge transport in amorphous ZrO_2 and HfO_2 films

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Atomic and electronic structure of sputtered ZrO_2 and HfO_2 were studied by X-ray diffraction, extended X-ray absorption fine structure (EXAFS) spectroscopy using synchrotron radiation, photoemission and electron energy loss spectroscopy. Sputtered films were amorphous. The mean Zr-O distance estimated from EXAFS was 2.15 Å. After annealing in air at 800°C the tetragonal phase was detected by X-ray diffraction. Valence band of amorphous ZrO_2 and HfO_2 consists of two sub-bands separated with ionic gap. The lower sub-band is composed mainly with O 2s states, the top valence sub-band consists of O 2p and Zr, Hf 4d, Zr 5s bonding states. The ZrO_2 valance band top position determined by ultraviolet photoemission spectroscopy is located 7.5 eV from vacuum level. The current in amorphous ZrO_2 and HfO_2 exponentially grows with increasing of electric field and temperature. Two possible mechanism of charge transport discussed: Pool-Frenkel effect and multi-phonon trap ionization.

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