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Electronic States of Hafnium and Vanadium oxide in Silicon Gate Stack Structure CHIYU ZHU, FU TANG, XIN LIU, Arizona State University, JIALING YANG, ROBERT NEMANICH, Arizona State University — Vanadium oxide (VO_2) is a narrow band gap material with a metal-insulator transition (MIT) at less than 100C. Hafnium oxide (HfO_2) is currently the preferred high-k material for gate dielectrics. To utilize VO_2 in a charge storage device, it is necessary to understand the band relationships between VO_2, HfO_2, and Si substrate. In this study, a 2nm thick VO_2 layer is embedded in a dielectric stack structure between an oxidized n-type Si(100) surface and a 2nm HfO_2 layer. The in situ experiments are carried out in an UHV multi-chamber system. After each growth step, the surface is characterized using XPS and UPS. After the initial plasma cleaning and oxidation treatment the Si substrate displayed essentially flat bands at the surface. After deposition of the VO_2 layer, the Si 2p peak shifted to lower binding energy, and the Si 2p associated with the SiO_2 layer also was shifted, indicating an internal field in the SiO_2. The VO_2 valence band maximum (VBM) was identified at 0.6 eV below the Fermi level (E_F). This ultra thin VO_2 exhibits the metal-insulator transition at a temperature higher than thicker films. As a comparison, a 100nm thick film of VO_2 on Si showed a MIT at 60C. After the HfO_2 deposition, the Si 2p substrate feature returned to the initial value indicating a return to flat band conditions. The UPS indicated the VBM of HfO_2 at 4.0 eV below E_F. This work is supported by the NSF (DMR-0805353).

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