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XPS measurements of interface dipole switching at the a-Al₂O₃/Si interface STEPHANIE FERNANDEZ-PENA, Geneva University, D.P. KUMAR, Yale University, Z. ZHANG, Argonne National Laboratory, A.M. KOLPAK, MIT, S. ISMAIL-BEIGI, C.H. AHN, F.J. WALKER, Yale University — In this work, we describe work on polarization switching at a high-k oxide-silicon interface. The procedure involves inserting a monolayer (ML) of ZrO₂ in-between an amorphous-Al₂O₃ and Si. Theoretical calculations using density functional theory (DFT) predict that the ZrO₂ should display two stable configurations of the polarization. Deposition of the ZrO₂ in UHV is used to avoid SiO₂ formation. The device is transferred in vacuum and the interface chemistry analyzed using x-ray photoelectron spectroscopy (XPS) to determine the oxidation state of the Si. When the ZrO₂ is in direct contact with the Si, chemical shifts as large as 0.58 [eV] are observed, implying a polar interface. In addition, XPS measurements on devices under applied voltage, along with electron transport measurements, show a switching of the interface dipole of 0.25 [eV]. These voltage dependent XPS results are consistent with the magnitude and direction of hysteresis loops observed in Capacitance-Voltage measurements. Finally, the microscopic structure has been investigated using extended x-ray absorption fine structure (EXAFS) at the Zr K-edge. The results are compared to DFT-calculated atomic positions.

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