X-Ray Photoelectron Spectroscopy Analysis of Electronic Band Structure for MIM capacitor interfaces

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Abstract

Metal-Insulator-Metal (MIM) capacitors play a crucial role in many applications including dynamic random access memories (DRAM), radiofrequency and analog circuits, and high power microprocessor units. For the DRAM applications, the understanding of the electronic band structure of the interface between the high-k dielectric and metal is crucial to design an effective strategy to control the leakage current. Future DRAM MIM capacitors aim at an increasingly thinner oxide layer with equivalent oxide thicknesses below 0.5 nm [1], posing challenges in probing interfacial properties using conventional metrology methods.

In this work, we report an entirely XPS-based workflow to determine the interfacial band structure of TiN/ZrO_2/TiN stacks. The TiN/ZrO_2/TiN stacks were deposited on Si substrates by magnetron sputtering of TiN and atomic layer deposition of ZrO_2. XPS is a surface-sensitive technique, probing only the top 6-10 nm of the material being analyzed. Conventionally, XPS is used to analyze the composition, chemical states, and valence band structures of materials. In our case, we also employ XPS to determine the work function of TiN via cut-off energy measurement and the bandgap of the ultrathin ZrO_2 layer via examining the onset of energy loss in O1s core-level spectra [2]. An electronic band model of the interface is proposed based on the combined analyses, allowing us to determine barrier height and providing insight into the potential leakage of the stack.

[1] S. Y. Lee et al., Appl. Phys. Lett. 105 (2014) 201603

[2] M. T. Nichols et al., J. Appl. Phys. 115 (2014) 094105

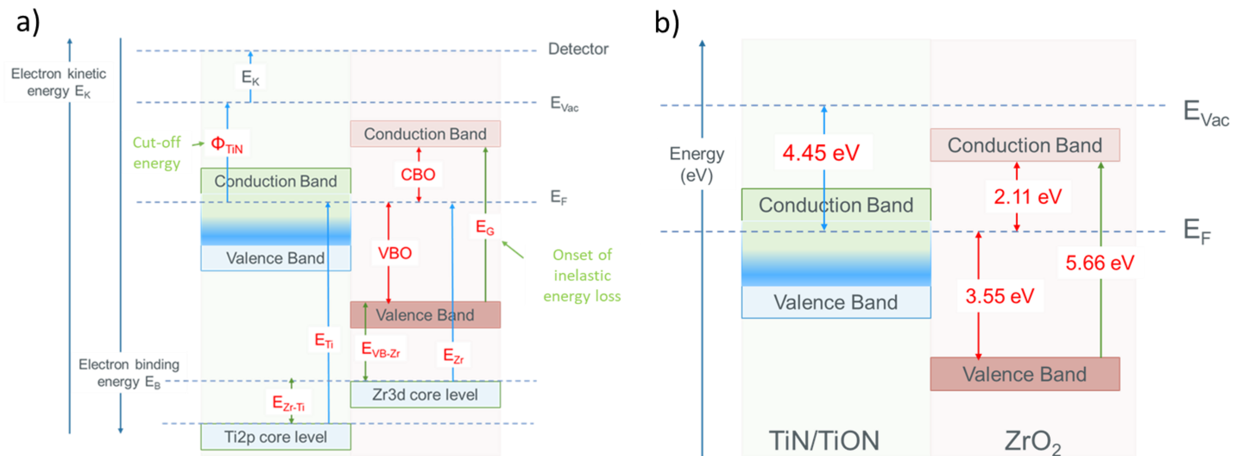

Figure 1. (a) XPS analysis workflow and (b) proposed band structure model for the TiN/ZrO_2 interface.