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Resonant photo-ionization of charged oxygen vacancy defects in Si/SiO2/HfO2 film stacks observed by second-harmonic generation. J. PRICE, M. C. DOWNER, University of Texas, Austin — The semiconductor industry recently achieved a historic milestone with the introduction of high-k gate dielectrics. However, much effort continues to focus on characterizing defects in these materials that promote charge trapping. Using internal multi-photon photoemission (IMPE) and time-dependent electrostatic field-induced second harmonic (TD-EFISH) generation, we probe the charge trapping kinetics in Si/SiO2/HfO2 gate stacks. During IMPE charging, the TD-EFISH response of the HfO2 film uniquely increases and then decreases when irradiated at the characteristic three-photon energy of 4.71 eV. The decrease in TD-EFISH is explained by resonant three-photon excitation of HfO2-induced negatively charged oxygen vacancy defects in the SiO2 interfacial layer, and subsequent removal of its negative charge by tunneling to the Si substrate. This interpretation is supported by spectroscopic ellipsometry and electron spin resonance measurements, and ab initio calculations, which identify the 4.71 eV transition with this defect. Photo-ionization of this defect also explains hysteresis in the TD-EFISH response when charges trapped at the surface are quenched between successive IMPE charging cycles. The results demonstrate that second harmonic generation can potentially be used as an in situ, real time monitor of charge trapping kinetics prior to device fabrication.

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