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Atomic-level imaging and properties of stray Hf atoms in Si-SiO_2-HfO_2 nanoscale structures.[1]

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The aberration-corrected scanning transmission electron microscope (STEM) provides a new level of sensitivity for analyzing nanoscale oxide films. The sub-Ångstrom probe provides much improved resolution, but equally important, greatly increased sensitivity to individual atoms. Single Hf atoms are visible within the nanometer thick SiO_2 interlayer between a HfO_2 dielectric and the Si substrate. Furthermore, the depth of focus of the aberration-corrected STEM is greatly reduced, and Hf atoms can be located in depth to better than 1 nm precision. Strikingly, no Hf atoms are seen to be in contact with the Si substrate, and exhibit preferred distances from the interface. First-principles density-functional calculations find that the energy of single Hf atoms rises sharply if they approach closer than $\sim$0.3 nm, in agreement with observations. The Hf atoms introduce localized states within the Si band gap, which are detected by electron energy loss spectroscopy. These states may mediate leakage currents. The effect of the stray Hf atoms on the electron mobility in the Si channel has been calculated using a novel first-principles approach and found to be consistent with measured mobility values. Work performed in collaboration with K. van Benthem, S. N. Rashkeev, M. H. Evans, and S. T. Pantelides.

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