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### **3D Location of Single Hf Atoms at a Si/SiO<sub>2</sub>/HfO<sub>2</sub>/p-Si Gate Dielectric**

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## 3D location of single Hf atoms at a Si/SiO<sub>2</sub>/HfO<sub>2</sub>/p-Si gate dielectric

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The three-dimensional location of single atoms has recently been addressed to be the main issue for controlling properties and life-times of semi-conductor devices (for instance field-effect transistors) due to a segregation or pinning of dopant atoms at the Si/dielectric interfaces.

Aberration-corrected scanning transmission electron microscopy (STEM) is an ideal tool to study the atomic and electronic structure as well as the segregation behavior at semiconductor hetero-structures with unprecedented detail and a laterally resolution of 0.61 Angstroms has recently been achieved. To gain 3D information about the single Hf atom distribution at the Si/SiO<sub>2</sub>/HfO<sub>2</sub> interface a through-focus series technique was applied for recording high-angle annular dark-field images in a VG HB603 U dedicated STEM. The usage of rather large convergence angles (20 to 30 mrad) provides a limited depth of focus, and, therefore, a spatial resolution of around 1-3 nm parallel to the optical axis. Additional 3D reconstruction techniques, such as deconvolution of the recorded image stacks with a three-dimensional point-spread function, were used to enhance the accuracy in determining the vertical atom positions. As a result, single Hf atoms can be located with an accuracy of 0.61 Angstroms laterally, and better than 1 nm vertically.

It was possible to locate single Hf atoms at various depths within the SiO<sub>2</sub> layer of 1 nm thickness, located between the single crystalline silicon substrate and the poly-crystalline HfO<sub>2</sub> film. Reconstructed data sets show that Hf atoms are randomly distributed within the volume of the SiO<sub>2</sub> layer. A preferred segregation of Hf atoms to the Si/SiO<sub>2</sub> surface was not observed.

Complementary, atomically resolved electron energy loss spectroscopy allows study of the electronic structure of the interface. Preliminary studies of the Si L-2,3 and Hf O<sub>2,3</sub> edges across the interfaces will be shown.