Characterization of ultrathin ferroelectric oxide films using X-ray photoelectron spectroscopy

Popular science abstract

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Increasing the operational speed of computers, while decreasing their energy dissipation with regard to the fast growing use of artificial intelligence in a broad range of applications, forms one of the main motivations for research in the field of low power computation. The main components of a computer, known as transistors, have undergone extensive optimization over time. Generally, they come in slightly different variations, but nowadays the CMOS-type is the one most in use. CMOS stands for the complementary metal oxide semiconductor setup of the devices representing its three layers from top to bottom.

Transistors can be compared to small switches controlling the current flow within the central processing unit (CPU) of the computer. The voltage applied on the metal top contact determines a possible charge flow through the semiconductor substrate and the oxide layer serves as an insulating layer preventing any charge exchange between the top contact and the substrate. The insulating layer is commonly made of doped HfO_2. Transistors are also found in the memory units located separately to the CPU. The retrieval of data between these units is limiting the computational speed and consumes additional power.

A new direction of research in the field has developed dedicated to designing so called neuromorphic computational systems. As the word neuro suggests, this method resembles the operation mode of a brain; the memory and computational modules are combined into one common network removing long paths of data retrieval. One way of designing such systems is to extend the transistors to still follow the CMOS structure, but with an oxide layer that shows to have ferroelectric characteristics.

Ferroelectricity might remind you of the phenomenon of ferromagnetism, which refers to permanent magnets that remain stable after adapting a spontaneous magnetization state and whose orientation of poles can be reversed through a strong enough, external magnetic field. The resemblance in names is not a coincidence. Ferroelectricty refers to the adaption of a spontaneous polarization in a material leading to a net electric dipole moment and the possibility to reverse the orientation. This property is due to the adaption of certain crystal structures of the material. Similarly to the phenomenon in magnetism, the orientation can be reversed by an external electric field. In the final devices the two polarization states represent a 0 and 1 signal as used in binary code and each insulating dielectric can be turned into a memory unit cell located within the CPU.

Luckily in the material of HfO_2, which has been used as the insulating dielectric for quite some time now, a phase transition can be induced through high temperatures, such that the atomic arrangement changes into a ferroelectric structure. However, a commercialization of these new transistor models has so far been prevented by a lingering device performance. he high temperatures needed for obtaining a ferroelectric structure during the fabrication can cause unwanted side effects affecting the elemental composition of the layers and the quality of the interface.

The aim of this work was to improve understanding of what thermal conditions are necessary to induce the required phase change and what side effects are being induced along with the thermal annealing. Two sample structures were analyzed through data produced by a hard X-ray photoelectron spectroscopy experiment and an X-ray absorption spectroscopy one. The first method was used to track changes in the electronic structure in the samples and the second to visualize changes in the atomic arrangement of the samples. The results have shown how the phase transition was successfully induced to a very clearly ordered atomic arrangement pointing to the formation of the ferroelectric structure. This alteration on the atomic scale was preserved even after the heating. The electronic structure was observed to change at the same temperatures as evident from the electrons detected. The electronic structure determines how tightly electrons are bound to their corresponding nuclei, or in other words how much energy they have. One could observe how in both samples the energy shifted first to lower values and suddenly increased to even higher values compared to the initial conditions at the transition temperature.