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Editorial: Advanced characterization methods for HfO_2/ZrO_2-based ferroelectrics

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Editorial on the Research Topic
Advanced characterization methods for HfO_2/ZrO_2-based ferroelectrics

Ferroelectric HfO_2 and ZrO_2-based materials are unconventional ferroelectrics compared to historically dominant perovskite-based ferroelectrics. These differences from conventional perovskite ferroelectrics are distinctly seen in HfO_2-ZrO_2's fluorite-based structure that exhibits a rich polymorphism of competing crystal phases, enhanced ferroelectric behavior when scaling film thicknesses down to 10 nm and below, and a one order of magnitude lower relative permittivity and higher coercive field. Both the complex interplay of the fluorite crystal phases, as well as the intrinsic material and/or ferroelectric properties associated with them, have made ferroelectric HfO_2-ZrO_2-based ferroelectrics simultaneously challenging and interesting to characterize. Due in strong part to the nanoscale thicknesses of these fluorite-based ferroelectric films, the device behavior is an inseparable combination of the ferroelectric film properties (i.e., structure, crystalline orientation, grain size) and the material stack structure that encapsulates it into a two or three terminal device (i.e., interfaces, dielectric layers, electrode materials). Each article comprising this Research Topic on advanced characterization methods for HfO_2/ZrO_2-based ferroelectric illustrates different ways in which the intrinsic material properties or the ferroelectric film's interaction with the device stack can be characterized to gain physical insight into this unconventional ferroelectric material system.

Surface energy effects and grain size are often attributed to the predominant stabilization of either the non-polar tetragonal, monoclinic, or the polar orthorhombic phases in polycrystalline HfO_2–ZrO_2 films. It is generally observed that the polar orthorhombic phase is stabilized somewhere between the non-polar tetragonal and monoclinic phase boundaries, and that these non-polar phases are very sensitive to grain size in both HfO_2 and ZrO_2. Since the preferred crystal phase-dependence on grain size can be sensitive to stoichiometry (for instance, in $Hf_{1-x}Zr_xO_2$ or Si-doped HfO_2), it can be anticipated that there may be a complex interplay between grain-size engineering and ferroelectric film composition. In "Effect of Al_2O_3 interlayers on the microstructure and electrical response of ferroelectric doped HfO_2 thin films" by Lederer et al., the grain-size and composition dependence of ferroelectric $Hf_{1-x}Zr_xO_2$ and Si-doped HfO_2 is investigated in detail in which 1, 2, and 3 Al_2O_3 interlayers are used to control grain size while adjusting the stoichiometry of the fluorite-structured ferroelectric films. Using a combination of structural techniques, such as grazing-incidence X-ray diffraction and Kikuchi diffraction, as

well as electrical characterization to assess the ferroelectric and electric-field cycling properties, the work strikingly shows how stack engineering can be combined with the rich polymorphism to optimize fluorite-structured films for ferroelectric applications, such as front-of-line integration of $Hf_{1-x}Zr_xO_2$ due to the improved temperature robustness aided by the Al_2O_3 interlayers.

Other types of interlayers are often found in ferroelectric-based devices as either an intentional or unintentional consequence of the fabricated device stack, most frequently as dielectric interfacial layers between a ferroelectric-metal or ferroelectric-semiconductor interface. While the high coercive field of HfO_2-ZrO_2-based ferroelectrics makes it more robust to depolarization fields caused by interfacial dead layers compared to perovskite ferroelectrics, the typical 6–10 nm fluorite ferroelectric film thickness can still lead to large depolarization fields that can impact the ferroelectric behavior. Depolarization effects can lead to poor performance in data retention tests for ferroelectric random access memory (FRAM) capacitors and ferroelectric field effect transistors (FeFETs), and thus pose a considerable reliability challenge. In "Investigating charge trapping in ferroelectric thin films through transient measurements" by Lancaster et al., the loss of remanent polarization as a consequence of interfacial layers of Al_2O_3 in $Hf_{0.5}Zr_{0.5}O_2$ ferroelectric capacitors is presented to assess the competing effects of depolarization and charge trapping at the ferroelectric-dielectric interface. In particular, the dependence of the polarization loss on pulse-width and delay time with a specially designed variant of the positive-up-negative-down (PUND) was proposed as a new technique to better assess the influence of charge injection on polarization loss.

While the ferroelectric-dielectric interface plays an important role in conventional CMOS-based FeFET behavior and reliability, there is interest in making FeFETs out of semiconducting oxide channels that may be suited for neuromorphic computing applications. The electrostatic control of the semiconducting oxide channel and the corresponding high and low resistance states are performance metrics of note for the construction of this class of artificial synapse. In "Physical modeling of HZO-based ferroelectric field-effect transistors with a WOx channel" by Wen et al., simulations are presented that illustrate the potential for using ferroelectric HfO_2-ZrO_2 with a WO_x semiconducting channel to achieve artificial synaptic devices for neural networks. While scaling the ferroelectric film thickness and semiconducting oxide layer thickness were found to enhance the margin between the on and off resistance, a double-gated structure was found to enhance the on/off resistance ratio by a factor of 13 compared to back-gated structures. Thus, the results provide an interesting framework that can help guide the characterization of synaptic-based devices utilizing ferroelectric HfO_2-ZrO_2 and WO_x.

The last article in the Research Topic "Simulation of XRD, Raman and IR spectrum for phase identification in doped HfO_2 and ZrO_2" by Kersch et al., performed *ab initio* simulations of the phases in HfO_2 and ZrO_2 with resulting X-ray diffraction, Raman, and infrared patterns. Since most experimentally reported HfO_2-ZrO_2-based ferroelectric films are polycrystalline and often contain more than one phase, the accurate quantification of the presence of each crystal phase is important to understand the resulting device behavior. However, phase quantification using X-ray diffraction only is extremely difficult in HfO_2 and ZrO_2 polycrystalline films due to the close similarity in the tetragonal and orthorhombic diffraction patterns. The reported Raman and infrared spectroscopy for crystal structures in HfO_2 and ZrO_2 can thus provide important reference patterns that experimentalists can use to more accurately quantify the phase composition in fluorite ferroelectric films.

The articles on grain-size engineering, interfacial effects involving charge trapping and depolarization, conducting oxide transistors with ferroelectric gates, and the *ab initio* simulations of the XRD, Raman, and infrared signatures of the crystalline phases capture a small cross-section of the fascinating complexity of ferroelectric HfO_2 and ZrO_2. This Research Topic on advanced characterization methods for HfO_2/ZrO_2-based ferroelectrics provides important insights into the material and device-level behavior for these unconventional ferroelectric materials.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

Conflict of interest

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