SCIENCE CHINA
Information Sciences

• PERSPECTIVE •

June 2025, Vol. 68, Iss. 6, 160407:1–160407:3
https://doi.org/10.1007/s11432-025-4372-4

Special Topic: Novel Memory Materials and Devices: Ferroelectrics and Oxide Semiconductors

Prospects and challenges of HfO_2-based ferroelectric devices

Shinichi TAKAGI, Mitsuru TAKENAKA* & Kasidit TOPRASERTPONG

Department of Electrical Engineering and Information Systems, The University of Tokyo, Tokyo 113-8656, Japan

Received 21 January 2025/Revised 31 March 2025/Accepted 1 April 2025/Published online 14 May 2025

Citation Takagi S, Takenaka M, Toprasertpong K. Prospects and challenges of HfO_2-based ferroelectric devices. Sci China Inf Sci, 2025, 68(6): 160407, https://doi.org/10.1007/s11432-025-4372-4

Ferroelectric materials are characterized by their ability to exhibit spontaneous electric polarization, which can be reversed by an external electric field. This property has made them indispensable in applications such as non-volatile memories, capacitors, and sensors. Conventional ferroelectrics, such as perovskite oxides (e.g., $Pb(Zr,Ti)O_3$ or PZT), have been widely studied and utilized; however, their integration with advanced semiconductor technology is hindered by issues such as poor thickness scalability and incompatibility with standard CMOS process. Thus, the discovery of doped hafnium oxide (HfO_2)-based ferroelectric films in 2011 by a German group [1] revolutionized the field of ferroelectric materials, paving the way for highly scalable and silicon-compatible ferroelectric devices. The spontaneous polarization in these films originates from the movement of oxygen atoms within an orthorhombic crystal phase characterized by a non-centrosymmetric structure. This phase emerges amidst other possible crystal phases, such as amorphous, monoclinic, and cubic, depending on processing conditions and dopant concentrations. A particularly noteworthy dopant, Zr, enables ferroelectricity in $Hf_{1-x}Zr_xO_2$ (HZO) films across a wide range of compositions, with low and mid-Zr contents favoring ferroelectricity and higher Zr contents inducing antiferroelectric properties due to the tetragonal phase.

Compared to traditional perovskite ferroelectrics like PZT or SBT, which require relatively thick films (50–200 nm) and noble metal electrodes, HfO_2-based materials offer superior scalability. They function effectively at thicknesses below 10 nm and are highly compatible with the Si CMOS platform. HfO_2-based films achieve comparable remanent polarization (P_r) of 10–40 μC/cm^2 at ultrathin thicknesses with easily processed electrodes like TiN. In addition, the easy formation of HfO_2-based films by atomic layer deposition (ALD) enables the integration into 3D trench structures and 3D integration. Notably, polycrystalline HZO films formed by ALD and subsequent annealing have the maximum P_r at the thickness of around 6 nm with maintaining almost constant coercive fields (E_c) of 1–2 MV/cm, though the physical origin of these properties is not clear yet. Another advantage of HfO_2-based ferroelectric films is excellent hydrogen resistance, which cannot be obtained for the perovskite ferroelectrics without requiring a passivation layer. These unique characteristics position HfO_2-based ferroelectrics as promising candidates for highly scaled, energy-efficient, and Si-integrated devices. However, their highly coercive fields introduce reliability concerns.

Typical ferroelectric devices include MFM capacitors for FeRAM, FeFETs, and FTJs, as shown in Figure 1. Those devices have potential applications in memory, logic, and AI (Artificial Intelligence) computations. FeRAM and FeFET memories, in particular, enable low energy write operation due to voltage writing with acceptable read/write speed. FeFETs are also being explored for NAND flash memory for reduction in operation voltage. Additionally, ferroelectric memories are well-suited for AI computing due to their analogue memory function. Neuromorphic architecture and circuits are effective in drastically reducing the AI computation power. The HfO_2-based ferroelectric devices are suitable for hardware to realize such neuromorphic systems on the Si CMOS platform. This article highlights the expectations and challenges of the HfO_2-based ferroelectric devices, focusing on FeRAM and FeFETs for memory and AI applications.

High-density FeRAM has been demonstrated by many companies and research institutes. A key challenge is achieving MFM capacitors with high polarization, high reliability, sufficient retention time, and low voltage operation, while maintaining a low thermal budget compatible with back-end processes. Among these factors, write/read endurance is the most crucial issue, requiring innovative strategies to extend cycling capabilities. We have demonstrated that the HZO thickness scaling enables low voltage operation and improves endurance caused by HZO film breakdown. This improvement is attributed to the reduction in energy of hot electrons generated during write/read operations [2]. However, we have also found the trade-offs between HZO thickness, annealing temperature, and wake-up properties. For instance, thinning HZO to 4 nm significantly lowers operating voltage but increases crystallization temperature and worsens wake-up behavior.

Another challenge is fatigue of polarization and imprint-

* Corresponding author (email: takagi@ee.t.u-tokyo.ac.jp)

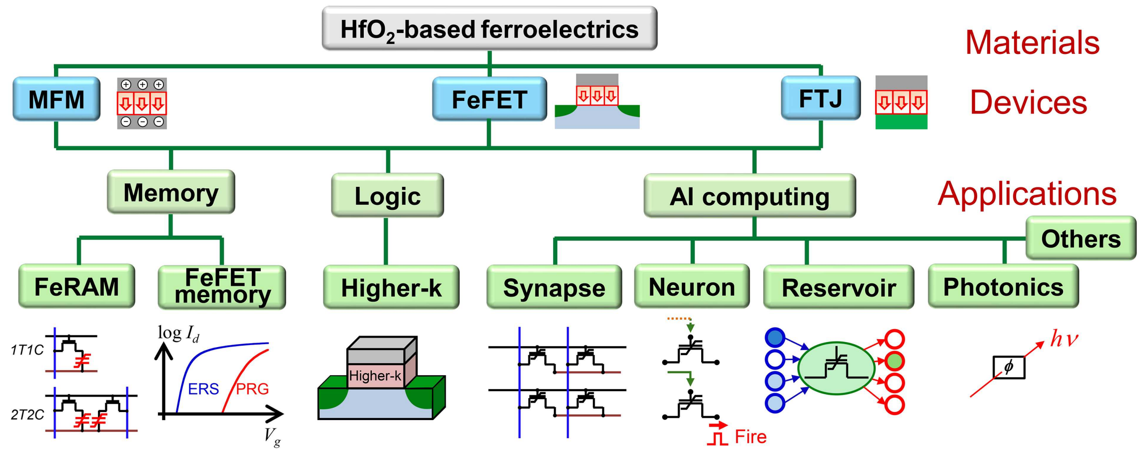

Figure 1 (Color online) A variety of applications of HfO_2-based ferroelectric materials and devices.

induced retention loss. Operating at low electric fields gradually reduces the $2P_r$ value over cycling, which is a failure mode known as fatigue. Interestingly, this fatigue can be recovered by applying a higher operating voltage, suggesting that this degradation is not permanent. Additionally, imprint effects in HfO_2-based ferroelectrics cause a continuous shift in P-V characteristics in the standby state, leading to retention degradation of the opposite state [3]. These instabilities such as fatigue, imprint, and recovery of polarization are well explained by domain pinning under multi-domain switching, local charge trapping/de-trapping at defect sites, and diffusion of charged defects. However, a universal and quantitative model to represent these instabilities has not been established yet. Such a model is crucial for improving the reliability of FeRAM. The optimization of metal electrodes, doping into HZO films, and annealing conditions can also be expected to solve the reliability issues.

HfO_2-based FeFETs hold a great promise for low-voltage and low-power non-volatile memory applications. This is because the electric field applied to the ferroelectric film is used for writing, enabling non-destructive readout at low voltage. Recently, NAND flash memory cell structures based on HfO_2-based ferroelectric FeFETs, where the charge trap layer is replaced by a ferroelectric film, have been widely studied [4]. This is one of the most promising near-term applications of FeFETs. Here, a charge trap layer and an interfacial layer are often inserted between the gate electrode and the ferroelectric films to increase the memory window. Proper gate stack design is critical to balancing memory window, retention, and fatigue.

A simple FeFET composed of metal-ferroelectric-interfacial layer-semiconductor (MFIS) structures is also promising for non-volatile memory embedded with logic circuits. However, a large density of carrier traps strongly affects the memory operation and reliability [5, 6], leading to a reduction in the memory window and a long read-delay-time after the write operation. FeFETs have two aspects in the memory operation: polarization switching memory function and trap memory function, both of which compete in terms of a memory window. Electrons and holes repeat trapping into and de-trapping from these traps during the program and erase operation. As a result, the memory window narrowing with increasing cycle number is caused by the generation of such electron and hole traps during cycling [7]. The physical picture of these traps is still not well understood, but they are believed to be located at or near the ferroelectric/interfacial layer interface. Thus, interfacial layer engineering to suppress trap generation is essential for improving endurance due to memory window narrowing. From this viewpoint, strong attention has recently been paid to oxide semiconductor channel (OS) FeFETs due to their potential to eliminate interfacial layers. However, the interface properties between OS and HfO_2-based ferroelectrics are complicated and must be carefully optimized for reliable FeFET operation.

Interestingly, a high density of electron traps in Si FeFETs can also have positive effects on memory characteristics. These traps increase the electric field across ferroelectrics, resulting in trap-assisted polarization switching [8] and a reduction in the depolarization field during the hold condition [9]. Beyond identifying the physical nature of traps in the gate stack of FeFETs, it is crucial to establish trap-property-aware optimized device operation to achieve well-balanced memory characteristics. For future research on HZO memory devices, in addition to further optimization of HZO film quality and a better understanding of trap properties and trap generation mechanisms, studies on the impact of polycrystalline HZO structures on the ferroelectric behavior of small-size HZO films and devices are essential.

FeFETs are also attractive for AI computing due to the analog memory behavior. The explosive increase in the energy demand of AI computation is a serious challenge, making the hardwareization of AI computation an urgent issue for the future widespread use of AI technologies. FeFETs with multiple localized polarization domains exhibit analog memory characteristics, making them suitable as artificial synapses. Polarization reversal of small-area FeFETs occurs through a "polarization domain nucleation" process [10], enabling accumulative and stochastic behavior similar to artificial neurons. The analog memory function leads to the application to synaptic weights in the cross-bar array for deep neural network (DNN) calculations. FeFETs benefit from symmetry and high-speed weight updates. Also, the neuron-like and stochastic firing functions, and the spike timing dependent plasticity (STDP) function in FeFETs can be utilized for spiking neural network (SNN) calculations. Several demonstrations have shown the feasibility of FeFETs in these AI architectures. Another exciting direction is integrating FeFETs with Si photonic integrated circuits (PIC), using optical phase shifters for reconfiguring AI computing [11].

Beyond direct AI applications, we have proposed and experimentally demonstrated a Si-CMOS-compatible physical reservoir computing scheme using HZO/Si FeFETs [12]. This method exploits the transient current response of Si FeFETs as virtual nodes in AI calculations. We have successfully applied this approach to nonlinear time-series prediction and speech recognition. We have experimentally shown an accuracy of 98.1% for classifying the audio waveforms of '0' to '9' spoken digits. This FeFET-based reservoir computing approach holds great potential for future AI applications by combining FeFET arrays with existing CMOS circuits and new circuit technology.

In general, emerging memory technologies such as HZO-based FeRAM and FeFETs hold a greater promise for AI applications compared to conventional non-volatile memory applications. This is because the stringent requirements for retention and variability in AI computing can be relaxed in certain cases. Furthermore, unique properties of HZO, such as inherent stochasticity and dynamic time-dependent responses, may enable novel AI applications. Exploring AI computing architectures that leverage these distinctive HZO memory characteristics represents an intriguing research direction.

Acknowledgements This work was supported by Japan Science and Technology Agency (JST) CREST (Grant No. JPMJCR20C3) and Japan Science and Technology Agency (JSPS) KAKENHI, Japan (Grant No. 23K20951).

References

1 Böscke T S, Müller J, Bräuhaus D, et al. Ferroelectricity in hafnium oxide thin films. Appl Phys Lett, 2011, 99: 102903

2 Toprasertpong K, Tahara K, Hikosaka Y, et al. Low operating voltage, improved breakdown tolerance, and high endurance in $Hf_{0.5}Zr_{0.5}O_2$ ferroelectric capacitors achieved by thickness scaling down to 4 nm for embedded ferroelectric memory. ACS Appl Mater Interfaces, 2022, 14: 51137–51148

3 Mueller S, Muller J, Schroeder U, et al. Reliability characteristics of ferroelectric Si:HfO_2 thin films for memory applications. IEEE Trans Device Mater Relib, 2013, 13: 93–97

4 Lee J G, Kim J, Suh D I, et al. Memory window expansion for ferroelectric FET based multilevel NVM: hybrid solution with combination of polarization and injected charges. In: Proceedings of IEEE International Memory Workshop, 2022

5 Toprasertpong K, Takenaka M, Takagi S. Direct observation of interface charge behaviors in FeFET by quasi-static split C-V and Hall techniques: revealing FeFET operation. In: Proceedings of International Electron Devices Meeting (IEDM), 2019. 570–573

6 Ichihara R, Suzuki K, Kusai H, et al. Re-examination of $V_{\rm th}$ window and reliability in HfO_2 FeFET based on the direct extraction of spontaneous polarization and trap charge during memory operation. In: Proceedings of IEEE Symposium on VLSI Technology, 2020

7 Toprasertpong K, Takenaka M, Takagi S. On the strong coupling of polarization and charge trapping in HfO_2/Si-based ferroelectric field-effect transistors: overview of device operation and reliability. Appl Phys A, 2022, 128: 1114

8 Cho S K, Toprasertpong K, Takenaka M, et al. Unveiling memory-window narrowing mechanism after bipolar cycling in HZO/Si FeFETs: critical role of hole trap generation and carrier de-trapping behavior. In: Proceedings of IEEE International Electron Devices Meeting (IEDM), 2024

9 Otomo M, Toprasertpong K, Cai Z, et al. Revealing mechanism of non-accumulative disturb and approach toward disturb suppression in HZO/Si FeFET memory. In: Proceedings of IEEE Symposium on VLSI Technology & Circuits, 2024

10 Mulaosmanovic H, Ocker J, Müller S, et al. Switching kinetics in nanoscale hafnium oxide based ferroelectric field-effect transistors. ACS Appl Mater Interfaces, 2017, 9: 3792–3798

11 Taki K, Sekine N, Watanabe K, et al. Nonvolatile optical phase shift in ferroelectric hafnium zirconium oxide. Nat Commun, 2024, 15: 3549

12 Toprasertpong K, Nako E, Wang Z, et al. Reservoir computing on a silicon platform with a ferroelectric field-effect transistor. Commun Eng, 2022, 1: 21