Next generation information storage using hafnia-based ferroelectrics: Back to the future?

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Hafnia-based ferroelectrics offer exciting potential for applications in both computer logic and memory, with the corresponding direct improvement in computational performance. This preview aims to introduce and share this exponentially growing excitement to the wider community, by highlighting the recent review by Park et al.[1]

Modern technology is heavily reliant on efficient information storage and processing. The continuous advancements in transistor-packing densities have led to increasingly powerful devices, a progression commonly referred to as "Moore's Law." This progress was exemplified in 2012 when a team at the University of Tennessee demonstrated that a commercially available handheld Apple iPad2 outperformed the world's fastest supercomputer from 1985, the ∼2.5 ton behemoth Cray-2.[2] However, the rapid pace of technological advancement is now facing significant challenges as we approach the perceived limits of miniaturization. In response, researchers are actively exploring innovative hardware solutions to overcome these limitations and continue this rapid technological progress.

Ferroelectrics (see Box 1) have long been recognized for their inherent functional properties that make them attractive candidates for computer memory. These

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Box 1

Ferroelectrics are materials exhibiting a spontaneous polarization, which can be switched between at least two symmetrically equivalent orientations. In a "proper" ferroelectric, this is often evidenced via a polarization hysteresis loop, where the polar order is switched with an electric field.[5]

materials can be switched between different polarized states with an electric field, making them well suited for binary information storage. Compared to memory devices that require the use of magnetic fields or spin-polarized currents, electric field switching typically consumes less energy, which adds to their appeal.[3] Historically, this potential has led to extensive research in both academia and industry, notably resulting in their use as random access memory (RAM) in the Sony Playstation 2 computer games console manufactured with a 0.5 μm complementary metal-oxide-semiconductor (CMOS) process.[4] Following the peak in interest, Park et al. attribute the subsequent decline in interest to two main factors. First, the integration of many ferroelectrics with existing CMOS processes proved to be a challenging task. Second, some undesirable side effects, associated with miniaturization of ferroelectrics, imposed stringent limitations on component size reduction. One notable effect is the surface charge-related depolarizing field, which acts to destabilize polar ordering and, everything else being equal, scales inversely with film thickness. In other words, while bulk ferroelectrics are conceptually ideal for computer memory, they begin to lose their desirable properties once they are fabricated in a CMOS-compatible manner and become thin enough for practical applications. This limitation, which is directly correlated with the surface-bound polarization charges, was expected to be present in all ferroelectrics, thereby posing an inherent constraint on their miniaturization potential.

In this context, the discovery of a ferroelectric material with stable and switchable polarization at nanoscale sample thickness, fabricated using CMOS-compatible methods and composed of readily available elements, would be an immensely exciting achievement. In 2011, Böscke et al.[6] published precisely such a breakthrough when they reported the presence of ferroelectric behavior ($P \sim 10$ μC/cm^2 with a coercive field of 1 MV/cm) in a ~10-nm-thick thin-film based on the two-element system hafnium oxide. The significance of this discovery was further amplified by the fact that hafnium oxide was already being utilized by Intel as a gate insulator in their Penryn processor, and the corresponding fluorite crystal structure had been extensively studied as a "high-k" dielectric in CMOS systems.[7] This immediately hinted at the possibility of integrating ferroelectric properties into existing metal-oxide-semiconductor field-effect-transistors (MOSFETs). In other words, a small amount of dopant and subsequent annealing was potentially all that was required to make existing MOSFETs applicable to non-volatile data storage.[1]

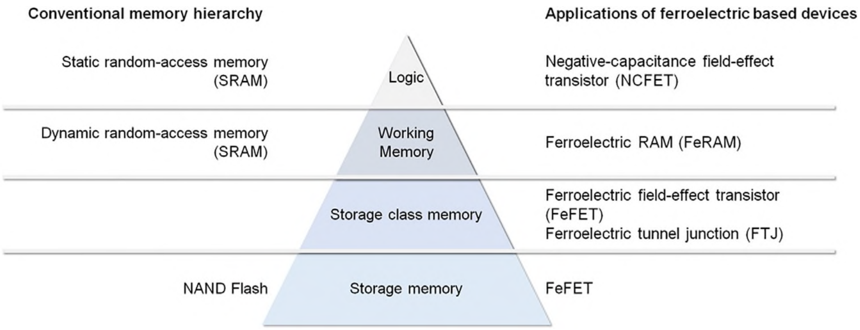

Figure 1. Potential applications of ferroelectric-based information devices, in the context of von Neumann computing

Image recreated based on work from Park et al.[1]

This breakthrough was not just of industrial interest, but has sparked a reconsideration of what materials are interesting in the ferroelectrics community. Traditionally, much research effort has focused on perovskite structures, which include community favorite materials like Pb(Zr,Ti)O_3, BaTiO_3, and BiFeO_3. However, the opportunities demonstrated by HfO_2 in its non-perovskite structure have prompted a renewed exploration of other crystal systems with unconventional properties. Exciting recent results from non-perovskite systems include the negative capacitance associated with unconventional movement of domain walls in Cu-Cl boracites,[8] the strain gradient-driven conductivity observed in lacunar spinels (with their lack of inversion domains[9]), and even the intriguing absence of conducting domain walls in lead germanate.[10] These reports signify a renewed interest in different material classes within the community as it becomes clear that there is a vast amount of exciting science yet to be reported.

On a more applications focused context, this work by Park et al.[1] provides a comprehensive description of the properties of hafnia-based ferroelectrics, as well explaining the associated fabrication questions and challenges needed to scale them down for device application. Their description of the potential of ferroelectrics is effectively illustrated by explaining how these materials can be applied in various applications and architectures, as depicted in Figure 1. This includes exploring possibilities beyond the traditional von Neumann computing

Box 2

Park et al. describe negative capacitance as the phenomenon where the change in electric field across the ferroelectric layer is negative, while the change in polarization state is positive. Others might describe it as the local amplification of the effective electric field across a dielectric, caused by, e.g., the induced alignment of polarization in an incipient ferroelectric that is electrostatically coupled to the dielectric. The exact nature of this exciting topic is still contentious, and readers are encouraged to consult recent reviews, such as by Íñiguez et al., for a discussion.[11]

paradigm, such as in neuromorphic computing and processing-in-memory. One particularly captivating prospect is the utilization of hafnia-based ferroelectrics for stable negative capacitance (see Box 2), which holds the promise of achieving lower power operation and avoiding the so-called ''Boltzmann tyranny.''

A crucial aspect to consider for future devices is stabilization of the ferroelectric phase, which poses a challenge in HfO_2 due to the existence of stable polymorphs. These include monoclinic ($P2_1/c$), tetragonal ($P4_2/nmc$), and orthorhombic ($Pca2_1$) phases, with only the latter exhibiting ferroelectric properties. Park et al.[1] make it evident that a combination of driving factors is necessary to achieve stabilization of the desired ferroelectric orthorhombic phase, with much effort focused on finding an optimized combination. Various processes are discussed in this regard, but Park et al. link these all with inducing strains within the material. These approaches encompass the use of a capping layer, control of thickness and grain size, selection of suitable substrates, and specific annealing conditions. The first aim of these is to reduce the free energy difference between the tetragonal and monoclinic phase (often done via doping or surface energy), so that during the first annealing step, the sample crystalizes in a metastable tetragonal phase, rather than the monoclinic phase. The second annealing step is the stabilizing of the desired orthorhombic phase from the tetragonal phase. This tetragonal-orthorhombic phase transition is martensitic in character, indicating a preference for high cooling rates to facilitate the nucleation of the orthorhombic structure.[1] However, it should be noted that the high temperatures and rapid cooling rates associated with these processes could pose challenges in terms of CMOS fabrication. Therefore, once the material properties are better understood, these processes will need to be carefully optimized for practical implementation.

Reducing the thickness of ferroelectric films introduces several universal challenges that persist, albeit potentially with a diminished impact, in the antifluorite structure. Among these challenges, one prominent issue arises from the increased significance of interface layers, which occupy a relatively larger volume fraction in thinner films and exert a substantial influence on the overall material behavior. Additionally, the inherent stability of the ferroelectric phases is expected to scale with the reciprocal of film thickness, suggesting at some film thickness ferroelectricity should not be stable.[3] This effect elevates the energetic cost of maintaining the ferroelectric phase, thereby impacting its stability and performance.[1] Furthermore, the empirical Kay-Dunn relationship, commonly observed in conventional ferroelectrics, suggests that the coercive field, which represents the electric field required to switch the polarization directions, should increase in thinner films. Alongside these fundamental challenges, various material-specific engineering-based hurdles arise in terms of process optimization, ensuring device-to-device consistency and achieving material stability. For instance, empirical evidence suggests that in HfO_2, higher annealing temperatures are required to crystallize the tetragonal phase as film thickness decreases. This is problematic since this heightened temperature also promotes the formation of undesired point defects like oxygen vacancies. Addressing these multifaceted challenges is paramount for reducing variations and enhancing the reliability of ferroelectric-based devices.

In summary, the work by Park et al. provides an elegant and captivating overview of the current state of hafnia-based ferroelectrics. They successfully explain the fundamental origin of ferroelectricity in these materials and explore their potential applications in both current von Neumann architectures and next-generation devices. Additionally, the authors shed light on the challenges that must be addressed to fully unlock the potential of hafnia-based ferroelectrics. The growing interest in non-perovskite structures and the significance of hafnia-based ferroelectrics suggest promising hardware advancements in future computing systems and is also a boon for ferroelectrics research in general. Park et al.'s manuscript makes a valuable contribution by comprehensively explaining the current state of the field and advancing our understanding of hafnia-based ferroelectrics, while acknowledging the remaining challenges that need to be overcome.

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DECLARATION OF INTERESTS

The author declares no competing interests.

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