Design and Development of Nitride Ferroelectric Memory Devices

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Abstract. To address the inherent “memory wall” bottleneck of the von Neumann computing architecture and meet the growing demand for high-energy-efficiency non-volatile storage, ferroelectric memory technology is regaining widespread attention from both academia and industry. However, traditional perovskite-based ferroelectric materials, such as lead zirconate titanate (PZT), face inherent limitations in CMOS process compatibility and environmental regulations, making seamless integration with advanced logic processes challenging. In recent years, perovskite-structured nitride ferroelectric materials, exemplified by aluminum scandium nitride (AlScN), have emerged as a leading alternative solution. Their lead-free nature, excellent thermal stability, and potential compatibility with back-end-of-line (BEOL) processes offer critical opportunities for developing next-generation memory, neuromorphic computing, and electronics for extreme environments. This paper aims to systematically review the research background and core advantages of nitride ferroelectric materials relative to traditional materials. It discusses key challenges in material preparation and device integration, elucidates the correlation mechanisms between microstructure and macroscopic properties, and introduces representative device architectures and application prospects based on this material system. Finally, it presents outlooks on material engineering, interfaces and reliability, device architecture innovation, and heterogeneous integration with emerging semiconductors.

Keywords: Nitride Ferroelectric Materials; Aluminum Scandium Nitride; Ferroelectric Memory Devices; CMOS Compatibility; Interface Engineering.

1. Introduction

The core characteristic of ferroelectric materials lies in their internal spontaneous polarization, which an external electric field can reversibly control. This unique bistable or multistable property forms the physical foundation for constructing nonvolatile memory cells. Historically, research has long focused on perovskite structures, with lead zirconate titanate ($Pb(Zr, Ti)O_3$, PZT) as a prime example, garnering significant attention for its exceptional piezoelectric and ferroelectric responses. However, compatibility issues with standard CMOS processes pose a major obstacle to its application in advanced logic circuits.

The strategic value of ferroelectric materials lies in their dual support for next-generation information technology: high-density storage and efficient computing. First, in the storage domain, their bistable polarization enables nonvolatile data retention. More importantly, under optimized device structures and operating conditions, ferroelectric memory can exhibit write latency and low-power characteristics comparable to volatile memory (e.g., DRAM). Second, beyond traditional storage, the progressive, partially controllable polarization reversal behavior of ferroelectric materials can simulate the plasticity of biological synapses. This provides the physical foundation for constructing efficient in-memory computing and neuromorphic computing hardware, considered one of the key technological pathways to alleviate the von Neumann bottleneck. Moreover, the inherent coupling between ferroelectricity and the piezoelectric effect grants it irreplaceable application value in microelectromechanical systems (MEMS), high-precision sensors, actuators, and energy harvesting.

Despite the superior performance of traditional materials like PZT, their development faces several insurmountable bottlenecks, which also serve as core drivers for advancing new material systems: Poor CMOS process compatibility: PZT contains lead, a contaminant strictly prohibited in semiconductor manufacturing lines, whose diffusion severely degrades transistor performance. Environmental pollution concerns: Lead's toxicity renders it non-compliant with increasingly stringent environmental regulations. High processing temperatures: PZT's ferroelectric phase crystallization typically requires elevated annealing temperatures, conflicting with the thermal budget constraints of CMOS logic circuits' back-end-of-line (BEOL) processes. Fatigue and retention performance: PZT devices exhibit polarization decay (fatigue) after repeated electrical cycles, and their data retention capability faces challenges during scaling and in high-temperature environments. These issues become particularly pronounced with reduced feature sizes and elevated temperatures.

2. Core Advantages of Ferroelectric Nitride Materials

AlN is a wide-bandgap semiconductor with a hexagonal wurtzite structure. When Sc is introduced into AlN, Sc atoms partially replace Al atoms. Due to Sc's larger ionic radius compared to Al, the Sc–N bond becomes softer and longer, inducing local lattice distortion. AlN exhibits high hardness, low dielectric constant, and excellent thermal stability, but its piezoelectric properties are limited. After Sc doping, enhanced lattice distortion amplifies the polarization effect, significantly improving both piezoelectric and dielectric properties while maintaining good thermal stability. It should be pointed out that ScAIN is compatible with CMOS technology even in harsh environments. Among the commonly used CMOS-compatible metals, molybdenum has a high melting point (about 2160°C), low coefficient of thermal expansion (5×10^{-6}°C^{-1} at 20°C), and low resistivity ($5\times10^{-8}\Omega$m), making it an ideal metal for CMOS manufacturing processes.[1]

To overcome the limitations of traditional materials, perovskite-structured ferroelectric nitride materials represented by aluminum scandium nitride (AlScN) have rapidly emerged. They offer numerous core advantages: Compared to traditional perovskite materials, the AlScN-based nitride ferroelectric system demonstrates a series of fundamental benefits, primarily summarized as process integration compatibility, superior intrinsic physical properties, and robustness under extreme conditions.

2.1 Process Integration Compatibility

One of AlScN's core advantages lies in its high compatibility potential with standard semiconductor processes, particularly back-end-of-line (BEOL) processes. Firstly, as a III-V group nitride, AlScN aligns with traditional AlN and GaN process systems. It exhibits excellent chemical stability and does not undergo violent reactions during conventional etching, deposition, or thermal treatment processes. Compared to mainstream ferroelectric materials like HfO_2, AlScN requires lower preparation temperatures, enabling deposition and crystallization within the BEOL process compatibility range (typically <400°C). This compatibility stems from its chemical inertness, thermal stability, and process homogeneity with the nitride system.

AlN-based memristors have emerged as particularly noteworthy due to their exceptional properties, including ultrafast switching speed, small switching current, substantial on/off ratio, controllable material growth, and compatibility with complementary metal-oxide-semiconductor (CMOS) processes.[2]

Secondly, through techniques such as reactive magnetron sputtering, high-quality films can be deposited at temperatures significantly lower than the crystallization temperatures of traditional ferroelectric materials ($\leqslant$ 400 °C, compliant with BEOL thermal budgets). More importantly, AlScN's ferroelectricity stems from its intrinsic wurtzite structure, eliminating the need for additional high-temperature annealing to induce specific crystalline phases. This stands in stark contrast to HfO_2-based ferroelectric materials, which require precise thermal processing to form the metastable orthorhombic phase. This process's simplicity and low-temperature characteristics establish a foundation for its three-dimensional (3D) monolithic integration on logic chips. Its scalability has been demonstrated through heterointegration with two-dimensional semiconductors such as MoS_2.

Liu et al. studied a transistor-free ScAIN-based ferroelectric diode array, which realizes data storage, search, and neural network operation on sub-50 nm thick FeDs. In this study, the authors designed a fully BEOL-compatible architecture using two ScAIN field-programmable ferroelectric diodes in parallel.[1]

2.2 Superior Physical Properties

The AlN lattice itself adopts a polar wurtzite structure. Upon introducing Sc, localized lattice distortion and a “softening effect” reduce the polarization reversal barrier, enhancing spontaneous polarization. The combination of significant ionic displacement and non-centrosymmetric structure generates a substantial switchable polarization. This phenomenon relates to lattice distortion, local symmetry breaking, and energy barrier modulation. Consequently, at the physical property level, AlScN demonstrates potential surpassing existing mainstream ferroelectric materials. Its residual polarization (P_r) can exceed 100 μC/cm², several times that of HfO_2-based materials, providing greater margin for device miniaturization and multilevel storage. Simultaneously, AlScN possesses a relatively high coercive field (E_c), indicating exceptional resistance to polarization disturbance and facilitating long-term data retention. While high E_c poses challenges for operating voltage, this can be effectively managed through thin-film thickness reduction and strain engineering. Furthermore, its low dielectric constant (κ ≈ 12–18) helps reduce gate leakage current and enhances electrostatic control capabilities in field-effect transistor (FE-FET) structures. Simultaneously, increasing Sc doping concentration (typically 10–40%) significantly enhances AlScN's piezoelectric constants d_{3333} and e_{3333}, achieving values several times higher than pure AlN. This occurs because Sc's hexagonal structure more closely resembles the hexagonal rocksalt phase. When introduced into the AlN lattice, it lowers the energy barrier along the polarization direction. The resulting lattice softening facilitates easier atomic displacement under external fields, thereby enhancing polarization. Additionally, the ASAM shows excellent resistive switching performance with ultrafast switching speed (<5 ns), low operation voltage (<0.5 V), and ultralow power consumption as small as 0.2 pJ.[2]

2.3 Robustness in Extreme Environments

Both AlN and ScN belong to the III-V group of nitrides, where the N－Al and N－Sc bonds exhibit strong covalent characteristics (high bond energy and strong directionality). This strong covalent nature determines that the bonds remain resistant to breaking even at elevated lattice thermal vibration energies, thereby maintaining robust thermal stability.

AlScN shows superior thermal stability; FeTFTs with AlScN/AlN/AlScN multi-layer (t_AlN=30 nm) maintain stable retention characteristics up to 125 ° C, and even at 185 ° C, stable hysteresis curves are observed over 100 cycles.[3]

Nitrides exhibit strong surface chemical inertness and excellent oxidation and corrosion resistance, making them suitable for extreme operating conditions. AlScN exhibits outstanding thermal and chemical stability. Experiments confirm its ferroelectric properties remain intact at temperatures up to 1000 °C, coupled with exceptional radiation resistance. These characteristics make it an ideal candidate material for non-volatile storage and sensing applications in extreme environments such as aerospace, automotive electronics, and deep-earth exploration.

3. The Intrinsic Relationship Between Microstructure and Ferroelectric Properties

3.1 Basic Mechanism

The ferroelectricity of AlScN does not originate from conventional phase transitions but results from precise control over the energy barrier surfaces of its wurtzite lattice through alloy engineering. Its intrinsic physical mechanism can be explained as follows:

Pure AlN belongs to the polar $P6_3mc$ space group and possesses intrinsic spontaneous polarization. However, due to the extremely high energy barrier required for polarization reversal (generally believed to involve a metastable layered hexagonal phase transition state), it exhibits behavior characteristic of a non-switchable polar dielectric rather than a ferroelectric material. Introducing Sc^{3+} ions with larger ionic radii at Al^{3+} sites induces significant local lattice distortion, thereby reshaping the system's energy landscape. Specifically, Sc insertion elevates the energy of the stable wurtzite ground state while substantially lowering the activation energy required for transition to the metastable state. Upon reaching a critical Sc concentration, the energy-displacement curve evolves from a deep single potential well into a relatively flat double well, with each well corresponding to one of two stable polarized states along the c-axis. Macroscopically, this reduction in the energy barrier manifests as lattice softening (i.e., a decrease in the elastic constant C_{33}). This enables the relative displacement of cations and nitrogen ions along the c-axis under an external electric field, thereby achieving polarization reversal.

3.2 Key Microstructural Parameters

Microscopically, the ferroelectricity of AlScN is determined by the displacement of ions in the lattice; the off-center displacement is described by the parameter u, which is defined as the ratio of the metal-nitrogen bond length parallel to the c-axis to the lattice parameter c, and the typical u value for AlScN is ≈ 0.38.[4]

The observed acceleration of ferroelectric switching with increasing temperature indicates that the process in AlScN is primarily driven by ionic displacement. This suggests that, unlike in HZO, the switching behavior of AlScN is less affected by extrinsic factors such as domain wall motion or chemical defects. Several mutually coupled microscopic factors jointly determine the key ferroelectric parameters (P_r, E_c) of AlScN: Sc concentration is the core variable regulating the height of the energy barrier. As concentration increases, E_c typically decreases, while P_r reaches an optimized value within a specific concentration range (approximately 20 – 43 at%). Beyond this range, phase separation occurs, leading to the precipitation of the non-ferroelectric rock salt phase ScN and resulting in performance degradation. Simultaneously, the spatial uniformity of Sc atom distribution within the lattice is critical; local clustering can create domain wall pinning centers, affecting the homogeneity of switching characteristics. Crystal Texture and Stress State. Since the polarization vector strictly aligns with the c-axis [0001] direction of the wurtzite structure, the film must exhibit a highly oriented texture to ensure the applied electric field can effectively drive polarization reversal. Furthermore, residual stresses within the film can serve as an effective means to fine-tune E_c. For instance, constructing multilayer structures by intercalating dielectric layers such as AIN between AlScN layers allows decoupling and synergistic optimization of P_{r} and E_c through interlayer stresses and electric field redistribution.

4. Potential Application Directions and Key Device Structure Overview

Due to their unique physical properties and process compatibility, AlScN-based ferroelectric devices demonstrate broad application prospects across multiple cutting-edge technology domains, primarily encompassing next-generation computing architectures, extreme environment electronics, and high-performance sensing systems:

4.1 Next-Generation Computing Architecture

In the computing domain, AlScN holds promise for simultaneously addressing energy efficiency bottlenecks in both storage and computation. First, as a core material for high-density non-volatile memory (NVM), it can be used to construct ferroelectric random-access memory (FeRAM) and ferroelectric field-effect transistors (FeFETs). Its back-end-of-line (BEOL) compatibility makes it particularly suitable for monolithic integration with advanced logic circuits, enabling the development of high-performance embedded or on-chip storage solutions. Second, in neuromorphic computing and in-memory computing, AlScN devices exhibit progressive, pulse-programmable polarization reversal characteristics. This enables them to effectively simulate the plasticity of biological synapses, providing a crucial physical foundation for constructing energy-efficient artificial synapse devices and neural network hardware accelerators. A reconfigurable compute-in-memory system utilizing field-programmable ferroelectric diodes based on AlScN has been developed, representing a key step toward next-generation computing architectures. The incorporation of a 30 nm-thick AlScN ferroelectric film into an MFeS capacitor structure provides a robust platform for the future realization of AlScN/SiC-based MFeS-FETs, addressing critical demands in high-temperature memory technologies and bridging an essential gap in high-temperature digital integrated circuits.[5]

4.2 Extreme Environment Electronics

AlScN's exceptional thermal stability makes it an ideal material for electronics in extreme environments. In demanding applications such as aerospace, deep-earth exploration, and automotive powertrain systems, AlScN-based storage and sensing systems ensure reliable operation under high-temperature and high-radiation conditions. This meets the future demands of intelligent equipment for data persistence and in situ sensing capabilities. For example， AlScN-based FeTFTs with a multilayer architecture exhibit stable operation at elevated temperatures, maintaining long-term retention up to 125 °C and reliable cyclic endurance up to 185 °C. These characteristics make them well-suited for electronics operating in extreme environments, where thermal stability is a critical requirement.[3]

4.3 High-Performance Sensing and Actuating Systems

Furthermore, leveraging its significant piezoelectric-ferroelectric coupling effect, AlScN can be utilized to fabricate high-performance sensors and microelectromechanical systems (MEMS). Its robust electromechanical conversion capability, combined with non-volatile polarization states, holds promise for achieving performance breakthroughs in applications such as RF filters, energy harvesters, and precision actuators.

AlScN has also been applied in several key device structures, with the following three representing the primary ones:

Ferroelectric Diode (Fe-Diode, M–F–M/Heterojunction Barrier) is a relatively simple device structure, typically consisting of a metal/AlScN/metal or a heterojunction with a semiconductor/functional layer, such as Ni/AlScN/Pt. Its operating mechanism closely resembles an interface Schottky barrier/polarization-modulated band bending (rather than a simple “tunneling barrier” change). Reversing the polarization direction alters the forward/reverse barrier height and conduction mechanism, yielding high/low resistance states and intrinsic rectification. This makes it suitable for high-density cross arrays and offers the advantage of simplified readout. To suppress crosstalk and sneak paths, integrator/stacked structures and array algorithms can be optimized.

Ferroelectric Field-Effect Transistor (FE-FET) utilizes a ferroelectric layer as the gate dielectric/gate stack, it modulates channel carriers through polarization reversal, thereby altering the threshold voltage V_TH to achieve “0/1” or multi-level storage. FeFET employs a ferroelectric layer as the gate dielectric (or part thereof). By altering the ferroelectric layer's polarization direction (upward or downward), it effectively modulates the carrier concentration in the underlying semiconductor channel, thereby changing the transistor's threshold voltage (Vth). A high Vth and a low Vth correspond to the two logic states “0” and “1,” respectively. The read operation of this device is non-destructive and facilitates high-density integration. By combining AlScN with a two-dimensional MoS_2 channel, FeFET devices exhibiting a large memory window and high on/off current ratio have been demonstrated. In conventional metal–oxide–semiconductor field-effect transistors (MOSFETs), the gate voltage applied across the oxide insulator modulates carrier accumulation or depletion in the semiconductor channel, thereby enabling the fundamental transistor functions of switching and amplification, forming the cornerstone of modern electronics. When ferroelectrics are employed as gate insulators, ferroelectric field-effect transistors (FeFETs) exhibit remarkable enhancements. The polarization charge of typical ferroelectrics is one to two orders of magnitude greater than that of conventional oxide dielectrics, enabling more efficient and nonvolatile modulation of the channel conductance.[6]

Ferroelectric field-effect transistors (FeFETs) are realized by integrating AlScN with a two-dimensional MoS_2 channel in a metal–ferroelectric–metal–insulator–semiconductor (MFMIS) architecture. The structure features a floating gate whose area ratio ($A_{(MIS)}$ / $A_{(FE)}$) can be adjusted to optimize the capacitance matching within the gate stack. Through effective charge compensation, charge trapping is significantly suppressed, enabling a ferroelectricity-driven memory window (MW) to be achieved under low operating voltages [4].

5. Material Preparation Challenges

Despite AlScN's immense application potential, achieving high performance and reliability at the device level still requires overcoming several critical challenges in material preparation and process integration.

5.1 Low-Temperature Deposition and Ferroelectric Properties

A comparison based on the fabrication process shows that PZT crystallizes at a lower temperature than SBT and is more suitable for state-of-the-art low-temperature CMOS processes.[7]

Although AlScN holds potential for low-temperature deposition, achieving high residual polarization ($P\_{_r}$), low coercive field (E_c), and excellent cycling stability simultaneously within the BEOL-compatible thermal budget (≤ 400 °C) presents a complex multi-parameter optimization challenge. This necessitates finding a precise equilibrium between the Sc composition (typically within the 20–40 at% range), film stress and texture, thickness, and deposition kinetics.

5.2 Interface Engineering and Defect Control

The quality of the interface between AlScN films and electrodes or semiconductor channels directly determines the device's leakage current, imprint effect, and fatigue characteristics. Interface trap states or fixed charges not only reduce device reliability but may also shield applied electric fields, leading to degraded switching windows. Therefore, introducing interface modification layers (such as ultrathin dielectric layers), optimizing surface treatment processes, and selecting electrodes with matching work functions are crucial for stabilizing the interface potential barrier and suppressing defect states. The interface between the polysilicon plug and the diffusion barrier layers is physically and electrically enhanced by preparing a buffer oxide layer, such as $CoSiO_2$, for maintaining an ohmic contact. However, it was observed that the BCs randomly fail at a given annealing temperature due to the formation of insulating SiO_2.[8]

5.3 Composition Uniformity and Scalability

In physical vapor deposition processes such as reactive magnetron sputtering, ensuring high uniformity of Sc composition at the wafer level while suppressing phase separation poses a significant process challenge. Non-uniform Sc distribution directly leads to variability in device electrical properties (e.g., V_th, E_c). To address this issue, the industry has conducted extensive research in target design (e.g., Al-Sc alloy targets, coaxial targets) and process control (e.g., substrate rotation, high-power pulsed magnetron sputtering, HiPIMS) to enhance film uniformity and reproducibility. Currently, there is no established approach for depositing films with a strongly preferred orientation using atomic layer deposition (ALD). Moreover, inducing such a preferred orientation in thick HfO_2-based films grown on bottom electrodes other than silicon remains unresolved, highlighting an urgent need for practical solutions to enable real-world applications.[9]

6. Future Outlook

Despite significant progress in ferroelectric nitride technology, achieving the leap from laboratory validation to large-scale commercial application still requires systematic R&D and breakthroughs in several key areas.

First, material synthesis and process integration form the foundation. Future research must focus on developing low-temperature deposition techniques fully compatible with advanced CMOS nodes. This entails not only deep optimization of existing sputtering processes (such as HiPIMS) but also exploration of novel methods like atomic layer deposition (ALD), which offer precise thickness control and conformal coverage capabilities. The core objective is to precisely control the coercive field (E_c) through techniques like multi-level doping or strain engineering, while meeting back-end-of-line (BEOL) thermal budgets. This aims to reduce operating voltages without sacrificing the core advantages of high residual polarization (P_r) and low leakage.

Second, interface engineering and device reliability are critical determinants of technological success. It is essential to deeply investigate the physicochemical mechanisms at the ferroelectric layer/electrode and ferroelectric layer/semiconductor interfaces, clarifying the origin and evolution of defect states. Based on this understanding, designing and introducing functional interface modification layers holds promise for effectively passivating traps and stabilizing interface barriers, thereby fundamentally enhancing device endurance and data retention capability.

Third, innovation in device structure and system architecture is the core pathway to increasing storage density. To overcome the physical limitations of two-dimensional planar scaling, future R&D will focus on three-dimensional vertical integration, such as developing 3D-NAND-like vertical FeFETs and stacked crossbar arrays. This requires synergistic optimization of device design, array interconnects, and selector units. Additionally, for neuromorphic computing applications, improving the linearity and consistency of multi-level storage states represents a critical technological bottleneck for practical implementation.

Finally, heterogeneous integration will open entirely new application domains for nitride ferroelectrics. By combining AlScN's nonvolatility with the high-power/high-frequency characteristics of wide-bandgap semiconductors (e.g., GaN, SiC) or the unique optoelectronic/mechanical properties of two-dimensional materials, multifunctional integrated systems with disruptive potential can be developed. These systems are poised to play pivotal roles in next-generation power electronics, RF communications, and flexible electronics.

7. Conclusion

Represented by AlScN, the nitride ferroelectric system is emerging as a key alternative to traditional oxide ferroelectrics due to its unique combination of material physics, process compatibility, and application versatility. Its scalability and high performance have been preliminarily validated at the array level, particularly in heterointegration with two-dimensional semiconductors. Nevertheless, fully realizing their potential requires overcoming critical engineering challenges, including low-temperature high-quality film deposition, interface defect control, and the trade-off between write voltage and endurance. Looking ahead, with the continuous advancement of materials engineering, interface science, and device-architecture co-design, nitride ferroelectrics hold promise as the core hardware enabler for a new computing-memory paradigm that integrates high energy efficiency, high density, and strong robustness.

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