Multiscale Modeling of Ferroelectric Memories: Insights into Performances and Reliability

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***Abstract*— Despite large efforts in research of HfO_2- based ferroelectric (FE) random access memories (FRAM), mechanisms underlying the device behavior of and its reliability (premature degradation) are poorly understood. To tackle this issue, we used a multiscale modeling framework that allows investigating the interplay between the FE switching, defects and polycrystalline nature of the HfO_2 material. This multiscale model allows connecting the electrical performances of FE devices (e.g. switching) to the atomic material properties, including defects and morphology (e.g. material phase). We used this simulation platform to both study wake-up process and the device-to-device variability in different memory architectures, i.e. capacitor- based FRAM and ferroelectric tunnel junction (FTJ) and the ferroelectric FET (FeFET) subjected to high field program/erase stress.**

Keywords*— *FRAM; FTJ; FeFET; ferroelectric HfO_2;

I. INTRODUCTION

Due to the high-speed operation and low-power required for altering the polarization state as well as the non-volatility, ferroelectric (FE) memories are long time envisioned as one of the most promising memory solutions [1]. However, contamination and CMOS incompatibility caused that the state-of-the-art perovskite (PZT)-based ferroelectrics stopped scaling at 90 nm technology nodes and PZT-based devices never exploited their full market potential [2,3]. On the other side the discovery of the FE properties of HfO_2 [4] stimulated an intense research [5-11] toward CMOS compatible FE memories (FM), that can be implemented by either capacitor-based (FRAM) [12], ferroelectric tunnel junction (FTJ) [13-15] or transistor-based (FeFET) [16] solutions. However, despite the great interest in this technology, the performances and variability/reliability of FE memories have not been unambiguously understood yet.

HfO_2-based FE devices suffer from ionic transport (e.g. drift of O interstitials and vacancies) and the simultaneous presence of multiple phases [5,6], which can significantly increase the device variability. In addition, the high field [5,8] required for switching causes the material degradation (e.g. O vacancy/ion generation), which eventually results in the premature dielectric breakdown responsible of the closure of the memory window (MW) [7-9]. In order to contrast such premature reliability phenomena, anti-ferroelectric (AFE) solutions have been proposed, which engineer the material systems offering significantly improved endurance [17,18] with penalty of a slightly reduced retention [19] compared to FE equivalents.

A consistent description and quantitative understanding of all these aspects requires a multiscale modeling framework, connecting the material properties to the electrical device performances, which is described in the next Section. We use multiscale approach to understand the FE memory device behavior and underlying physical mechanisms. By understanding the underlying physics, we are able not only to predict reliability and variability of single cells but also to engineer novel, superior devices at array level.

II. MULTISCALE MODEL

The multiscale model describing the device operations is comprised of two main parts consistently connected, which address the charge transport and stress-induced material modifications, respectively, which is crucial to model device aging and reliability phenomena [20-25]. The individual contributions of interstitial ions and vacancies are included, along with their diffusion and generation processes and the FE properties of the film, Fig.1.

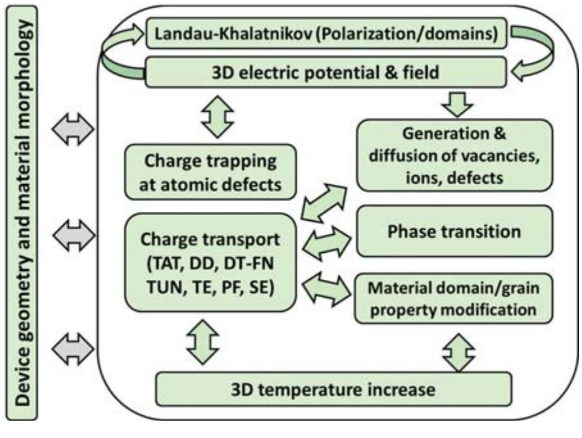

Fig. 1. Flow chart and Schematic illustration of the multiscale modelling platform presented for the simulation of emerging memory devices [20,21]. The ab-initio section for the calculation of the fundamental material and defect properties (represented with material morphology section) is connected to the device modeling section, which is comprised of two parts addressing a) the charge transport (including charge trapping) within the device and b) the stress (operation) induced material changes (phase changes, defect generation and migration) occurring, within the material, during the device operation.

The electric potential within the Fe-device is calculated by solving the Poisson equation consistently with Landau-Khalatnikov formalism enriched with Ginzburg domain interaction term. Time dependent Ginzburg-Landau [26-31] model is described with the following equation:

$$-\rho\frac{dP}{dt} = 2\alpha P + 4\beta P^3 + 6\gamma P^5 + 2k\Delta P + \nabla\varphi, \qquad (1)$$

where ρ denotes damping coefficient, P polarization, α, β, γ Landau parameters, k-domain coupling factor and φ, electrostatic potential obtained using self-consistent approach. Model performance is illustrated in Fig.2, which shows the simulated evolution of the FE domain orientation over time upon the application of the external excitation field. The 2D domain map shows a clear domain reorientation from the initial random to a common oriented state, which proves that the model captures not only the reorientation but also the and nucleation occurring upon application of the electric field.

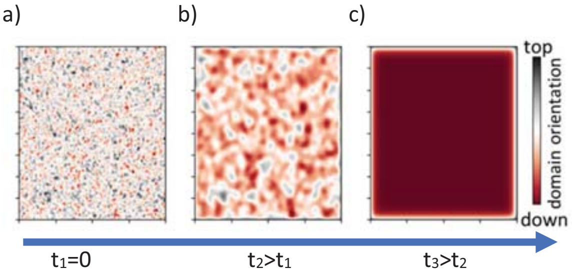

Fig. 2. Domain dynamic in 2D ilustrating nucleation processes within device (top view) while seting it into the erase state. a) intial randomly distributed polarization (without applied electric field); b) initial coalesncence of the domains and nucleation; c) whole device area set into erased-set (negative polarization state).

Thanks to the multiscale approach, the interaction between atomic defects and FE properties responsible for domain switching is physically described, which allows consistently modeling the device variability (defects treated individually) and reliability (defects i.e. oxygen ion, vacancy pairs are generated due to the high field, Section III). This modeling platform is thus essential for understanding the key material properties and microscopic mechanisms responsible for wake-up and fatigue, while accounting for the role played by defects, which can impede the nucleation of the domains and promote phase changes at same time.

III. SIMULATION OF FERROELECTRIC DEVICE VARIABILITY AND REALIABILITY

A. *Variability and Wake-up(increase of the MW)*

Random vacancy and charge distributions together with the phase fluctuations of polycrystalline FE HfO_2 film (Fig.3a) impact the nucleation of the domains and change the electrostatics of the active FE layer inducing modifications of the internal field [5,8]. The aforementioned effects and their entanglement are well captured by simulations that successfully reproduce wake-up, i.e. opening of the MW and the polarization hysteresis (see Fig. 3a-I) of FE devices. The wake-up and polymorph nature of the HfO_2 can cause a significant variability in FE tunnel junctions (FTJs), FeFETs and FRAMs, Fig.3a.

In pristine conditions, large portions of the HfO_2 layer are not orthorhombic/ferroelectric (even up to 50-70% of the film might be in non-switching tetragonal or monoclinic phase). In addition, a significant number of the FE-domains is thus pinned by the non-uniformly distribution of charges originated by oxygen vacancies, and the polarization orientation is random. During the wake-up phase, P_r can often triple due to the de-pinning of domains, the phase transformation, and the internal charge and vacancy redistribution. These internal material changes cause a severe memory window variability, which can even lead to the complete overlap binary logical "0" and "1" distributions.

We simulated the randomness of the polycrystalline film by accounting for both random orientation of domain polarization P_r and the random distribution of the defects. The local changes of the potential (internal field) due P_r magnitude and charged defects can bend the bands, thus affecting in turn the local tunneling probability, which generates fluctuations of the I_{ON}/I_{OFF} ratio in FTJ devices (see Fig.3b). As it can be seen in Fig. 3c both changes in wake-up (P_r increase with cycling) and/or ferroelectric properties nonuniformity over the wafer (polycrystalline nature of the binary oxides) of up to 30% resulted in negligible MW change, whereas a higher change resulted in strong I_{ON}/I_{OFF} fluctuations.

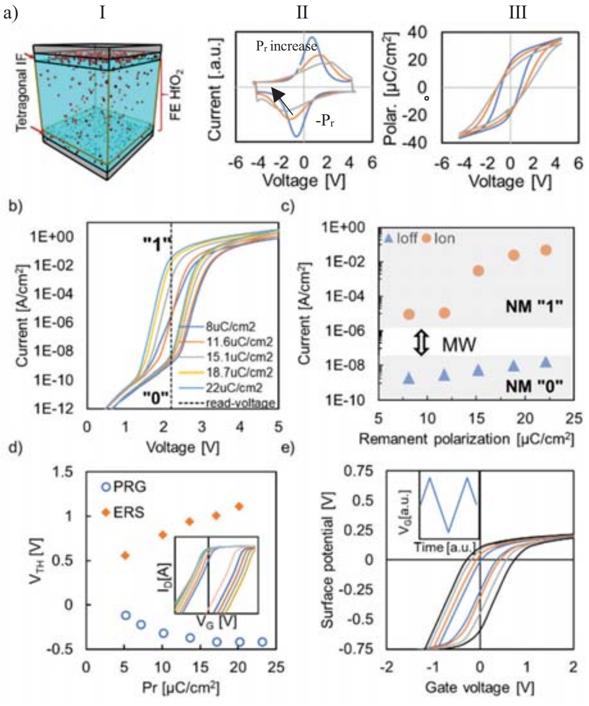

Fig. 3. a) Wake-up modeled through the ion/charge movement and phase transformation; (I) device geometry with ortorombic FE bulk, tetragonal (non-switching) interfaces and O-vacancies (red spheres); (II) current-voltage and coresponding (III) polarization-volate behavior with wake-up of the device. b) Fluctuation of the I_{ON} and I_{OFF} and c) MW variability of FTJ and d) MW variability of FeFET. e) Coresponding surface potential evolution depending on the switching variability of the device.

Analogously to FTJ, domain orientations and film polycrystallinity can result in a significant variability increase in ultra-scaled FeFETs. Fig. 3d-e shows that depending on the P_r, MW fluctuations affect both programmed (PRG) and erased (ERS) states. Interestingly, the PRG state is more immune against to P_r variability, which impacts strongly the surface potential (see Fig. 3e) of the negative polarity (ERS-state). Finally, MW saturates with P_r above 15 μC/cm².

B. Degradation of interfacial layer and fatigue

The high fields required for the overcoming of the switching barrier (coercive field, E_c) and switching of the FE layer can even increase with stack having the low-k interfacial (IF) layer, which act as a dead layer from FE perspective, but it experiences the highest field due to the electrostatics – there is a voltage divider between the low-k IF and high-k FE layers. Consequently, voltage required for memory operation has to be further increased, and this causes a very high field on IF layer of both FTJ and FeFET (see Fig. 4a and Fig. 5a respectively). Such high fields induce a significant defect generation due to atomic bond breakage, especially in the IF, which can be further increased by the alternating polarity switching inducing a significant charge flow (back and forth) across the interface. The increase of the defect density and consequent charge trapping inside the FeFET gate stack affects the device electrostatics, finally compensating its MW.

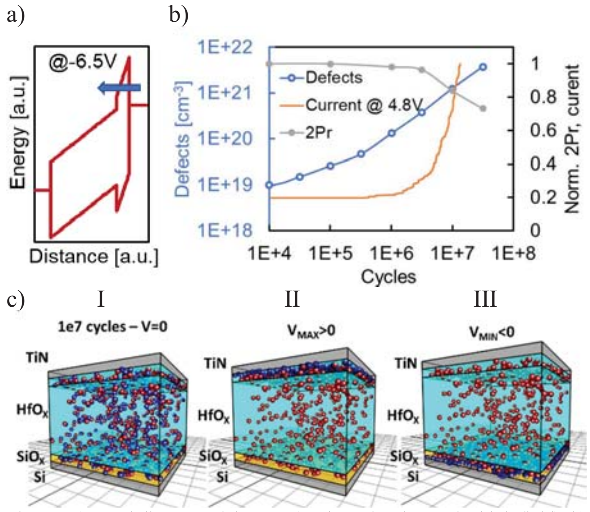

Fig. 4. a) Band diagram of the FTJ (IF degrades due to the high field). b) Defect density, norm. $2P_r$ and leakage current evolution with stress program/erase (PRG/ERS) cycles. c) Geometry of FTJ with O-vacancies (red spheres) and O$^-$ ions (blue spheres). I denotes the degraded device after 10^7 PRG/ERS cycles while II and III denote the shift of the O$^-$ ions (blue spheres)due to the application of positive (PRG) and negative (ERS) program pulse respectively.

Besides, generation of the vacancy-ion pairs due to bond breakage, the subsequent charge trapping alters the electrostatics of the device[5,8]. In the FTJ case shown in Fig.4c, O$^-$ ions attracted by the positive voltage applied on the top electrode reduce the electric field in the bulk, impacting the domain nucleation and resulting in drop of the P_r. However, reduction of P_r does not impact the ON state and ON/OFF ratio as long as P_r does not drop below 50% of its initial value (see Fig.3b-c). On the other side, OFF current is severely impacted by the defect generation.

As in the FTJ case, the high fields used for PRG/ERS operation in Fe-FET device can induce a strong charge injection to/from the channel. As the channel conductivity and the threshold voltage (V_{TH}) are impacted by both ferroelectric dipole and the charge trapped within the gate stack (both affects the device electrostatics), we used the simulations to analyze the FeFET behavior and separate the two contributions, i.e. the FE one from the charge trapping one. FE switching, and charge trapping are acting in opposing directions by shifting the V_{TH} towards more negative/positive for on same (positive) excitation on the gate. Namely, sweeping from negative to positive voltages and back charge trapping results in clockwise (CW) behavior, which is completely opposite what is observed for pure ferroelectric switching [19]. Consequently, strong injection from the channel partially compensates the MW (blue dashed trace Fig. 5b) of the FeFET decreasing the distance between high (red trace Fig.5b) and low (blue trace Fig.5b) V_{TH}.

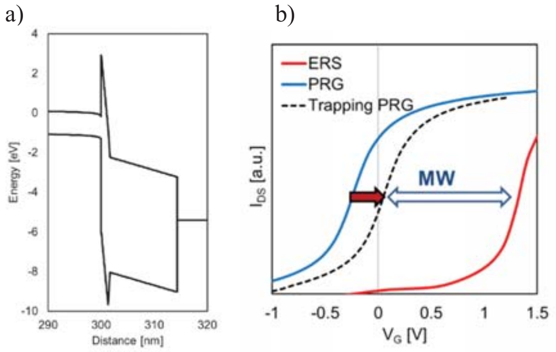

Fig. 5. a) Band diagram of the Si/SiO$_2$/Si:HfO$_2$/TiN FeFET under program condition of 5V. The high potential drop over IF is observed and it is accompanied with the strong electron injection from the channel that compensates the memory window b) of the FeFET. Blue and red trace denote low and high V_{TH}, whereas the dashed black line denotes the shift of the low V_{TH} due to the charge trapping.

IV. CONCLUSION

In this paper we presented a multiscale modeling of the ferroelectric memory devices. A comprehensive modeling framework was developed to investigate the reliability aspects of both capacitor- and transistor- based ferroelectric memories. We show the capability to fully describe the physical mechanisms behind the wake-up and fatigue, accounting for the polymorphism of the film and investigate the implication of the interplay between FE and defects variability on performances and variability of different FE memory devices.

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