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Experiment and Modeling of Dynamical Hysteresis in thin film Ferroelectrics

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Abstract

Polarization hysteresis in thin film ferroelectrics is studied based on a two-dimensional multi-domain time-dependent Landau-Khalatnikov model. An extraction method for ferroelectric parameters to calibrate the experimental hysteresis loop is proposed. Based on this approach, the frequency-dependent hysteresis loops in HZO ferroelectric capacitor measured by triangular waveforms are successfully reproduced.

I. Introduction

Recently, negative-capacitance FETs (NC-FETs) based on ferroelectrics (FEs) have gained great attention as a steep slope device for low power consumption [1]. Polarization dynamics of FE switching are key to NC effects, of which are generally treated as homogeneous single-domain state by either analytical or numerical simulation [2-4]. Nevertheless, since multi-domain state are preferable to reduce the electrostatic energy of the system, the use of homogeneous single-domain theory to model such NC effects is improper and will lead to inaccurate predictions and NC device design.

In this work, multi-domain time-dependent Landau-Khalatnikov model is used to describe the FE dynamics, and particularly an extraction method for FE parameters is proposed, which is useful to further NC-FET simulation.

II. Methods

Simulation model To describe the dynamical behaviors in ferroelectric thin films, a two-dimensional (2D) multi-domain time-dependent Landau-Khalatnikov (TDLK) model is used [5]. A ferroelectric thin film is consisted of $N\times N$ domains in the x-y plane which is perpendicular to the applied electric field. The polarization reversal of each domain (i, j) in the ferroelectric based on the TDLK model is expressed as:

$$\rho_{i,j}\frac{\partial P_{i,j}}{\partial t}=-\frac{\partial F_{i,j}}{\partial P_{i,j}}=-(2\alpha_{i,j}P_{i,j}+4\beta_{i,j}P_{i,j}^3+6\gamma_{i,j}P_{i,j}^5)+\frac{V}{T_{FE}} \quad (1)$$

for i and j = 1, 2, …, N, where ρ is the internal resistivity related to the domain switching, P is the polarization charge density, F is the free energy, (α, β, γ) are the Landau parameters, and V is the applied voltage. Particularly, (α, β, γ, ρ) for all domains follow Gaussian distributions with standard variation σ to consider the effect of the distribution of the spatial orientation of the crystallites in a polycrystalline film [6]. Here for simplicity, only variation of α is considered. Actually, since domain interaction is not included which is reasonable considering nucleation limited switching, parameter distribution with σ=0 is equivalent to single-domain state. Above dynamic equation is solved using Runge-Kutta algorithm with adaptive time step.

Fabrication and measurement Fig.1 shows the fabricated 10nm Zr-doped HfO_2 (HZO) FE capacitor with TiN as electrodes, which are annealed at 450°C. The electrical characteristics are measured by triangular waveform voltage.

III. Results and Discussions

Single-domain simulations Fig.2 shows the simulated P-V curves based on single-domain TDLK model, where 'S'-shaped P-V curve is obtained from static case with dP/dt=0, and hysteretic P-V curve is obtained from dynamical case with $dP/dt\neq0$ which is critical to describe the polarization switching. Fig.3 shows the simulated frequency-dependent P-V loops with internal resistivity ρ of 10 and 500 Ω·m respectively, indicating that the larger the resistivity is, the more dispersed the curves are.

Multi-domain simulations Fig.4(a) shows the 2D domain pattern of ferroelectric containing $N\times N$ domains, and Fig.4(b) shows corresponding clusters of P-V loops for each domain with Landau parameter α following Gaussian distribution as shown in Fig.4(c). Fig.5 shows the effect of domain number on the P-V loops. It can be seen that step-like switching occurs with only a few domains (e.g. four domain), which is potential for multi threshold voltage application. Fig.6 show the effect of standard deviation σ of Gaussian distribution, indicating that the smaller the σ is, the steeper the switching is, where multi-domain switching with σ=0 is equivalent to the single-domain case as expected.

Calibration and validation with experimental measurements A method to extract the HZO ferroelectric parameters from experimental measurements is proposed as follows. Step 1: static parameters of (α, β, γ) is extracted from the 'S'-shaped curve as shown in Fig.7. It should be noted that dashed curve is generally fitted, but solid curve is adopted in the simulation where both remnant polarization P_r and coercive field E_c are fitted to measurement. Step 2: from Fig. 8, dynamic parameter of resistivity ρ is extracted by comparison of measured and simulated frequency dependence of E_c normalized to E_c at 100Hz obtained from Fig.3. Step 3: domain number and related Gaussian distribution can be determined by fitting the slope of polarization switching as shown in Fig.9. Actually Step 2 performed by single domain case is reasonable, because the E_c remains almost unchanged as σ varies in multi-domain case. Based on above procedure, measured frequency-dependent P-V loops are successfully reproduced in Fig.10, which verifies the simulation method. Fig.11(a-f) shows domain evolution along the hysteresis loop in HZO FE capacitor as shown in Fig.10. Finally, Table I list all the extracted parameter in the simulation.

IV. Conclusions

A multi-domain time-dependent Landau-Khalatnikov model is used to describe the FE dynamics, and particularly an extraction method for FE parameters is proposed. The measured frequency-dependent hysteresis loops in thin film HZO FE capacitor are well reproduced by accounting for the effect of distribution of the spatial orientations of the crystallites.

Acknowledgements

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References

[1] S. Salahuddin *et al., Nano Lett.* 8, p. 405, 2008.

[2] A. Khan et al., *Nature Mater.* 14, p. 182, 2015.
[3] W.-X. You and P. Su, *IEEE TED*, 65, p. 4196, 2018
[4] H. Ota et al., *IEDM*, p. 197, 2018.
[5] M. Hoffmann et al., *Adv. Funct. Mater.* 26, p. 8683, 2016.

HZO FE capacitor fabrication

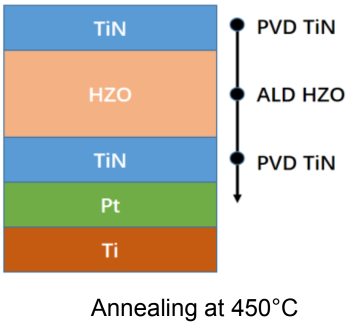


Fig.1 Device structure of fabricated 10nm HZO ferroelectric capacitor with TiN as electrodes. The capacitor area is 100μm×100μm.

Single-domain simulations

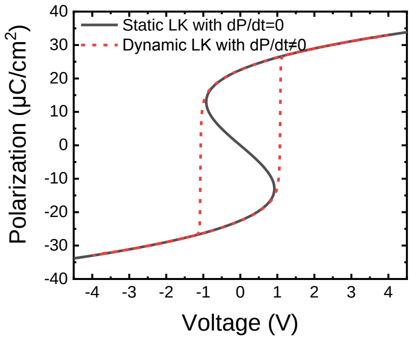


Fig.2 Simulated P-V curves based on static (solid, 'S'-shape) and dynamic (dash, hysteretic loop) single-domain TDLK model.

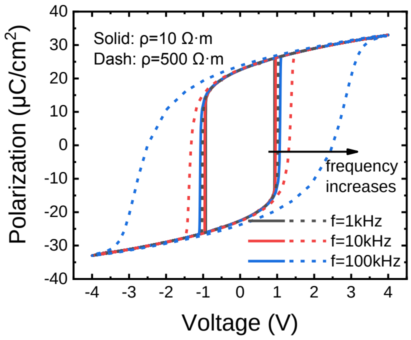
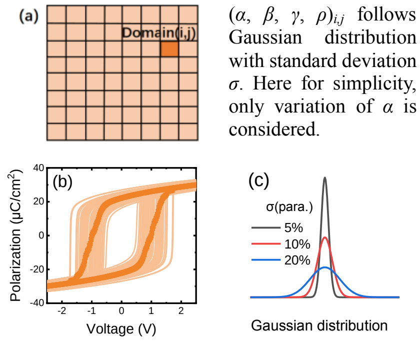


Fig.3 Simulated frequency-dependent P-V loops with different internal resistivity ρ, and the larger the ρ is, the more dispersed the curves are.

Multi-domain simulations



$(\alpha,\ \beta,\ \gamma,\ \rho)_{i,j}$ follows Gaussian distribution with standard deviation σ. Here for simplicity, only variation of α is considered.

Fig.4 (a) Two-dimensional pattern of FE contains $N\times N$ domains. (b) P-V curves of each domain with α following distribution as shown in (c).

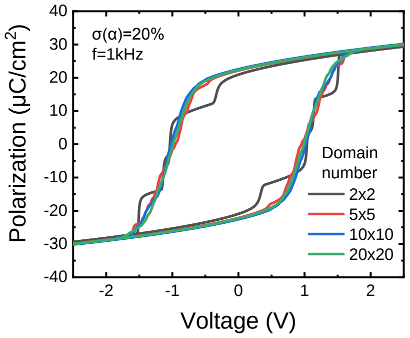


Fig.5 Simulated P-V curves with different domain numbers, where step-like switching occurs with only a few domains.

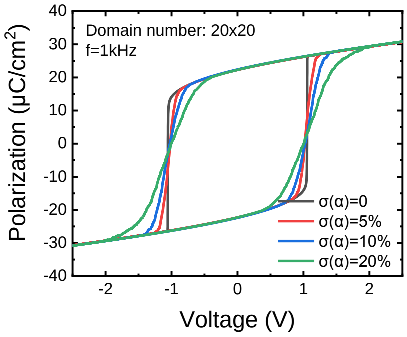


Fig.6 Simulated P-V curves with different standard deviation σ for Landau parameter α, and the smaller the σ is, the steeper the switching is.

Calibration and validation with experimental measurements

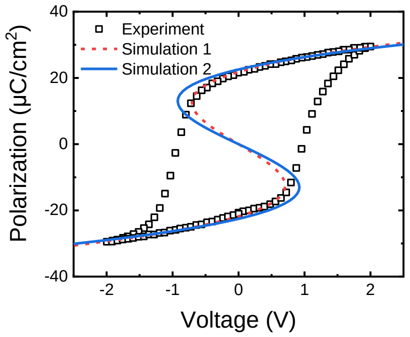


Fig.7 Measured P-V loop and simulated 'S'-shaped P-V curve based on static LK model, to extract the Landau parameters of α, β, and γ.

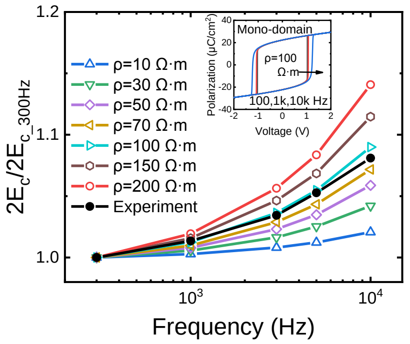


Fig.8 Measured and simulated frequency dependence of E_c normalized to E_c at 100Hz, to extract the dynamic parameter ρ.

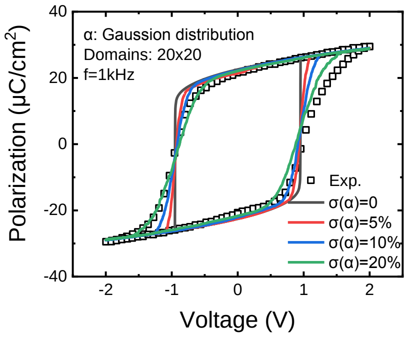


Fig.9 Measured and simulated P-V loops at 1kHz to extract the domain number N and Gaussian distribution for α.

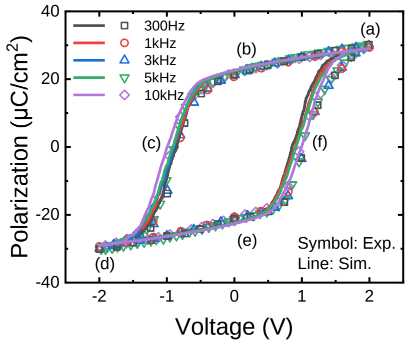


Fig.10 Measured and simulated frequency-dependent P-V loops, which shows an excellent agreement and verifies the simulation method.

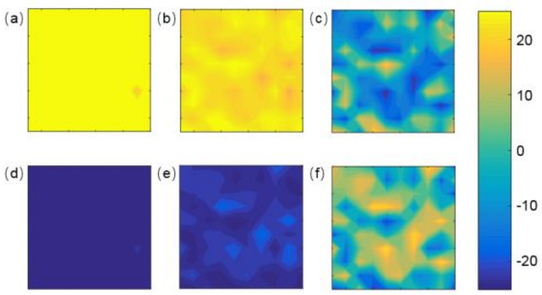


Fig.11 Domain evolution along the hysteresis loop in HZO FE as shown in Fig.10 at 1kHz, where (a) and (d) correspond to $\pm P_s$, (b) and (e) is for $\pm P_r$, and (c) and (f) is for $\pm E_c$, respectively.

Table I HZO ferroelectric parameters used in the simulations

α	-5.3×10^{8} *m/F*
β	5.22×10^{9} $m^5/F/C^2$
γ	0
ρ	100 *Ω·m*
T_{FE}	10 *nm*
$N_{domains}$	20×20
$\sigma_{Gaussion}$	20%×α

* Second-order phase transition of ferroelectric is considered in this work with γ=0.