A Theoretical Study of Multidomain Ferroelectric Switching Dynamics With a Physics-Based SPICE Circuit Model for Phase-Field Simulations

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Abstract—In this article, the multidomain nature of ferroelectric (FE) polarization switching dynamics in a metal–ferroelectric–metal (MFM) capacitor is explored through a physics-based phase-field approach, where the 3-D time-dependent Ginzburg–Landau (TDGL) equation and Poisson’s equation are self-consistently solved with the SPICE simulator. Systematically calibrated based on the experimental measurements, the model well captures transient negative capacitance (NC) in pulse switching dynamics, with domain interaction and viscosity being the key parameters. It is found that the influence of pulse amplitudes on voltage transient behaviors can be attributed to the fact that the FE free energy profile strongly depends on how the domains interact. In addition, we extract the domain viscosity dynamics during polarization switching according to the experimental measurements. For the first time, a physics-based circuit-compatible SPICE model for multidomain phase-field simulations is established to reveal the impact of domain interaction on the NC effect and microscopic domain evolution. The findings of this article may have important implications for the charge boost induced by the stabilization of NC in an FE/dielectric (DE) stack since the so-called capacitance matching needs to be designed at a specific operating voltage or frequency.

Index Terms—HfZrO2 (HZO) capacitor, multidomain ferroelectrics (FEs), phase-field simulations, SPICE circuit model.

I. INTRODUCTION

Since the discovery back in the 1920s [1], ferroelectric (FE) materials have attracted significant research attention because of the possibility to switch their polarization by an externally applied voltage and spontaneous polarization under zero bias. These unique properties make FEs promising materials for emerging nanoelectronic devices. One of the most fundamental yet important applications of FE materials is in FE capacitors, which consist of an FE layer sandwiched between two conducting metal contacts. Such a device structure is believed to have many prospective applications in both high-density nonvolatile memories and neuromorphic computing, including FE random access memories (FeRAMs), FE tunnel junctions (FTJs), and FE field-effect transistors (FeFETs) [2]–[4].

In recent decades, the relentless pursuit of Moore’s law comes to a bottleneck due to the fact that as the device dimensions shrink, the power density in circuits becomes a challenging concern [5]. Based on the Boltzmann statistics, the minimum voltage required for conventional CMOS transistors to achieve a tenfold increase in the channel current is larger than 60 mV/decade at room temperature. This subthreshold swing is considered as a fundamental limit for conventional CMOS transistors. To overcome this thermodynamic limit, [2] proposed to stabilize the transient nature of negative capacitance (NC) by replacing the conventional gate oxide with FE materials, which, in theory, may lead to an internal voltage boost due to the double-well energy profile of the FE. Since then, a considerable amount of research efforts has been put into a thorough understanding of both transient and stabilized NC effects [6]–[11]. In particular, recently discovered doped hafnium FE materials are intensively studied due to the CMOS process compatibility [12]–[14].

Transient NC was experimentally observed during polarization switching in an R-FE capacitor (RFEC) circuit [6], [10]. Such transient NC was considered to be a direct indication of the NC region during polarization switching from one state to the other state. To further characterize the switching dynamics of a HfZrO2 (HZO) capacitor, the transient responses of the voltage across an FE (VFE) were well measured experimentally with various pulse amplitudes in an RFEC circuit [15]. With the single-domain Landau–Khalatnikov theory, the transient NC and its link to the curvature of the free energy profile are explained by the mismatched switching rates of the polarization charge and the free charge provided by the external circuit [16]. From a multidomain perspective,
physics-based phase-field models highlighted the importance of spatially distributed FE grains and domain interaction in pulse switching dynamics [17]–[19]. Moreover, macroscopic transient NC trends in pulse switching experiments can be described by the Preisach model and the delayed responses of FE domains [20]. Alternatively, the observed voltage drop was explained with conventional domain-mediated FE switching mechanisms based on the Kolmogorov–Avrami–Ishibashi (KAI) theory of domain nucleation and growth [21], [22].

Despite all theoretical efforts to explain the experimental measurements of FE switching kinetics, quantitative frameworks that explore the voltage-dependent dynamic responses of FEs and the physical understanding of domain interaction based on experiments are still elusive. Therefore, it is critical to establish a physics-based theoretical model that can be calibrated with experimental measurements for the purpose of studying the multidomain nature of FEs. To elucidate how microscopic domain interaction can change the macroscopic transient NC behaviors, in this article, we adopt a 3-D multidomain phase-field approach that can describe measured domain switching dynamics with well-calibrated parameters. In addition, current FE circuit models in the literature are developed only in either 1-D or 2-D space, and the effect of domain interaction is not considered in those models [10], [23], [24]. For the first time, we develop a physics-based circuit-compatible SPICE model that self-consistently performs 3-D phase-field simulations to further investigate multidomain FE characteristics in an RFEC circuit. With this approach, we model the polarization switching under different voltage pulses and the corresponding transient NC behaviors. By analyzing the effects of domain interaction on the free energy profile, it is shown that the free energy curvature strongly depends on the applied voltage. This finding implies that the depolarization-driven charge boost realized in an FE/dielectric (DE) stack [11] needs to be designed under a specific voltage or frequency. Moreover, we show that the effect of domain interaction cannot be simply viewed as a local effective electric field based on the fact that the gradient free energy significantly affects the total free energy landscape. By further calibrating the transient $V_{FE}$ with experiments, we obtain dynamic domain viscosity responses in the pulse measurements.

This article is organized as follows. In Section II, a general phase-field formalism is presented to describe the polarization switching dynamics of multidomain FEs. Based on the phase-field formulations described in Section II, a circuit-compatible model is developed and implemented with the SPICE simulator in Section III. In Section IV, the simulations results reveal the effects of domain interaction on HZO switching dynamics and the free energy profile. In Section V, we conclude this article by highlighting the multidomain nature of HZO polarization switching and the importance of the SPICE implementation.

II. Phase-Field Formalism

In order to capture the multidomain nature of HZO thin films, we adopt a comprehensive phase-field framework that considers the contributions from the bulk free energy, gradient free energy, electric free energy, and elastic free energy. Under this physics-based framework, the order parameter is a 3-D polarization vector field $\mathbf{P}(\mathbf{r}, t) = (P_1, P_2, P_3)$ as a function of space $\mathbf{r} = (x_1, x_2, x_3)$ and time $t$. The temporal evolution of $\mathbf{P}$ is described by the time-dependent Ginzburg–Landau (TDGL) equation

$$\frac{\partial P_i(\mathbf{r}, t)}{\partial t} = -L \frac{\delta F(P_i, \nabla P_i)}{\delta P_i(\mathbf{r}, t)}$$

$$= -L \left[ \frac{\delta (f_{\text{bulk}} + f_{\text{elec}} + f_{\text{elas}})}{\delta P_i} - \nabla \cdot \frac{\partial f_{\text{elas}}}{\partial \nabla P_i} \right]$$

(1)

where $L$ is the kinetic coefficient (inversely proportional to domain viscosity), and $i = 1, 2, 3$ stands for $x$-, $y$-, and $z$-directions, respectively, [25]–[29]. In general, the total free energy functional $F$ includes the bulk Landau free energy $f_{\text{bulk}}$, the gradient free energy $f_{\text{elas}}$, the electric free energy $f_{\text{elec}}$, and the elastic free energy $f_{\text{elas}}$ over the film volume $V$: $F = \int (f_{\text{bulk}} + f_{\text{elec}} + f_{\text{elas}}) dV$. However, due to the lack of discussion of elastic conditions in HZO thin films in the literature, the elastic energy contributions are excluded to highlight the effect of gradient free energy in this article.

The Landau free energy density can be expanded as

$$f_{\text{bulk}} = a_1 (P_1^2 + P_2^2 + P_3^2) + a_{11} (P_1^4 + P_2^4 + P_3^4)$$

$$+ a_{12} (P_1^2 P_2^2 + P_2^2 P_3^2 + P_3^2 P_1^2) + a_{111} (P_1^6 + P_2^6 + P_3^6)$$

$$+ a_{112} (P_1^4 (P_2^2 + P_3^2) + P_2^4 (P_1^2 + P_3^2) + P_3^4 (P_1^2 + P_2^2))$$

$$+ a_{123} (P_1^2 P_2^2 P_3^2)$$

(2)

where $\{a_i\}$, $\{a_{ij}\}$, and $\{a_{ijk}\}$ are Landau expansion coefficients [30].

The gradient free energy results from the spatial gradients of the polarization and thus can be expressed as

$$f_{\text{grad}}(P_{i,j}) = \frac{1}{2} G_{11} [P_{1,j}^2 + P_{2,j}^2 + P_{3,j}^2]$$

$$+ \frac{1}{2} G_{44} [2P_{1,1}^2 + 2P_{2,1}^2 + 2P_{3,1}^2 + 2P_{1,2}^2 + 2P_{1,3}^2 + 2P_{2,3}^2 + 2P_{3,1}^2]$$

$$= \frac{1}{2} G_{11} [P_{1,j}^2 + P_{2,j}^2 + P_{3,j}^2 + P_{1,2}^2 + P_{2,3}^2 + P_{3,1}^2]$$

$$+ P_{3,2}^2 + P_{1,3}^2 + P_{2,1}^2$$

(3)

where $P_{i,j} = (\partial P_i / \partial x_j)$ is the spatial derivative of $\mathbf{P}$, $\{G_{ij}\}$ are the gradient coefficients that account for the FE domain interaction, and the second equality comes from $G_{44} = G_{11}/2$ [28].

The electric energy density can be calculated as

$$f_{\text{elec}} = -\frac{1}{2} \epsilon_0 \kappa \mathbf{E} \cdot (\mathbf{E} + P_i)$$

(4)

where $\epsilon_0$ is the vacuum permittivity, $\mathbf{E}$ is the total electric field in the FE, $\kappa$ is the background DE constant that accounts for non-FE switching charges, and $\mathbf{P}$ is the FE-contributed polarization obtained from the TDGL equation [29], [31], [32]. The electric displacement field $D_i = \epsilon_0 \kappa \mathbf{E} + P_i$ satisfies the electrostatic equation $D_{i,j} = 0$ if there are no space charges.
inside the film [29]. Poisson’s equation (5) is obtained with \(E\) replaced by the potential gradient \(-\nabla \phi\)

\[
e_{0}k(\phi_{11} + \phi_{22} + \phi_{33}) = (P_{1,1} + P_{2,2} + P_{3,3})
\]

which is subject to the out-of-plane boundary conditions (BCs)

\[
\phi(z = 0) = V_{\text{FE}} \\
\phi(z = t_{\text{FE}}) = 0.
\]

The in-plane BCs are assumed to be periodic due to the fact that top metal contacts are patterned on a continuous FE thin film in experiments [28], [33].

With the aforementioned energy contributions, the governing TDGL equation can be numerically solved by the SPICE simulator with periodic BCs in the in-plane directions and zero BCs in the out-of-plane direction [28], [29], [33].

III. SPICE CIRCUIT MODEL

In this section, we develop the equivalent circuits of the TDGL equation and Poisson’s equation so as to solve for the polarization and potential distributions self-consistently with the SPICE simulator.

A. TDGL Equation

The mathematical form of (1) is similar to the voltage–current relationship of a unit capacitor (\(C = 1\)) [34]. In other words

\[
dV(P_{i}) = I(V(P_{1}), V(P_{2}), V(P_{3}), V_{\text{FE}}) \Rightarrow C \frac{dV}{dt} = I
\]

where \(V(P_{i})\), \(i = 1, 2, 3\) is the voltage representation of the polarization in the SPICE simulator and \(I\) is a voltage-controlled current source as a function of polarization and FE voltage. It is noteworthy that the gradient energy contributions in the right-hand side of (1) can be simplified as

\[
\nabla \cdot \frac{\partial f_{G}}{\partial \nabla P_{i}} = \left( \frac{\partial}{\partial x} \frac{\partial f_{G}}{\partial P_{i,1}} + \frac{\partial}{\partial y} \frac{\partial f_{G}}{\partial P_{i,2}} + \frac{\partial}{\partial z} \frac{\partial f_{G}}{\partial P_{i,3}} \right) G_{11}(P_{i,1} + P_{i,2} + P_{i,3}) = G_{11}\nabla^{2} P_{i}.
\]

With the finite-difference discretization, the Laplacian of a variable can be expressed as

\[
\nabla^{2} P_{i} = \frac{P_{i}(m + 1, n, k) + P_{i}(m - 1, n, k) - 2P_{i}(m, n, k)}{dx^{2}} + \frac{P_{i}(m, n + 1, k) + P_{i}(m, n - 1, k) - 2P_{i}(m, n, k)}{dy^{2}} + \frac{P_{i}(m, n, k + 1) + P_{i}(m, n, k - 1) - 2P_{i}(m, n, k)}{dz^{2}}
\]

where \(\{dx, dy, dz\}\) are the numerical grid spacing and \(\{m, n, k\}\) are discrete indices in each dimension.

(B) Poisson’s Equation

To obtain the multidomain potential profile and the corresponding local electric field, we discretize (5) as

\[
\nabla^{2} \phi = \frac{\phi_{m+1,n,k} + \phi_{m-1,n,k} - 2\phi_{m,n,k}}{dx^{2}} + \frac{\phi_{m,n+1,k} + \phi_{m,n-1,k} - 2\phi_{m,n,k}}{dy^{2}} + \frac{\phi_{m,n,k+1} + \phi_{m,n,k-1} - 2\phi_{m,n,k}}{dz^{2}} = g(\mathbf{P})
\]

where \(g(\mathbf{P}) = (P_{1,1} + P_{2,2} + P_{3,3})/(e_{0}k)\). By rearranging (10), one obtains

\[
\phi_{m,n,k} = -g(\mathbf{P}) + \frac{\phi_{m+1,n,k} + \phi_{m-1,n,k}}{dx^{2}} + \frac{\phi_{m,n+1,k} + \phi_{m,n-1,k}}{dy^{2}} + \frac{\phi_{m,n,k+1} + \phi_{m,n,k-1}}{dz^{2}} = I(\mathbf{P}, \phi_{m,n,k})
\]

where \(\phi_{m,n,k}\) represents \((P_{z,1}/t_{\text{FE}} + \lambda_{1}/\epsilon_{1} + \lambda_{2}/\epsilon_{2})\) is the screening charge density due to out-of-plane polarization and \(\lambda_{1,2}\) and \(\epsilon_{1,2}\) are the screening lengths and relative DE constants of contacts \(1, 2\), respectively. The equivalent circuit diagrams of (1) and (5) are summarized in Fig. 1. Note that it is important to distinguish the total free charge density and polarization in an RFEC circuit [16]. In Fig. 2, the current flowing through the FE capacitor \(I_{R}\) can be calculated as

\[
I_{R} = \frac{dQ_{\text{FE}}}{dt} = \frac{d}{dt} \left( \epsilon_{0}k \frac{V_{\text{FE}}}{t_{\text{FE}}} + P_{z} A \right)
\]

where \(\epsilon_{0}\) is the free charge, \(A\) is the capacitor cross-sectional area, and \(P_{z}\) is the average polarization in the out-of-plane direction. Note that it is more convenient to implement the contact module with Verilog-A based on (13).
It is noteworthy that the measured charge is the total free charge $Q_{FE}$ instead of polarization charge according to (13).

**IV. RESULTS AND DISCUSSION**

Based on the phase-field formalism, we solve the TDGL equation (1) and Poisson’s equation (5) for polarization charge and potential distributions to investigate the pulse switching dynamics of multidomain HZO capacitors in an RFEC circuit. In this article, the baseline experimental measurements are extracted from [15], which demonstrated the transient responses of a TiN/Hf$_{0.7}$Zr$_{0.3}$O$_2$/TiN capacitor under various pulse amplitudes. The parameters used in this article are summarized in Table I.

### Table I: Parameters Used for HZO in This Article

| Parameter          | Value     |
|--------------------|-----------|
| $(\lambda/c)_{1,2}$ (Å) | 0.06, 0.06 |
| $\kappa$            | 35        |
| $t_{FE}$ (nm)       | 10 [15]   |
| $\alpha_0$ (m$^2$/F) | $-4 \times 10^8$ [16] |
| $\alpha_{111}$ (m$^3$C$^{-2}$/F) | $3.7 \times 10^9$ [16] |
| $G_{11}$ (m$^3$/F)  | dynamic   |
| $L$ (μm)$^{-1}$     | $2 \times 10^{-4}$ or dynamic |
| $R$ (Ω)             | 20k [15]  |
| Area (m$^2$)        | $7 \times 10^{-9}$ [15] |

To validate the numerical accuracy of the proposed SPICE model, we also solve the TDGL equation (1) and Poisson’s equation (5) in MATLAB using the semi-implicit Fourier spectral method [36]. Fig. 3 shows the simulated transient responses from the SPICE simulator compared to those from the Fourier spectral method with the same numerical settings and BCs. A negative voltage pulse is applied to the steady-state domain state to obtain the initial conditions for the pulse measurements.

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A. **SPICE Model Initialization and Validation**

In our simulations, the FE film is discretized into $10 \times 10 \times 10$ rectangular cells with the grid size being 1 nm in each dimension. For further analyses, we first obtain the steady-state multidomain polarization distributions and potential profile under zero bias with polarization initialized with a zero-mean normal distribution. A negative voltage pulse is applied to the steady-state domain state to obtain the initial conditions for the pulse measurements.

To validate the numerical accuracy of the proposed SPICE model, we also solve the TDGL equation (1) and Poisson’s equation (5) in MATLAB using the semi-implicit Fourier spectral method [36]. Fig. 3 shows the simulated transient responses from the SPICE simulator compared to those from the Fourier spectral method with the same numerical settings and BCs. A negative voltage pulse is applied to the steady-state domain state to obtain the initial conditions for the pulse measurements.

B. **Effects of $G_{11}$ on the Transient Responses**

From the experimental measurements in [15], the charge in the steady state is found to be suppressed at smaller pulse amplitudes. With our model, we find that the measured saturation free charges at various pulse amplitudes do not

![Fig. 2. RFEC circuit diagram used in [15] and this article.](image)

![Fig. 3. Comparisons between the semiimplicit Fourier spectral method and SPICE circuit simulations of (a) $P_z$ and (b) $V_{FE}$ with $G_{11} = 1 \times 10^{-9}$ (m$^3$/F) at a pulse amplitude of 4 V.](image)

![Fig. 4. SPICE simulations of (a) charge switching dynamics and (b) $V_{FE}$ transient responses with various $G_{11}$ values under a voltage pulse of 4 V (dashed line). (c) and (d) Transient responses of $Q_{FE}$ and $V_{FE}$ with $G_{11}$ correction under various pulse amplitudes.](image)
match those predicted by the phase-field approach with a constant $G_{11}$. As a result, we propose that the gradient coefficient $G_{11}$ (and hence domain interaction) depends on the applied voltage. To verify this argument, we first examine how $G_{11}$ affects the transient behaviors at a pulse amplitude of 4 V. In Fig. 4(a), the saturation charge decreases significantly as $G_{11}$ increases, which indicates that stronger domain interaction tends to suppress polarization switching. Moreover, the experimental measurements in [15] also show that the transient voltage drop disappears as the pulse voltage decreases. This finding is also captured by increasing $G_{11}$. As shown in Fig. 4(b), $V_{FE}$ dynamics acts like a normal DE capacitor and the voltage drop is no longer to be seen as domain interaction gets stronger (or larger $G_{11}$). Next, we extract the $G_{11}$ value for each pulse amplitude based on the saturation total free charge measured in [15]. With extracted $G_{11}$, Fig. 4(c) and (d) shows the transient responses of $Q_{FE}$ and $V_{FE}$ at various pulse amplitudes, which are qualitatively consistent with the experimental observations. Therefore, these simulation results imply that domain interaction of the HZO thin film is weaker under a larger voltage, which may be attributed to the breaking of spatial domain coupling under a large electric field. It is also noteworthy that in this framework, we find that the effect of $G_{11}$ is mainly on the average polarization rather than the spatial variations because of the relatively uniform initial domain state. In reality, the polarization spatial variations would be induced by the inevitable defects inside the FE films, which play an important role in the domain-wall boundaries and, thus, polarization, switching behaviors [37]. Therefore, further theoretical studies of domain interaction mechanisms may rely on more experimental investigations of domain formation and domain-wall characteristics of Zr-doped HfO$_2$ thin films.

**C. Effects of $G_{11}$ on the Free Energy Curvature**

Now, we have shown that $G_{11}$ is dependent on the applied voltage and investigate the effects of domain interaction on the transient response in terms of the free energy dynamics. Fig. 5(a)–(c) shows the free energy dynamics when polarization switches from the negative state to the positive state under a pulse of 4 V with increasing $G_{11}$. Without domain interaction ($G_{11} = 0 \ m^3/F$), the bulk free energy exhibits an NC region (negative curvature) during polarization switching. With a nonzero $G_{11}$, the gradient free energy due to FE domain interaction shows a quadratic shape and, thus, turns the negative curvature of the bulk free energy into a positive one as $G_{11}$ increases. Note that the extracted gradient free energy as a function of polarization is consistent with the parabolic shape obtained from the first-principles calculations [38]. The corresponding free energy curvatures ($\partial^2 U/\partial P_z^2$) near-zero polarization are plotted in Fig. 5(d)–(f). The positive curvature of the total free energy with a larger $G_{11}$ explains how stronger domain interaction can suppress the transient NC. Since $G_{11}$ is voltage-dependent, the energy profile at various voltages depends on how FE domains interact.

The voltage dependence of the free energy curvature implies that FE capacitance can only be matched with a constant DE capacitance for charge boost at a specific voltage based on the fact that the total free energy curvature is directly related to the FE capacitance [6], [16]. Moreover, in Fig. 4(c) and (d), we use a constant $G_{11}$ to simulate the switching dynamics at a given applied pulse due to the short rise time of the pulse. In reality, $G_{11}$ varies when the applied voltage switches from low to high. This indicates that the frequency of the applied pulse affects the FE–DE capacitance matching as well.
Note that the electric free energy has a mathematical form as in (4) and, hence, does not affect the energy curvature, as can be seen in Fig. 5(d)-(f), which demonstrate that $G_{\text{tot}}^2 = (d^2 f_{\text{tot}}/d^2 P) = 0$. As a result, our simulations also show that the gradient energy contribution $G_{11} \nabla^2 P$ cannot be simply treated as an effective interaction electric field because the existence of gradient free energy changes the curvature of the total free energy landscape [19].

D. Dynamic Kinetic Coefficient

Fig. 6(a) shows the extracted $G_{11}$ at each pulse amplitude based on the experimentally measured FE free charge in the steady state. With extracted $G_{11}$ and a constant kinetic coefficient $L$, the measured saturation polarization can be well captured by the phase-field framework. However, the voltage responses during the transient NC are not consistent with experiments. Therefore, we adopt a dynamic $L$ to further characterize the domain viscosity variations during polarization switching. Fig. 6(b) shows the transient kinetic coefficient $L$ at various pulse amplitudes. When $V_{\text{FE}}$ is below the coercive voltage, the constant $L$ represents the inherent DE response. The larger $L$ in the time interval between the gray dashed lines indicates that the polarization switching speeds up due to the unstable nature of the NC region. As the FE capacitance goes back to a positive value, $L$ decreases and the transient $V_{\text{FE}}$ recovers to a normal DE response. For smaller pulse amplitudes, the energy curvature is positive during polarization switching due to stronger domain interaction. Therefore, the transient responses of the FE are similar to DE responses without a voltage drop. Compared with measurements in [15], the simulation results of total free charge $Q_{\text{FE}}$ and FE voltage $V_{\text{FE}}$ with various pulse amplitudes are shown in Fig. 6(c)-(d).

Note that the time interval where $L$ increases may depend on the external circuit components because the increase in $L$ indicates the occurrence of polarization reversal.

Although our simulations show reasonable trends of the measured transient responses, there are some discrepancies between the simulations and experiments, which may result from the elastic free energy. Because HZO materials are not classical perovskites, the crystal structures and the related elastic contributions to the total free energy need further experimental investigations, which is beyond the scope of this article. Further simulations that include broad distributions of bulk Landau parameters show insignificant impacts on the transient responses and confirm the dominant effects of the gradient coefficient (see the Appendix for details). However, the gradient and kinetic coefficients may also have spatial distributions due to the multidomain nature of HZO [10], [18].

E. Comparison With the Preisach-Based Approach

In a previous work [20], a Preisach model combined with the delayed responses of FE domains was used to well describe the macroscopic transient NC trends in pulse switching experiments. Such a Preisach-based approach simulates the polarization switching with the assumption that each domain cell has a different switching threshold voltage and responds instantaneously. The FE switching delay is modeled using Merz’s law, which states that FE polarization switching has a characteristic time depending on the activation field and the applied field [39]. Based on Merz’s law, when the external field is larger than the activation field of the domain cell, the delay time constant decreases exponentially. The smaller delay under a larger external field is qualitatively consistent with the increasing kinetic coefficient as the pulse amplitude increases, as shown in Fig. 6(b).

The advantage of the Preisach-based approach as a circuit-compatible model is that it well captures FE switching characteristics in a more computation efficient manner.
However, for ultrascaled devices that contain few grains, the Preisach-based approach may not be suitable because it is based on the parameter distribution of a large domain ensemble [40], [41]. Moreover, the Preisach model approximates the FE switching dynamics well when the domains only have up and down orientations [42]. In this article, we choose a phenomenological approach for a deeper understanding of microscopic switching mechanisms from the perspective of the thermodynamic free energy. In contrast to the Preisach-based approach, such a thermodynamic phase-field model is not only effective in incorporating free energy contributions but also useful for the studies of domain structures and the FE-paraelectric phase transitions. In addition, the proposed way of solving TDGL and Poisson’s equation in the SPICE simulator can be applied to other physics-based partial differential equations of a similar form.

V. CONCLUSION

In summary, the first physics-based circuit-compatible SPICE model for multidomain FE materials is developed and calibrated with experimental measurements. With this model, we investigate the effect of domain interaction on the transient responses of HZO capacitors under a voltage pulse in an RFEC circuit. We find that FE domain interaction depends on the applied voltage and plays an important role in the dynamic responses of polarization switching and the transient NC effect. By studying how domain interaction affects the total free energy curvature, we show that the effect of domain interaction cannot be viewed as an effective electric field. More importantly, as the domain interaction becomes stronger and stronger, the negative curvature of free energy around zero polarization turns positive. Therefore, the voltage-dependent domain interaction indicates that FE-DE capacitance matching can only be achieved at a specific voltage and frequency. Furthermore, the dynamic nature of FE domain viscosity at a voltage pulse is explored based on the experimental measurements. This article explores the physical roles that phenomenological parameters play in microscopic switching mechanisms for multidomain HZO capacitors, and the proposed circuit model shows the potential for the analyses of HfO$_2$-based FEAs at device and circuit levels.

APPENDIX

DISTRIBUTIONS OF PHENOMENOLOGICAL PARAMETERS

In this article, the spatial distributions of phenomenological parameters are neglected for the purpose of studying the domain interaction in HZO capacitors based on the experimental measurements [15]. In reality, the phenomenological parameters for multidomain FE HZO capacitors may have spatial distributions, which were assumed to be Gaussian distributions for each cell of the multidomain FE film [10]. Besides the simulations in the main text, we also perform the transient simulations with Gaussian-distributed bulk Landau parameters, $\{\alpha_1, \alpha_{11}, \alpha_{111}\}$. In [10], the mean ($\mu$) is the single-domain value and the corresponding standard deviation ($\sigma$) is around 10% of the mean value. To validate the analyses, a relatively broad spatial distribution with a standard deviation of 20% is used here, as listed in Table II. Fig. 7 shows the transient NC responses with and without spatially distributed bulk parameters at different pulse amplitudes. It is found that the broad distributions of Landau parameters have an insignificant impact on the transient NC behaviors under the domain interaction effect, which highlights that the important role domain interaction plays in the FE dynamic responses. Furthermore, it is noteworthy that the switching responses may also be affected by the nucleation process or grain structures [43]–[45]. Thus, the circuit compatibility and computing efficiency would depend on how these polycrystalline effects are implemented.

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