Analytical modeling and Dynamics of Multi-Domains in Negative-Capacitance MFIS-FETs

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Abstract—Analytical modeling and dynamics of multidomain in metal-ferroelectric-insulator-semiconductor (MFIS)-FETs are presented in this paper. The formation of multi-domain (MD) leads to oscillations in the conduction band in the channel and periodicity in the local electric field in the ferroelectric region. The impact of 2-D local electric field on the MD switching is captured in the model using the domain wall velocity concept. The optimum values of oxide thickness, ferroelectric thickness and channel length are calculated which corresponds to mono-domain device operation. Deviation from the optimum device parameters causes the transition of mono-domain state to multi-domain state in the ferroelectric. This work can be used as a guideline for designing MFIS-NCFETs, which provides the device parameters that leads to monodomain state in the MFIS-NCFET.

I. INTRODUCTION AND METHODOLOGY

The formation of multi-domains (MD) in ferroelectric (FE) is an inevitable process during the minimization of system energy [1]. To simplify the analysis, most of the of MFIS-NCFET studies consider only mono-domain condition in the ferroelectric region [2]-[7]. Few very studies have included the impact of MD impact on the ferroelectric. However, these reported papers have neglected the study of state transition, domain wall velocity and the optimization of device. Besides, these studies are based on the numerical solutions of phase field equations [8]-[12].

The divergence in the spontaneous polarization is responsible for the formation of MD in the FE region [1]. To study the impact of MD on FE, $180^\circ$ strip domain pattern is assumed in the ferroelectric region, which is a valid and realistic assumption, for the temperature less than the Curie temperature [1]. Using this assumption, the polarization associated with each domain can be expressed in the form of a Fourier series (1). The 2-D Poisson equation with the divergence of spontaneous polarization term is solved using Green’s function approach [15]. This solution is completely analytical and explicit in nature. The obtained potential function of the FE region ($\phi_{MD}(x,y)$) is used to calculate the domain wall velocity ($V_{dw}$) and the switching of domains is captured by $V_{dw}$ concept [13]-[14]. The domain period ($T_D$) is not known in $\phi_{MD}(x,y)$. Hence, to calculate the $T_D$, first, we consider the equilibrium condition ($V_{gs} = V_{ds} = 0$ $V$) in the MFIS-NCFET. Later, the net thermodynamic energy of the system is minimized to calculate the equilibrium domain period ($T_{D0}$) [16]. The obtained $T_{D0}$ is used in (4) to derive the complete expression of $\phi_{MD}(x,y)$ which valid only for the equilibrium state. The next step is to obtain the value of the domain period and domain wall velocity for a nonzero gate/drain voltage. An iterative procedure is used to calculate the alignment of each domain with the 2-D local field (see Fig. 1). The obtained angle is further used to calculate the voltage-dependent polarization and the domain period for the nonzero applied gate/drain voltage. Finally, the $\phi_{MD}(x,y)$ is updated with the new domain period (for nonzero gate/drain voltage), and, $V_{dw}$ is calculated for any value of applied $V_{gs}$ and $V_{ds}$.

II. RESULTS AND DISCUSSION

Fig. 2 shows the equilibrium domain formation in MFIS-NCFET with the default parameters used in this paper. Fig. 3(a), shows the conduction band profiles plotted at the mid-channel, for various domain periods ($T_D$). As the number of domains increases, the oscillations in $E_c$ increase, due to increment in the periodicity of adjacent positive and negative charges, in the FE region. Fig. 4(a), shows the drain current for the various $T_D$ values, indicates that smaller number of domains (larger $T_D$) reduces the OFF current. Fig. 4(b), shows the subthreshold slope (SS) as a function of $T_D$, for various ferroelectric thickness ($t_{fe}$) values, as the number of domains increases, SS starts to degrade, due to MD effect. Maximum two domains exist for $T_D > L/2$, hence, SS begins to saturate at its minimum value, as $T_D$ approaches to the L/2 limit.

Fig. 5(a), shows the switching of domain’s polarization with variation in the applied gate voltage ($V_{gs}$). As $V_{gs}$ increases, the vertical direction ferroelectric electric field increases, and this in turn, increases the domain wall velocity in the lateral direction [13]. Moment of the upward-facing domains in the x-direction causes gradual reduction in the number of downward-facing domains and this is defined as the switching of domains [14]. Due to this switching of domains oscillations in $E_c$, decrease as $V_{gs}$ increases in Fig. 5(b). Additionally, the period of upward-facing domains ($x_c$) also increases with the increment in $V_{gs}$, and this is another way to define the domain switching in the FE region. Fig. 6, shows the variation in lateral direction E-field of FE ($E_{x,fe}$) with $V_{gs}$. Similar to Fig. 5(b) higher $V_{gs}$ increases $x_c$. Hence, at higher $V_{gs}$ smaller number of oscillations in $E_{x,fe}$ is observed.

Fig. 7(a), shows the variation of lateral-directional polarization ($P_{x,x}$) of the domains with drain voltage ($V_{ds}$). Domains near drain end experience strong lateral E field, hence, their orientation angle ($\theta_x$) is larger than to domains near source end (see Fig. 1). Therefore, the magnitude of $P_{x,x}$ increases gradually, as domain approaches near drain end. On the other hand, as can be seen in Fig. 7(b), the magnitude of vertical-direction polarization ($P_{yz}$) decreases near drain end, due to reduction in the y-direction polarization vector component. Further, $V_{ds}$ also contributes to domain wall velocity and, hence, the switching of domains also takes place with variation in $V_{ds}$, as evident from Fig. 7(a) and (b). Fig. 8 and Fig. 9 show the variation $E_c$ and $E_{x,fe}$ with $V_{ds}$. As $V_{ds}$ increases, $T_D$ increases due to the gradual alignment of the polarization in the lateral direction (switching of domains) or along lateral-E field.

According to [13], domain wall velocity increase exponentially with increases in the net 2-D local electric field. Hence, switching of the MD increases, as net E field increases. Fig. 10(a) and Fig. 10(b) show the $V_{dw}$ for various $L$ and $V_{ds}$ values. Shorter $L$ or higher $V_{ds}$ enhances the lateral E field which increases the magnitude of $V_{dw}$. However, as $t_{fe}$ increases $V_{dw}$ decreases, due to reduced vertical E field at higher insulator thickness. Therefore, the switching of domains can be significantly controlled by the 2-
According to [16] at the higher \( t_{ox} \) monodomain state shows an abrupt transition to multidomain state. The maximum value of \( t_{ox} \), at which the transition takes place is calculated using (9) by putting \( T_D = L \), which represents the extremum of the thermodynamic potential \( (\xi) \) [17]. Subsequently, \( \xi \) is minimized with \( t_{ox} (\partial \xi / \partial t_{ox} = 0) \), to find out the maximum value of \( t_{ox} \), at which the system can exist in the monodomain state, with the minimum thermodynamic energy. Fig. 11(a), shows that as channel length increases (for fixed \( t_{ox} \)), monodomain states starts to shift towards the multidomain state. Therefore, a new device is more likely to have multidomain states and, hence, reduced NC effect. Fig. 11(b), shows the transition of states with variation in \( t_{fe} \). At larger \( t_{fe} \), multidomain state transitions into monodomain state, which is the opposite compared with L. Fig. 11(a) and (b), can be used as device design guidelines, to obtain the optimum values of \( t_{fe}, t_{ox} \) and \( L \) to operate devices in the monodomain region (stronger NC region).

### III. Conclusion

Formation of multi-domains is an essential process to minimize the total system energy. The switching of multi-domains does not directly depend on the gate/drain voltage. Instead, 2-D local electric field is responsible for the switching. Each domain in the FE region moves with a different \( V_{dw} \) due to different E field in each domain. Each domain has dissimilar polarization vector which depends on the local E field of the domain. The transition from monodomain to multidomain depends mainly on \( t_{fe}, t_{ax} \) and the \( L \). The optimum set of physical parameters, to operate the device in monodomain state can be predicted by the model.

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**Spontaneous Polarization Profile (180° strip domains with the domain wall thickness \( d_w \))**

\[
P_{s0} = 20 \, \mu C/cm^2
\]

\[
P_s(x) = P_{s0} \sum \left( (a_j + c_j) \cos(k_jx) + (b_j + d_j) \sin(k_jx) \right)
\]

\[a_j = \cos(k_jd_w) - 1 + \cos(k_ja_1) - \cos(k_ja_2); c_j = \cos(k_ja_2) - \cos(k_ja_3) + \cos(k_ja_3) - \cos(k_ja_4)
\]

\[b_j = \sin(k_jd_w) - \sin(k_ja_2) + \sin(k_ja_2); d_j = \sin(k_ja_2) - \sin(k_ja_3) + \sin(k_ja_3) - \sin(k_ja_4)
\]

### 2-D Potential modeling

\[
\frac{\partial \phi^2}{\partial x^2} + \frac{\partial \phi^2}{\partial y^2} = \frac{\Delta P_s}{\epsilon_{fe}}
\]

**Ferroelectric Region**

\[
\phi_{fe}(x,y) = \frac{2}{t_{fe}} \sum_{m=1}^{\infty} \frac{\sin(k_{m}t_{fe} - y)}{k_{m}\cosh(k_{m}t_{fe})} \bigg[ A_1\sinh(k_{m}L - x) + A_2\sinh(k_{m}(L - x)) \bigg] + \phi_{pol}(x,y)
\]

\[
\phi_{pol}(x,y) = \frac{4P_s}{d_wT_Dt_{fe}\epsilon_{fe}} \sum_{n=1}^{\infty} \frac{\sin(k_{n}t_{fe})}{k_{n}\sinh(k_{n}L)} \sum_{j=1}^{\infty} \frac{(b_j + d_j)t_j - (a_j + c_j)t_j}{k_jk_j^2 + k_j^3}
\]

**Oxide region**

\[
\phi_{ox}(x,y) = \frac{2}{t_{ox}} \sum_{m=1}^{\infty} \frac{\cos(k_{m}t_{fe} + t_{ox} - y)}{\sinh(k_{m}L)} \bigg[ B_1\sinh(k_{m}L - x) + B_2\sinh(k_{m}(L - x)) \bigg] + \frac{2}{t_{ox}} \sum_{m=1}^{\infty} \frac{\sin(k_{m}x)}{k_{m}\sinh(k_{m}t_{ox})} \bigg( D_1\cosh(k_{m}(t_{fe} + t_{ox} - y)) - D_2\cosh(k_{m}(t_{fe} - y)) \bigg)
\]

**Channel region:**

\[
\varphi_{si}(x,y) = \frac{F_g}{2q} \sum_{m=1}^{\infty} \frac{\sin(k_{m}x)D_2}{k_{m}\sinh(k_{m}t_{ox})} \bigg( \cosh(k_{m}(t_{fe} + t_{ax} + t_{si} - y)) + \cosh(k_{m}(t_{fe} + t_{ax} - y)) \bigg)
\]

Where, \( A_1, A_2, B_1, B_2 \) are the boundary gap that are evaluated by considering linear potential profiles along the \( x=0 \) and \( x=L \) line. \( D_1^m \) and \( D_2^m \) are Fourier series coefficients which are evaluated by the potential continuity conditions at \( (x,t_{fe}) \) and \( (x,t_{fe}+t_{ox}) \) boundary interfaces and \( P_{s0}^m = \int_0^L P_s(x) \sin(k_{mx}) \, dx \).
Modeling of domain switching and domain wall velocity

Initially, the system is considered to be in the equilibrium state. Hence the work produces by the voltage sources and the energy of the electric field is expressed as (\(\xi\)) [16]:

\[
\xi = E_{LGD} - 2q\Phi_{fe}(x_v,0) + \int E_{fe}^2/8\pi \quad (9)
\]

Where, \(E_{LGD}\) is standard Landau-Ginzburg-Devonshire functional at zero electric field and \(E_{fe}\) is the 2-D electric field in ferroelectric.

\[
\frac{\partial \xi}{\partial x_1} = 0, \quad (a) \rightarrow T_{D_0} \sim 2x_1 (x_1 = x_2), \quad P_{sx}^{i-1} (x) \quad (10)
\]

\(V_{gs} = V_{ds} = 0\) is the equilibrium condition of domain formations, due to the gradient in spontaneous polarization. Eq. (9) is the condition of minimization of net thermodynamic potential [17], which is used to calculate the equilibrium domain period \((T_{D0})\).

The value of \(\theta_z\) is obtained from (12) used to determine the x and y direction polarization components as:

\[
P_{sx}^i(x, \theta) = P_{sx}^{i-1} \sum \cos(\theta_z^{i-1}); \quad P_{sy}^i(x, \theta) = P_{sy}^{i-1} \sum \cos(\theta_z^{i-1}). \quad (13)
\]

\[
P_{sz}^i = \sqrt{\left(P_{sz}^2\right) + \left(P_{sz}^2\right)} \quad (14)
\]

Eq. (14) is used in (10) to calculate the updated \(P_{sz}^i\). Subsequently, (12) is updated to obtain new \(\theta_z\). An iterative procedure among (10), (12), and (14) is used to obtain the accurate orientation and magnitude of the \(z^{th}\) domain polarization. Note that, due to hyperbolic functions in the electric fields, only 3-4 iterations needed for the convergence.

![Equilibrium domain formation in MFIS-NCFET](image)

**Fig. 2:** Equilibrium domain formation in MFIS-NCFET. Default Parameters: \(t_{ox} = 0.5 \text{ nm}, t_{fe} = 6 \text{ nm}, \phi_m = 4.4 \text{ eV}, \text{S/D doping } = 1 \times 10^{20} \text{cm}^{-3}, V_{gs} = 0 \text{ V}\) and \(V_{ds} = 0.7 \text{ V}\). The material parameters of HfO\(_2\) ferroelectric are taken from [14].

**Fig. 4:** Leakage current increases with domains concentration in the FE region (due to downward shift in the conduction band (see Fig. 3 (b)). (b) SS also degrades with the formation of multdomain, SS saturates to its minimum value, as period approaches to L.

**Fig. 3:** Conduction band energy, plotted in the middle of the channel for various domain periods \((T_D)\). (a) The oscillations in \(E_c\) increase as \(T_D\) decreases. However, magnitude of the oscillations decreases as \(T_D\) decreases, hence, there are no visible oscillations at smaller \(T_D\). (b) Multidomain formations shift the conduction band downwards, hence, degrades the subthreshold performance of the device. Model is validated with the numerical COMSOL simulations [18].

\[
\phi_{fe}(x,y) \rightarrow E_{fe}(x_d, t_{fe}/2), \quad (11) \rightarrow \Delta = (x_1 - x_2) \rightarrow
\]

\[
\frac{da}{dt} = -2V_{dw} \sim -2\exp\left(-\frac{E_{act}}{q_{act}^{i+k}}\right) \rightarrow T_{D}^{i-1} \rightarrow
\]

\[
\theta_{z}^{i-1} = \tan^{-1}\left(\frac{E_{x,fe}^{i-1}}{E_{y,fe}^{i-1}}\right) \quad (12)
\]

Where, \(i\) is the switching time of the domain [14], \(E_{x,fe}\) and \(E_{y,fe}\) are ferroelectric electric fields in \(x, y\) directions respectively, \(x_d = 2x_1/2 + (z - 1)x_2/2\) \(z\) is an integer that represents the \(z^{th}\) domain in the ferroelectric region and, \(z_{max} = 2L/T_{D0}\). \(V_{dw}\) is the domain wall velocity [13], which depends on the 2-D local electric fields. The switching of domains is captured by the moment of domain wall in the FE region.

![Domain switching with the gate voltage](image)

**Fig. 5:** (a) Domain switching with the gate voltage. As \(V_{gs}\) increases, downward-facing domain starts to align with the applied E field, to minimize the potential energy of the system. (b) Due to the switching of domains with increase in \(V_{gs}\) the period of upward domain increases, hence, rate of oscillations decreases.
An abrupt transition from monodomain to multidomain state is observed with increase in insulator thickness. (a) The multidomain state is more probable in the long channel device compared to the short channel device. (b) Larger $t_\text{ox}$ devices are more favorable to the monodomain state.

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