Invited Paper

Device simulation of negative-capacitance field-effect transistors with a uniaxial ferroelectric gate insulator

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Abstract: We model the behavior of uniaxial ferroelectrics and simulate planar negative-capacitance (NC) field-effect transistors (FETs) having a gate insulating film made of a uniaxial ferroelectric. The behavior of such NC FETs strongly depends on the direction of the ferroelectric polarization axis. When the direction is away from being parallel to the ferroelectric film to some extent, the ferroelectric polarization becomes larger than the paraelectric polarization and the ferroelectric film begins to act as a negative capacitor. The NC FETs can then be switched on and off more steeply than conventional metal–oxide–semiconductor FETs. This NC effect is maximized at that moment and becomes weaker as the direction approaches perpendicular to the ferroelectric film.

Key Words: negative capacitance, ferroelectric, field-effect transistor, steep-slope transistor, device simulation, TCAD

1. Introduction

The demand for integrated circuits to reduce the power consumption has been growing for applications in portable, wearable \([1, 2]\), and implantable electronic devices \([1, 3]\) and wireless sensor networks \([4, 5]\). An effective way is to lower the operating voltage, which requires constituent transistors to be switched on and off steeply within a narrow voltage range, or to have a low subthreshold swing \(S\). Since the best value of \(S\) for conventional metal–oxide–semiconductor (MOS) field-effect transistors (FETs) is limited to about 60mV/decade at room temperature, the introduction of new physical phenomena such as quantum tunneling of carriers \([6]\) has been considered so far to overcome this limitation. Negative capacitance (NC) of ferroelectric materials is also one such phenomenon \([7]\) and FETs harnessing this are referred to as NC FETs. NC FETs have similar structures to MOS FETs and in most cases a ferroelectric thin film is inserted into their gate stack as a gate insulator. The ferroelectric film reduces the voltage applied to its underlying structure at a low gate voltage \(V_G\), while enhances it at a high \(V_G\). Owing to this \(V_G\) modulation, the underlying structure experiences a larger variation in the applied voltage than a given variation in \(V_G\); consequently, the drain current steeply
increases or decreases. NC FETs have recently been studied widely and intensively and their steep switching with an $S$ of less than 60 mV/decade has already been reported by a number of research groups [8–10]. Simulation will play an important role in the development of such studies by assisting the understanding of the behavior, prediction of the performance, and exploration of the suitable structure and material of NC FETs. It is therefore urgently needed to establish the simulation method for NC FETs, especially compatible with device simulators in technology computer-aided design (TCAD) systems, because those simulators are universally used for the simulation of standard electronic devices including MOS FETs.

A typical simulation method is intended mainly for an NC FET having a metal film beneath a ferroelectric film in the gate stack. In this method, such an NC FET is divided into two components: the ferroelectric capacitor sandwiched between the internal metal film and gate electrode and the remaining FET structure. They are simulated separately and then the results obtained for the FET structure are corrected on the basis of the voltage across the ferroelectric capacitor [11–16]. Although this method assumes that the polarization is uniform in the ferroelectric film, some recently proposed methods take into account the nonuniformity of the polarization [17, 18]. Owing to the difference in algorithms or core calculation techniques, it seems to be difficult to fully incorporate these methods into device simulators.

We have considered the simulation methods of NC FETs using our original homemade device simulator named Impulse TCAD [19, 20]. Owing to its high customizability that all device properties and all equations governing them can be defined by users, we successfully realized the simulation of NC FETs and revealed their interesting features such as reverse drain-induced barrier lowering, negative drain conductance, and fringing field effect [21–23]. Recently, we proposed a new simulation method taking into account nonuniform polarization fields in ferroelectrics [24]. It has complete applicability not only to Impulse TCAD but also to other standard device simulators, and high extensibility as well, which enables device simulators, for example, to take into account a nature of ferroelectrics that the polarization vectors tend to have the same direction and magnitude. In this method, the polarization vectors are assumed to potentially point in any directions; however, some materials, including hafnia of recent great interest, exhibit uniaxial ferroelectricity [25, 26], that is, the polarization vectors can only point in one direction or the opposite direction in such materials. In this paper, we model uniaxial ferroelectrics in a form that can be used in standard TCAD device simulators and simulate the behavior of planar NC FETs having a gate insulating film made of a uniaxial ferroelectric on Impulse TCAD. Then we investigate the relationship between the polarization axis and the performance of such NC FETs and find that their switching becomes steep only when the angle between the polarization axis and the ferroelectric film is within a certain range.

2. Simulation method

2.1 Governing equations for uniaxial ferroelectrics

In the simulation of NC FETs, the polarization field in the ferroelectric film is a key target. We assumed that it can be written as

\[ P_{\text{FE}} = P d + P_p. \] (1)

The first term on the right side is the component representing the uniaxial ferroelectricity, which is parallel to the unit vector $d$ and whose magnitude is $|P|$. Also, the second term represents the paraelectric component and it was assumed to be simply proportional to the electric field $E$ as

\[ P_p = \chi_p \varepsilon_0 E, \] (2)

where $\varepsilon_0$ is the permittivity of vacuum. The polarization field $P_{\text{FE}}$ interacts with $E$ and affects the behavior of NC FETs. Introducing the electric potential $\psi$ instead of directly dealing with $E$, which is given by $-\nabla \psi$, we can write the energy functional of the ferroelectric film as [17, 20]

\[ U[\psi, P] = \int \alpha P^2 + \beta P^4 + \gamma P^6 + \frac{\delta}{2} |\nabla P|^2 + \frac{1}{2\chi_p \varepsilon_0} |P_p|^2 + (\rho - \nabla \cdot P_{\text{FE}})\psi - \frac{\varepsilon_0}{2} |-\nabla \psi|^2 \, dV, \] (3)
where $\alpha$, $\beta$, $\gamma$, and $\delta$ are material parameters and $\rho$ is the charge density. When the ferroelectric film is in a stable state, this energy is expected not to change with infinitesimal variations in $\psi$ and $P$. The conditions for $\psi$ and $P$ to meet this expectation leads to the following two equations,

$$\nabla \cdot (\varepsilon_p E + Pd) - \rho = 0 \quad (4)$$

and

$$2\alpha P + 4\beta P^3 + 6\gamma P^5 - \delta \nabla \cdot (\nabla P) - d \cdot E = 0, \quad (5)$$

where $\varepsilon_p$ is equal to $(1 + \chi_p)\varepsilon_0$. The first equation is known as Poisson’s equation, and the second equation is referred to as the Landau–Khalatnikov (LK) equation in this paper because it is also derived from the LK model [7, 24, 27]. These two equations govern $\psi$ and $P$ in the ferroelectric film in a steady state.

2.2 Solution of the governing equations in device simulation

The first step in numerical computation is generally to discretize the equation to be solved. To do so, a finite volume method is often used in device simulation. In that method, a target device is divided into polyhedrons including one node of a computational mesh, which polyhedrons are referred to as control volumes (CVs). In this paper, we assumed that each face of a CV is shared with an adjacent CV and intersects with the edge between the nodes of the two CVs at a right angle at the midpoint unless the face is a part of the device boundary, as shown in Fig. 1. Integrating an equation over a CV after describing the parameters and variables in the CV by their values at the associated node and adjacent nodes, we can derive the discretized form of the equation.

The discretized form of Poisson’s equation of Eq. (4) for a node $n$ can be written as

$$\sum_m (\varepsilon_p E_{nm} + P_{nm}) S_{nm} - \rho_n V_n = 0, \quad (6)$$

where the summation is taken over all adjacent nodes $m$, $V_n$ is the volume of $n$’s CV, and $S_{nm}$ is the area of the CV’s face shared with $m$’s CV. Also, $E_{nm}$ and $P_{nm}$ are the electric and ferroelectric polarization fields perpendicular to and on $S_{nm}$ and they were approximated as $E_{nm} = -(\psi_m - \psi_n)/\ell_{nm}$ and $P_{nm} = (P_n + P_m) d \cdot r_{nm}/2$, where $r_{nm}$ is the edge vector from $n$ to $m$ and $\ell_{nm}$ is its length. On the other hand, the LK equation of Eq. (5) can be discretized as

$$\sum_m -\delta P_m \ell_{nm} S_{nm} + (2\alpha P_n + 4\beta P^3_n + 6\gamma P^5_n - d \cdot E_n) V_n = 0.$$  

(7)

Here, $E_n$ is the electric field at $n$ and its component in each direction was approximated as

$$(E_n)_i = \frac{\sum_m E_{nm}(u_{nm})_i(|u_{nm})_i|S_{nm}}{\sum_m (|u_{nm})_i|S_{nm}}, \quad (8)$$
Fig. 2. Schematic views of planar NC FETs (a) with and (b) without an internal metal film. The regions labeled “G”, “S”, and “D” represent the gate, source, and drain electrodes, respectively. The thicknesses of the film components are shown in parentheses in their labels. The thickness of the gate oxide film $T_{\text{OX}}$ is 1 nm in (a) and 5 nm in (b).

where $i$ denotes the $x$, $y$, or $z$-direction and $u_{nm}$ is the unit vector of $r_{nm}$.

In device simulation, since the discretized equations are solved by the Newton–Raphson method, the Jacobians of the left sides of Eqs. (6) and (7) must be derived. Impulse TCAD, however, does this automatically and partially automates even the discretization of equations [20]. When solving the following equation with Impulse TCAD,

$$\nabla \cdot f + s = 0,$$

all a user has to do is to specify the discretized general forms of the inward flux term $f$ and the source term $s$ together with variables in the run script. Then Impulse TCAD discretizes this equation as

$$\sum_m f_{nm} S_{nm} + s_n V_n = 0$$

and derives the Jacobian of this left side automatically. For example, if $f_{nm}$ is specified as $-(\varepsilon_p E_{nm} + P_{nm})$ and $s_n$ as $\rho_n$, Impulse TCAD constructs Eq. (6).

3. Results and discussion

In this paper, we considered simple planar NC FETs as shown in Fig. 2 and assumed that the unit vector in the positive ferroelectric polarization direction $d$ is perpendicular to the gate width direction and has the form

$$d = (\cos \theta, 0, \sin \theta),$$

where $\theta$ is the angle between $d$ and the ferroelectric film. We simulated NC FETs with various values of this ferroelectric polarization angle $\theta$ and investigated the dependence of the behavior, especially the subthreshold swing, on $\theta$.

3.1 NC FETs with an MFMOS structure

First, we simulated the NC FET depicted in Fig. 2(a), which has a metal–ferroelectric–metal–oxide–semiconductor (MFMOS) structure, that is, whose gate stack consists of four layers, namely, a gate oxide film, an internal metal film, a ferroelectric film, and a gate electrode. This NC FET is of n-type and the acceptor concentration in the body are $6 \times 10^{17}$ cm$^{-3}$. The source/drain region has a depth of 50 nm and is formed by donors with a concentration of $1 \times 10^{20}$ cm$^{-3}$ from one edge of the body to a position just below the outer edge of the nearest gate sidewall. The donor concentration decreases with increasing distance from the source/drain region according to a Gaussian function and becomes equal to the acceptor concentration at a position just below the nearest gate edge. In the simulation, the gate length $L_G$ was set to 100 nm, and the gate oxide film thickness $T_{\text{OX}}$, internal metal film thickness, and ferroelectric film thickness $T_{\text{FE}}$ were set to 1, 4, and 10 nm. Also, the charge density $\rho$ in the ferroelectric film was set to zero, and the material parameters listed in Table I were used. The values of ferroelectric parameters $\alpha$, $\beta$, and $\gamma$ were chosen so that the remanent polarization $P_r$...
Table I. Parameters used in the simulation.

| Component      | Material | Parameter | Value                  |
|----------------|----------|-----------|------------------------|
| Body           | Si       | Permittivity $\varepsilon$ | 11.7$\varepsilon_0$ |
| Gate oxide film| SiO$_2$  | $\varepsilon$ | $3.95\varepsilon_0 T_{OX}/(1\text{nm})$ |
| Gate sidewall   | Si$_3$N$_4$ | $\varepsilon$ | 7.8$\varepsilon_0$ |
| Ferroelectric film | Hafnia | $\alpha$ | $-4.64 \times 10^8 \text{m}^3/\text{F}$ |
|                |          | $\beta$  | $-1.29 \times 10^8 \text{m}^5/\text{F}C^2$ |
|                |          | $\gamma$ | $9.88 \times 10^{10} \text{m}^9/\text{F}C^4$ |
|                |          | $\delta$ | $1.56 \times 10^{-8} \text{m}^3/\text{F}$ |
|                |          | $\varepsilon_p$ | 36$\varepsilon_0$ |

Fig. 3. (a) Relationship of the ferroelectric polarization $P_d$ and the electric field $E$ in the considered ferroelectric material plotted along the positive ferroelectric polarization direction $d$. NC states lie on the line A–B. (b) Contribution of $P_d$ to the permittivity divided by the permittivity of vacuum $\varepsilon_0$ and calculated for the NC states.

is 20 $\mu\text{C/cm}^2$, the coercive electric field $E_c$ is 1 MV/cm, and the ferroelectric polarization at $E_c$ is 0.67$P_r$, as shown in Fig. 3(a). On the line A–B in the figure, such a ferroelectric is in an NC state and the contribution of the ferroelectric polarization to the permittivity becomes negative, as shown in Fig. 3(b). The ferroelectric polarization angle $\theta$ was set to be perpendicular to the ferroelectric film, or $90^\circ$, the paraelectric permittivity $\varepsilon_p$ was set to 36$\varepsilon_0$, and the value of the remaining ferroelectric parameter $\delta$ was determined so that the domain wall thickness $T_{dw}$ is 10 nm, which is given by [28]

$$T_{dw} = \sqrt{\frac{6\delta}{-(2\alpha + \beta P_r^2)}}. \quad (12)$$

Figure 4(a) shows the drain current $I_D$ vs gate-to-source voltage $V_{GS}$ characteristics of the NC FET and the corresponding MOS FET at a drain-to-source voltage $V_{DS}$ of 0.05 V. That MOS FET is obtained by merging the ferroelectric film and internal metal film into the gate electrode in the NC FET. Comparing the two $I_D$–$V_{GS}$ characteristics, we can see that the $I_D$ of the NC FET varies more steeply than that of the MOS FET. This is because, in the NC FET, the gate voltage $V_G$ is modulated by the NC of the ferroelectric film. This $V_G$ modulation is shown in Fig. 4(b) as the voltage across the ferroelectric film $\Delta V_G$, to be precise, as the electric potential of the lower surface relative to that of the upper surface. The MOS structure under the ferroelectric film experiences $V_G + \Delta V_G$ as an effective gate voltage and this voltage determines the $I_D$ of the NC FET. The ferroelectric film forms a series capacitor together with the gate oxide film and the depletion layer under the semiconductor surface and the difference between $V_G$ and the flat band voltage is applied to this series capacitor.
Fig. 4. (a) Drain current $I_D$ vs gate-to-source voltage $V_{GS}$ characteristics of (solid line) the NC FET with an MFMOS structure shown in Fig. 2(a) and (dotted line) the corresponding MOS FET at a drain-to-source voltage $V_{DS}$ of 0.05 V. (b) Voltage across the ferroelectric film $\Delta V_G$ in the NC FET. In the simulation, the ferroelectric polarization angle $\theta$ was 90°, that is, perpendicular to the ferroelectric film.

Fig. 5. (a) $I_D$ and (b) $\Delta V_G$ in NC FETs with an MFMOS structure calculated for $\theta$'s of 0°, 30°, and 60° and a $V_{DS}$ of 0.05 V as a function of $V_{GS}$.

Thus, as $V_G$ increases, $\Delta V_G$ increases. Because the underlying MOS structure is subjected to this $\Delta V_G$ variation in addition to the $V_G$ variation, $I_D$ varies with $V_G$ more steeply in the NC FET.

Next, we simulated NC FETs with the same structure as above for different ferroelectric polarization angles $\theta$'s. Figures 5(a) and 5(b) show $I_D$ and $\Delta V_G$ in the NC FETs calculated for $\theta$'s of 0°, 30°, and 60° and a $V_{DS}$ of 0.05 V as a function of $V_{GS}$, and they indicate that the behavior of the NC FETs is strongly dependent on $\theta$. As can be seen from Fig. 5(b), the capacitance of the ferroelectric film is
Fig. 6. (a) Subthreshold swing $S$ of NC FETs with an MFMOS structure at a $V_{DS}$ of 0.05 V as a function of $\theta$. The dotted line represents the $S$ of the corresponding MOS FETs, whose value is 65.1 mV/decade. (b) Capacitance of the ferroelectric film $C_{FE}$ multiplied by $T_{FE}/\varepsilon_0$, where $T_{FE}$ is the thickness of the ferroelectric film. The gray areas represent the region of values of $\theta$ where the evaluation of $S$ failed.

no longer negative when $\theta$ is 0° or 30°.

Figure 6(a) shows the subthreshold swing $S$ of the NC FETs as a function of $\theta$. We calculated $S$ by dividing the $V_{GS}$ width required to increase $I_D$ from $I_{th}/10^3$ to $I_{th}$ by three, where $I_{th}$ is the $I_D$ when $V_{GS}$ is equal to the threshold voltage $V_{th}$, and is defined as $I_{th} = (W_G/L_G)10^{-7}$ A with $W_G$ being the gate width. In general, the $S$ of planar MOS FETs is given by [29]

$$S = \frac{k_B T}{q} \ln 10 \left( 1 + \frac{C_{dep}}{C_{ins}} \right),$$

where $k_B$ is the Boltzmann constant, $T$ is the operating temperature, $q$ is the elementary charge, and $C_{dep}$ is the capacitance of the depletion layer. Also, $C_{ins}$ is the capacitance of the gate insulator and is equal to that of the gate oxide film $C_{OX}$ in the considered MOS FETs. On the other hand, in the NC FETs, $C_{ins}$ is the series capacitance of the gate oxide film and ferroelectric film, and thus Eq. (13) can be rewritten as

$$S_{MFMOS} = \frac{k_B T}{q} \ln 10 \left( 1 + \frac{C_{dep}}{C_{OX}} + \frac{C_{dep}}{C_{FE}} \right).$$

This equation indicates that when the capacitance of the ferroelectric film $C_{FE}$ has a negative value, the NC FETs have a better $S$ than the MOS FETs. The capacitance $C_{FE}$ can be approximated as

$$C_{FE} \approx \frac{\sin^2 \theta}{2\alpha + 12\beta P^2 + 30\gamma P^4} \frac{1}{T_{FE}} + \frac{\varepsilon_p}{T_{FE}},$$

where the first term represents the contribution of the ferroelectric polarization $C_t$ and the second term represents the contribution of the paraelectric polarization and electric field $C_p$. Although $C_p$ is always positive, $C_t$ becomes negative when the ferroelectric film is in an NC state. Figure 6(b) shows $C_{FE}$ calculated as a function of $\theta$ with an assumption that both the ferroelectric polarization $Pd$ and the electric field $E$ are zero. When $V_{GS}$ is equal to $V_{th}$, the voltage across the ferroelectric film is considered to be lower than 0.4 V for most values of $\theta$, as can be inferred from Figs. 4 and 5. This means that, in the subthreshold region, the vertical electric field in the ferroelectric film $E_z$ ($\approx \Delta V_G/T_{FE}$) rarely exceeds 0.4 MV/cm. The electric field parallel to the ferroelectric polarization
axis \( E (\approx E_z \sin \theta) \) will certainly be weaker. Figure 3(b) indicates that \( C_f \) hardly changes with such \( E \) since the contribution of \( Pd \) to the permittivity plotted as a function of \( E \) in that figure is equal to \( C_f T_{FE}/\sin^2 \theta \). Also, \( C_p \) is constant for any electric field. Therefore, it can safely be assumed that \( C_{FE} \) takes the value shown in Fig. 6(b) in the subthreshold region. Then it is immediately apparent from Eq. (14) that when \( C_{FE} \) varies with \( \theta \) as shown in Fig. 6(b), \( S \) varies as shown in Fig. 6(a).

When the ferroelectric polarization axis is close to parallel to the ferroelectric film, that is, when \( \theta \) is close to 0° or 180°, \( C_f \) cannot cancel \( C_p \) and \( C_{FE} \) has a positive value; consequently, the NC FETs have a worse \( S \) than the MOS FETs. On the other hand, when the polarization axis is close to perpendicular to the ferroelectric film, that is, when \( \theta \) is close to 90°, \( C_f \) completely cancels \( C_p \) and \( C_{FE} \) becomes negative; consequently, the \( S \) of the NC FETs becomes better than that of the MOS FETs. The further \( \theta \) is from 90°, the closer the negative \( C_{FE} \) is to zero, and as can be seen from Eq. (14), the better \( S \) becomes in the NC FETs. Since \( C_{FE} \) is a series component of the gate-to-source capacitance \( C_{GS} \), if the negative \( C_{FE} \) is very close to zero, \( C_{GS} \) will become negative. A negative \( C_{GS} \) means that the number of carriers increases with decreasing \( V_{GS} \), that is, the lower \( V_{GS} \) becomes, the larger \( I_D \) flows. Although this will never occur in reality, it is not predictable how real NC FETs behave for a negative \( C_{GS} \). In Fig. 6(b), \( C_{FE} \) is zero when \( \theta \) is about 33° or 147°. When \( \theta \) was close to such an angle, the voltage across the ferroelectric film became very large. Then the simulation became unstable and we could not obtain \( I_D \) in the range of \( V_{GS} \) required to calculate \( S \). The range of values of \( \theta \) that caused such a situation are shown in gray in Fig. 6.

### 3.2 NC FETs with an MFOS structure

We also simulated the NC FETs shown in Fig. 2(b) with a metal–ferroelectric–oxide–semiconductor (MFOS) structure, i.e., without the internal metal film of the MFMOS structure. In our previous study [23], it was found that the performance of NC FETs is affected by the electrical coupling between the gate stack and the source/drain region through the gate sidewall. To avoid the change of such coupling, especially between a side surface of the ferroelectric film and the source/drain region, we obtained the MFOS structure corresponding to the above-mentioned MFMOS structure by merging the internal metal film into the gate oxide film in the MFMOS structure. Although the thickness of the gate oxide film in the MFOS structure then became 5 nm, in the simulation, the permittivity was increased by five times so that the capacitance did not change from before. Figure 7(a) shows the subthreshold swing \( S \) of such NC FETs at \( V_{DS} \) of 0.05 V as a function of the ferroelectric polarization angle \( \theta \). Comparing this figure with Fig. 6(a) with attention paid to the region of values of \( \theta \) where the \( S \) of an NC FET is better than that of the corresponding MOS FET, we can see that such an improvement in \( S \) is reduced by the absence of the internal metal film. This is due to an increase in the magnitude of the ferroelectric film capacitance \( C_{FE} \). In the presence of the internal metal film, the electric field applied to the ferroelectric film becomes almost uniform; however, in the absence of the internal metal film, the electric field varies in the direction and magnitude depending on the position. This non-uniformity of the electric field makes the simulation difficult to converge; consequently, the range of values of \( \theta \) where \( S \) could not be evaluated was extended. Since, as shown in Fig. 3(b), the contribution \( \varepsilon_f \) of the Ferroelectric polarization to the permittivity depends on the electric field, \( C_{FE} \) also differs depending on the position. Owing to a high electric potential in the source and drain regions, a relatively high electric field is applied to both edges of the ferroelectric film. In the MOS FET corresponding to the NC FET shown in Fig. 2(b), the electric field at both upper corners of the gate oxide film is higher than 0.5 MV/cm at a \( V_{GS} \) of 0 V. Such a relatively high electric field is applied to both lower corners of the ferroelectric film in the NC FET, although it is modulated by the ferroelectric film. Then, as seen in Fig. 3(b), the magnitude of \( \varepsilon_f \) increases and the magnitude of \( C_{FE} \) also increases. As a result, the \( V_G \) modulation by the ferroelectric film becomes weaker near its both edges and the improvement in \( S \) becomes smaller in the NC FET without the internal metal film than in that with the internal metal film.

So far, \( V_{DS} \) has been as low as 0.05 V and the electric field applied to the ferroelectric film has been approximately symmetrical about the center plane of the gate. As \( V_{DS} \) increases, however, this symmetry gradually disappears, as shown in Fig. 8. Then the symmetry of the behavior of NC FETs
Fig. 7. $S$ of NC FETs with an MFOS structure calculated for $V_{DS}$’s of (a) 0.05 V and (b) 1 V as a function of $\theta$. The values of $S$ of the corresponding MOS FETs, shown by the dotted lines, are 65.1 and 64.9 mV/decade.

Fig. 8. (a) Electric potential distribution in the MOS FETs corresponding to NC FETs with an MFOS structure at a $V_{GS}$ of 0.4 V and a $V_{DS}$ of 1 V. The black lines represent equipotential lines and the difference in the potential between two neighboring lines is 0.05 V. (b and c) Polarization fields in the ferroelectric films in the NC FETs with $\theta$’s of 45° and 135°. The electric potential distributions in the NC FETs are also shown by the equipotential lines.

with respect to the ferroelectric polarization angle $\theta$ measured from the normal of the ferroelectric film, 90°, such as the subthreshold swing $S$ shown in Figs. 6(a) and 7(a) may also disappear. As can be inferred from the electric field near both upper corner of the gate oxide film in MOS FETs shown
in Fig. 8(a), the electric field entering the ferroelectric film in NC FETs has an angle of about 45° at the source-side corner and has an angle of 135° at the drain-side corner. For this electric field, when \( \theta \) is 45°, the last term on the left side of Eq. (5), \( d \cdot E \), becomes about \( |E| \) at the source-side corner and becomes about zero at the drain-side corner. On the other hand, when \( \theta \) is 135°, the opposite occurs. Thus, when \( V_{DS} \) is high to some extent and the electric field entering each lower corner of the ferroelectric film has a different magnitude, an NC FET with a \( \theta \) of 45° probably shows different behavior than that with a \( \theta \) of 135°. If one set \( \theta \) to other than 90° to bring out better NC effects, this kind of behavioral asymmetry may have negative effects on the performance of some circuits where the source and drain of transistors are interchanged during operation. This is because, for the ferroelectric film, the interchange of source and drain means that the ferroelectric polarization angle is changed from \( \theta \) to \( 180° - \theta \). Finally, we simulated the NC FETs without an internal metal film for a high \( V_{DS} \) of 1 V. Figure 7(b) shows the dependence of their \( S \) on \( \theta \) and its symmetry still seems to be preserved. Comparing the electric potential distributions in the NC FETs with \( \theta \)'s of 45° and 135° respectively shown in Figs. 8(b) and 8(c), we can see that they are quite different near the drain-side edge of the ferroelectric film. This difference causes a difference in the electric potential distribution near the gate-drain edge of the semiconductor body, although it is smaller. In the other regions of the semiconductor body except for the region very close to the gate-source edge, however, such a difference is not clearly observed between the two NC FETs. They thus have a similar \( S \). This holds true for the other pairs of NC FETs.

4. Conclusions

We developed a method for standard device simulators to simulate the behavior of uniaxial ferroelectrics and incorporated it into our original homemade device simulator named Impulse TCAD, thereby realizing the simulation of planar NC FETs with a gate insulating film made of a uniaxial ferroelectric. The behavior of such NC FETs varies greatly depending on the direction of the ferroelectric polarization axis regardless of the presence or absence of an internal metal film. When the angle between the direction and the ferroelectric film becomes large to some extent, the ferroelectric polarization exceeds the paraelectric polarization and the ferroelectric film acts as a negative capacitor; consequently, the NC FETs can be switched on and off more steeply than the corresponding MOS FETs. This NC effect is maximized at that threshold angle and becomes weaker as the angle approaches perpendicular to the ferroelectric film. Choosing an angle close to the threshold angle as the ferroelectric polarization angle, however, should be avoided, because the NC of the ferroelectric film can potentially make the gate-to-source capacitance negative and then destabilize the behavior of the NC FETs in some operating conditions. When the angle is not perpendicular to the ferroelectric film, the behavior of NC FETs without an internal metal film may change by an interchange of the source and drain. This kind of asymmetry, however, was not observed in the NC FETs with a gate length of 100 nm and it might appear in the NC FETs having a shorter gate.

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