A Physics-Based Model for Mobile-Ionic Field-Effect Transistors With Steep Subthreshold Swing

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ABSTRACT A physics-based model and the corresponding simulation framework for the mobile-ionic field-effect transistor (MIFET) exhibiting the ferroelectric-like behaviors are innovatively proposed based on two-dimensional (2D) Poisson’s equation and non-equilibrium Green’s function (NEGF), coupling with ion drift-diffusion equations. The simulation framework captures the dynamic distribution of mobile ions’ concentrations within dielectric along the external electric field. TaN/amorphous-ZrO$_2$/TaN capacitors are experimentally characterized for the model calibration. It is proved that the mobile ions dominate the ferroelectric-like behaviors in MIFETs. Sub-60 mV/decade can be achieved in MIFETs based on the proposed model, which is consistent with the experimental results.

INDEX TERMS Subthreshold swing (SS), ZrO$_2$, ferroelectric-like, mobile-ionic field-effect transistor (MIFET).

I. INTRODUCTION

Nowadays, novel computing cells and architectures based on non-volatile memories (NVM) have been developing rapidly due to the potential for achieving low stand-by leakage and energy-efficient computing [1], [2], [3], [4]. However, traditional NVMs such as Flash have certain limitations including speed and endurance [1]. On the other hand, emerging two-terminal NVMs such as magnetic tunnel junctions, resistive RAMs, phase change memories and ferroelectric capacitor memories will face the issues of read disturbing and undesired current during programming/erasing [4], [5]. Therefore, novel three-terminal NVM devices are urgently needed to counter the limitations associated with the existing technologies. In recent years, some novel three-terminal NVMs with steep sub-threshold swing (SS), such as ferroelectric field-effect transistors (FeFETs) with poly-crystalline doped-HfO$_2$ gate insulator, and mobile-ionic field-effect transistors (MIFETs) with amorphous ferroelectric-like dielectrics (ZrO$_2$, Al$_2$O$_3$, La$_2$O$_3$, etc.), have been demonstrated with higher endurance and lower operation voltage [6], [7], [8], [9], [10], [11]. The working mechanism and fabricate process of FeFETs have been extensively analyzed with relatively complete theories [12], [13], [14], while the underlying mechanism of MIFETs cannot be explained by the traditional theories [10]. Some reports have claimed that the mechanism of amorphous films relies on the accumulation and dispersion of the mobile ions [10], [15], [16]. However, the model and the corresponding simulation framework related to mobile ions movement in amorphous dielectric under external field, which can predict the ferroelectric-like behavior, is yet to be understood.
In this paper, we propose a physics-based model describing mobile ions in the dielectrics of MIFETs based on the self-consistent two-dimensional (2D) Poisson's, non-equilibrium Green’s function (NEGF), and ion drift-diffusion (IDD) equations. The mechanism of mobile ions is well described to predict the non-volatile and steep SS characteristics in MIFETs, which are consistent with experiments.

II. MODELING AND SIMULATION METHODOLOGY

As illustrated in Fig. 1(a), an MIFET considering the migration and accumulation of oxygen vacancies \((V^{2+}_O)\) and negatively charged oxygen ions \((O^{2-})\) in the dielectric is simulated. The simulation framework is shown in Fig. 1(b). The proposed model for MIFET consists of three coupled parts, including the one-dimensional (1D) IDD equations for the concentration distribution of mobile ions \((n_{V/O})\) in the dielectric, the 2D Poisson’s equation for potential \((\phi)\) in the whole region of metal-oxide-semiconductor (MOS) and the 2D NEGF for charge density profile \((\rho)\) in the semiconductor channel region.

Ignoring the generation and recombination of ions for the simplification of the model, the IDD equations are formulated by combining the carrier transport equation and the continuity equation, as follows,

\[
\frac{\partial n_{V/O}}{\partial t} = D_{V/O} \frac{\partial^2 n_{V/O}}{\partial z^2} - \frac{\partial \left( v_{V/O} \cdot n_{V/O} \right)}{\partial z},
\]

where \(n_{V/O}, D_{V/O}\), and \(v_{V/O}\) represent the mobile ions concentration, the diffusion coefficient, and the drift velocity of the mobile \(V^{2+}_O/O^{2-}\) in the dielectric, respectively. In Eq. (1), \(z\) represents the position along the dielectric-semiconductor interface direction, and \(t\) represents time. The drift velocity of mobile ions is described by the point ion model of Mott and Gurney as [16]:

\[
v_{V/O} = \pm a_{V/O} f_{V/O} e^{- \frac{E_{av}/O}{kT}} \sinh \frac{2a_{V/O}E_z}{kT}
\]

where \(E_z\) is electric field intensity along the \(z\)-direction, \(a_{V/O}\) is effective hopping distance of \(V^{2+}_O/O^{2-}\), \(E_{av}/O\) is the average height of the potential barrier of \(V^{2+}_O/O^{2-}\), \(f_{V/O}\) is the attempt frequency \(V^{2+}_O/O^{2-}\), \(k\) is Boltzmann constant, \(T\) is temperature. The diffusion coefficient can be described as [17]:

\[
D_{V/O} = 2a^2 e^{- \frac{E_{av}/O}{kT}}
\]

Actually, the total number of mobile ions should be remained unchanged regardless the generation and recombination of mobile ions. Therefore, the boundary conditions should be:

\[
F|_{z=0} = D_{\frac{\partial n_{V/O}}{\partial z}}|_{z=0} - v_{V/O} n_{V/O} |_{z=0} = 0
\]

\[
F|_{z=L} = D_{\frac{\partial n_{V/O}}{\partial z}}|_{z=L} - v_{V/O} n_{V/O} |_{z=L} = 0
\]

where \(F\) is the ions flow, and \(L\) is the thickness of the film.

Here, we assume \(n_{V/O}\) in dielectric does not vary significantly along the \(x\)-direction. Therefore, 1D IDD equation is enough to describe the movement of \(V^{2+}_O\) and \(O^{2-}\) in the dielectric. Once \(n_{V/O}\) is obtained, we will extend these values uniformly to the \(x\)-direction and use them as the input of Poisson’s equation in the amorphous dielectric region, as shown in Fig. 1(b). For the semiconductor region, a self-consistent solution between Poisson’s equation and NEGF equation ensures the consistency between the charge distribution \((\rho)\) and the potential profile \((\phi)\).

In order to describe the characteristics of devices more accurately, instead of coupling the 1D Poisson’s equation in [16], we use the 2D Poisson’s equation as shown in Fig. 1(b),

\[
- \epsilon_0 \left[ \frac{\partial}{\partial x} \left( \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial z} \left( \frac{\partial \phi}{\partial z} \right) \right] = 2q \left( n_{V/O} - n_{O} \right) + \rho,
\]

where \(\epsilon_s\) and \(\epsilon_z\) are relative permittivity of the \(x\) and \(z\) directions, respectively. \(\epsilon_0\) is vacuum permittivity, and \(q\) is the charge of an electron. Here, \(\rho\) and \(\phi\) satisfy:

\[
\rho(\phi) = -q \left[ n(\phi) - p(\phi) - N_A + N_D \right],
\]

where \(n(\phi)\) and \(p(\phi)\) are the electron and hole concentrations, respectively, at a given \(\phi\). \(N_A\) and \(N_D\) are the concentrations of the acceptor and donor, respectively, in the semiconductor.

It is worth noting that the details of NEGF model has been described in [18], [19], and we list several key formulas in Fig. 1(b).

Hence, the whole modeling framework consists of three parts coupling with each other. In order to conduct the numerical modeling, a prediction-correction approach is proposed and used to solve the self-consistent problem, as shown in Fig. 2. Note that, the proposed model is applicable...
to this kind of amorphous dielectrics with ferroelectric-like behavior induced by mobile ions, including amorphous ZrO$_2$ [6], [7], amorphous Al$_2$O$_3$ [8], [9], [10], La$_2$O$_3$ [11], and so on. Note that, the existing numerical simulation solvers cannot solve this coupled problem. Therefore, we independently developed the solution algorithm based on the prediction-correction approach for the proposed model. In addition, our code is developed based on MATLAB v2021a environment.

III. RESULTS AND DISCUSSION

A. MODEL CALIBRATION

To verify the proposed model and extract the parameters for simulation based on the proposed modeling framework, positive-up, negative-down (PUND) measurements of a metal-insulator-metal (MIM) capacitor with 3.5 nm-thick amorphous (a)-ZrO$_2$ were carried out first. The details of the device fabrication process can be found in Refs. [6], [7]. The high-resolution transmission electron microscope (HRTEM) image of the MIM capacitor is shown in Fig. 3(a). Here, we have made a reasonable assumption that drift velocity of O$_2^-$ are much larger than those of V$_2^+$ according to previous study [19]. As shown in Figs. 3 (b, c), the induced charge on the metal can be extracted by Gauss’s law as follows

$$Q = Q_{MI} + D|_{z=zi},$$

where $zi = 2.5$ nm, $Q_{MI} = Q_O - Q_V$. $Q_{MI}$ is the total charge densities of mobile ions inside the selected Gaussian surface. $Q_O$ and $Q_V$ are O$^{2-}$ and V$^{2+}$ charge density inside the selected Gaussian surface, separately. The electric displacement vector is $D = \varepsilon_0\varepsilon_r E(z)$, which is a function of $z$.

The waveform of applied voltage of simulated PUND at a given frequency of 10 kHz within the voltage range $-4.5$ V $\sim$ 4.5 V and the corresponding current response are shown in Fig. 4 (a). The corresponding $Q$-$V$ curve is shown in Fig. 4 (b). The parameters are summarized in Fig. 4(c). Our simulation results have achieved good agreement with the measured $QPUND$-$V$ characteristics as plotted in Fig. 4 (d). This result demonstrates that the proposed modeling framework can reproduce the ferroelectric-like behaviors decently and get a deep insight into the underlying mechanism. Note that, the saturation charge density of $QPUND$ ($QPUND_{sat} = \pm 2.51 \ \mu C/cm^2$), cannot be simply defined by the maximum or minimum of $Q_{MI}$. Comparing Fig. 4 (b) with Fig. 4 (d), $QPUND_{sat}$ ($\pm 2.51 \ \mu C/cm^2$) are exactly equal to $Q$ at $V = 0$ V, while the minimum and maximum of $Q_{MI}$ are $-2.40 \ \mu C/cm^2$ and 5.95 $\mu C/cm^2$, respectively. Therefore, the minimum or maximum of $Q_{MI}$ cannot completely represent $QPUND_{sat}$, and the reasonable $Q_{MI}$ should be distributed in $-2.40 \sim 5.95 \ \mu C/cm^2$ in our simulation.
noted that hysteresis I_D-VGS curves induced by mobile ions without mobile ions, as illustrated in Fig. 5(b). It should be clearly, we mark ent states. In order to analyze the movement of ions more shown. (b) Comparison of I_D-VGS curves between the simulated results of MIFET and the normal FET without mobile ions at V_DS = 0.05 V. (c) The extracted SS curves from (b).

B. FERROELECTRIC-LIKE BEHAVIORS DETERMINED BY MOBILE IONS

The considered MIFET structure is shown in Fig. 5(a), where N_D = 10^{20} \text{ cm}^{-3} in source and drain region, N_A = 10^{12} \text{ cm}^{-3} in channel region. We compare the simulated I_D-V_DS curves under the 10 kHz triangular waveform at a 2.5 V to -2.5 V of the FETs with and without mobile ions, as illustrated in Fig. 5(b). It should be noted that hysteresis I_D-V_DS curves induced by mobile ions can also be extracted by simulation. The drain voltage (V_D) is 0.05 V. The proposed model successfully predicts the counterclockwise ferroelectric-type hysteresis. A larger current density compared with the MOSFETs without mobile ions is also obtained, which was proved in experiments [6], [7].

To illustrate the effects of movement of mobile ions in dielectric on the ferroelectric-like behaviors in MIFETs, we chose 8 states (A-H) on I_D-V_DS curves, as shown in Fig. 5(a), for insight of ions movement in the forward/reverse sweeps, where the sequence of A->B->C->D->E (for V_DS = -2.5 V, -2.0 V, -0.9 V, -0.4 V, 2.5 V) is the forward sweep, while E->F->G->H->A (for V_DS = 2.5 V, 2.0 V, -0.4 V, -0.9 V, -2.5 V) is for the reverse sweep. SS curves at a V_DS of 0.05 V of FETs with and without mobile ions are shown in Fig. 4(c), where states D and H correspond to the minimum SS during the forward and reverse sweeps, respectively. Fig. 6 shows the distributions of mobile V^2_O and O^2^- along the z-direction of MIFET for the different states. In order to analyze the movement of ions more clearly, we mark Q_O, Q_V and Q_M near the channel/dielectric interface (6-7 nm) and dielectric/gate interface (8.5-9.5 nm) in the Fig. 6. Here, we have made a reasonable assumption that the movement of V^2_O can be ignored compared to the movement of O^2^- [20] and the charge of V^2_O near the channel/dielectric interface (6-7 nm) and dielectric/gate interface (8.5-9.5 nm) remains constant (2.40 \mu C/cm^2). For the forward sweep, initially, the accumulated O^2^- charge near the channel/dielectric interface (6-7 nm) is 4.79 \mu C/cm^2 at a V_DS of -2.5 V (state A). As V_DS increases to -2.0 V (state B), due to that there is still a strong enough external electric field to make the drift of O^2^- greater than the diffusion of O^2^-, a small amount of O^2^- still moves to the channel/dielectric interface. Therefore, the accumulated O^2^- charge near the channel/dielectric interface (6-7 nm) increases to 5.26 \mu C/cm^2. With the increase of V_DS to -0.9 V (state C), the electric field in the z+ direction is not enough to maintain the high concentration of O^2^-. At the gate end, and O^2^- gradually starts to inject into the dielectric, accumulated O^2^- charge near the channel/dielectric interface (6-7 nm) decreasing to 4.22 \mu C/cm^2, while the one near the dielectric/gate interface (8.5-9.5 nm) increasing to 0.54 \mu C/cm^2. With a further increase of V_DS to 0.3 V (state D), more and more O^2^- moves to the gate metal/dielectric interface, and the accumulated O^2^- charge near the dielectric/gate interface increasing to 1.43 \mu C/cm^2. As V_DS continues to increase, up to V_DS = 2.5 V (state E), almost half of O^2^- ions accumulate at the gate metal/dielectric interface, and the accumulated O^2^- charge near the dielectric/gate interface increasing to 6.39 \mu C/cm^2. For the reverse sweeping, i.e., E->F->G->H->A, the process of O^2^- moving demonstrates quite the opposite. To verify the effect of mobile ion migration on ferroelectric-type hysteresis, the potential profiles in the whole region of MIFETs at states C, D, G, and H are shown in Fig. 7. It’s obvious that at states C and...
D, the surface potentials of the channel are lower than the ones of metal, while at states G and H, surface potential in the channel is higher than in gate metal. In other words, the surface potential should have been lower/higher than the gate potential, but due to the accumulation of mobile ions, the surface potential remained higher/lower than the gate potential. These phenomena mean that the mobile ions controlled by the $V_{GS}$ can dominate the surface potential of the channel, resulting in ferroelectric-type hysteresis.

The SS of a transistor can be evaluated by the surface potential amplification factor $A_{\varphi}$, which is expressed as [21]:

$$A_{\varphi} = \frac{\partial \varphi_s}{\partial V_{GS}}$$  \hspace{1cm} (8)

where $\varphi_s$ is the surface potential at the channel. We chose surface potential at the midpoint of the channel as the $\varphi_s$ for convenience, as shown in Fig. 7. The $\varphi_s$-$V_{GS}$ and $A_{\varphi}$-$V_{GS}$ curves of transistors with and without considering mobile ions are shown in Figs. 8 (a) and (b), respectively. MIFETs achieve a strong modulating efficiency of $\varphi_s$ with considering the mobile ions, which produces a steep sub-$kT/q$ SS.

Thanks to the amplification effect of the semiconductor surface potential caused by ions movement in the dielectric, MIFETs can realize ultra-steep SS both in forward and reverse sweep, which is consistent with the experimental results [22]. This trend is not limited to the ballistic NEGF model but is generally valid since the assumption of ballistic transport does not significantly change the interaction of the mobile ions in a dielectric with the underlying channel.

Note that, different from changing the resistance of the dielectric layer through the filament forming, or the increment of electronic traps concentration [23], [24], our model focuses on the influence of the movement and accumulation of mobile ions on the potential distribution of the whole device, so as to realize ultra-steep SS by dominating the surface potential of channel.

IV. CONCLUSION

We have innovatively proposed a physical-based model describing mobile ions movement in the dielectric of MIFET based on 2D Poisson’s, NEGF, and IDD equations. Using the corresponding simulation based on the modeling framework, we have described the important effects of mobile ions in amorphous dielectrics on SS characteristics of MIFETs. Furthermore, sub-60 mV/dec-sw characteristics of MIFETs have been achieved by simulation which is consistent with the experimental results [22].

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