# Importance of Self-Consistent and Transient Technology Computer-Aided Design Simulation of a Negative Capacitance Transistor

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#### Abstract

We discuss the importance of self-consistent technology computer-aided design (TCAD) simulation of negative capacitance transistors (NCFETs). To attain a fully coupled TCAD simulation, we applied an in-house TCAD module, named "Impulse TCAD.". With this approach, many unique characteristics such as the negative draininduced barrier-lowering effects can be predicted. The effectiveness of transient analysis in the case where the negative capacitance is unstable is also shown.

## 1. Introduction

The Internet of Things (IoT) is expected to be a new and smart platform in many industries owing to its capability to connect a tremendous number of electronic devices and collect their data. For an IoT network to be realized, high energy efficiency is a prerequisite for the large-scale integration (LSI) of the connected devices. For this reason, the negative capacitance transistor (NCFET) [1], which exploits a ferroelectric thin film as a gate insulator, has attracted much attention recently. In conventional metal-oxide-semiconductor field-effect transistors (MOSFETs), the physical limitation of the minimum subthreshold swing (SS) of 60 mV/decade constrains the reduction in the operation energy by decreasing the supply voltage. In NCFETs, however, the possibility of a steep SS of less than 60 mV/decade by harnessing the negative capacitance (NC) has been theoretically predicted [1]. Moreover, the discovery of ferroelectricity in orthorhombic HfO<sub>2</sub> in 2011 [2] has provided an excellent process compatibility between NCFETs and conventional MOSFETs because the high-k HfO<sub>2</sub> film is widely used as a gate insulator in state-of-the-art logic CMOS. Currently, a number of excellent demonstrations of NCFETs have been reported [3,4].

For improving the performances of NCFETs and for understanding their device physics, which exploit an elusive NC state, technology computer-aided design (TCAD) simulation is absolutely essential. There are two ways to simulate NCFETs using TCAD. The first one is through the so-called hybrid TCAD [5]. In this method, after the characteristics of conventional MOSFETs are simulated using TCAD, the effects of NC are factored in as a post-calculation. This is convenient but not necessarily self-consistent. The other one is through a fully coupled manner [6], in which both equations relating the transport and the NC are simultaneously and selfconsistently solved. Recently, we have developed an in-house TCAD simulation module, named "Impulse TCAD," which enables the self-consistent simulation of the device characteristics of NCFETs [6,7]. In this paper, we discuss the recent results obtained by Impulse TCAD including the short-channel effects and the effectiveness of the transient analysis of NCFETs.

# 2. Simulation Method

*Concept of the negative capacitance* 

Generally, the spontaneous polarization of an idealistic ferroelectric material is described by the Landau–Khalatnikov (LK) equation:

$$\rho \frac{dP}{dt} = -\nabla_P G \tag{1}$$
$$G = \alpha P^2 + \beta P^4 + \gamma P^6 - EP \tag{2}$$

where *P*, *E*, and *G* are the ferroelectric polarization, the electric field, and the Gibbs free energy, respectively.  $\alpha$ ,  $\beta$ , and  $\gamma$  are the ferroelectric material parameters.  $\rho$  is also a material parameter that accounts for the polarization switching speed. If we consider a steady state of d/dt = 0, Eq. (1) leads to

$$\mathbf{E} = 2\alpha P + 4\beta P^3 + 6\gamma P^5 \tag{3}$$

Figure 1 shows the typical *P*-*E* curves predicted by the LK equations [Eqs. (1) and (2)] for a metal (M)/ferroelectric (F)/metal (M) structure and an M/F/insulator (I)/M structure. In the MFM structure, the spontaneous polarization with hysteresis that can be observed in a ferroelectric material is obtained. In contrast, Eqs. (1) and (2) yield an S-shaped curve in an MFIM structure by choosing the appropriate thicknesses of the F and I layers. In the S-shaped curve, we can see a region in which the differential capacitance dP/dE is negative (NC state). This means that, because the NC state is unstable in an isolated F layer (MFM), it can be stabilized by stacking a paraelectric layer such as an I or a semiconducting (S) layer.



**Fig. 1** Typical P-E curves for MFM (green) and MFIM (red) stacks predicted by the LK equations [Eqs. (1) and (2)].

# Simulation framework

In our fully coupled TCAD tool, Impact TCAD, the concerned device structure is meshed like in conventional TCAD. After the meshing, the LK equations and the physical equations for MOSFET are solved simultaneously and self-consistently at every grid point in the transistor structure [6].

#### 3. Results and Discussion

## DC simulation of NCFETs

In general, DC characteristics such as the drain current  $I_D$  versus the gate voltage  $V_{GS}$  curve, the voltage is considered as the independent variable in the TCAD simulation. When we apply this approach to the simulation of NCFETs, we need to consider Eq. (3). Figure 2 shows the typical simulation results of double-gate (DG) NCFETs. In this simulation, the gate length was changed from 10 to 100 nm. As can be seen in Fig. 2, the threshold voltages shifted toward the positive side. Moreover, the SS values somewhat improved by reducing the gate length. This means that the short-channel effects in the NCFETs have the opposite trend. This tendency has been referred to as the negative (reverse) drain-induced barrier-lowering effects [6]. We have clarified that these phenomena are mainly attributable to the fringe coupling between the gate capacitance and the drain region [6].



**Fig. 2**  $I_{\rm D}$ - $V_{\rm GS}$  curves for DG-NCFETs simulated by a DC approach.

One inevitable challenge in this approach is that the prediction of on-current is sometimes very difficult, as can be seen in Fig. 2, because of the formation of the inversion layer, which results in instability of the NC state. On the other hand, Eq. (3) presumes that the NC state is always stable because this equation is derived from the condition  $\nabla_p G = 0$  [7]. We found that this contradiction leads to problems in obtaining a converged solution in TCAD simulation.

Transient TCAD simulation of NCFETs



**Fig. 3**  $I_{D}$ - $V_{GS}$  curve for DG-NCFETs simulated by a transient approach.

To avoid the difficulties in simulating the characteristics of NCFETS in the case where the NC state is unstable, we have recently proposed the use of a transient approach that considers the time-dependent LK equations [Eqs. (1) and (2)]. [7] In this method, time *t* is the independent parameter, even when simulating the DC performance. Figure 3 shows the typical simulated  $I_D$ - $V_{GS}$  curves of DG-NCFETs using the transient approach. In this simulation,  $I_D$ - $V_{GS}$  was calculated on the presumption that the gate voltage had a sine waveform. As can be seen in Fig. 3, in the transient method, we can predict the hysteresis, which is attributable to the instability of the NC state due to the formation of the inversion layer. The results suggest that transient TCAD is indispensable for simulating NCFETs even in the case where the NC state is unstable.

# 4. Conclusions

The self-consistent TCAD simulation of NCFETs can predict the various and unique characteristics of NCFETs. We believe that the fully self-consistent TCAD simulation based on the transient approach can be highly instrumental in providing a design guideline for NCFETs, which is a future promising option to realize highly energy-efficient LSIs.

## Acknowledgments

This work was supported by the Core Research for Evolutional Science and Technology (CREST, JPMJCR14F2) of Japan Science and Technology Agency (JST).

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