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An Extended Kolmogorov–Avrami–Ishibashi (EKAI) Model to Simulate Dynamic Characteristics of Polycrystalline-Ferroelectric-Gate Field-Effect Transistors

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Abstract: A physics-based model on polarization switching in ferroelectric polycrystalline films is proposed. The calculation results by the model agree well with experimental results regarding dynamic operations of ferroelectric-gate field-effect transistors (FeFETs). In the model, an angle θ for each grain in the ferroelectric polycrystal is defined, where θ is the angle between the spontaneous polarization and the film normal direction. Under a constant electric field for a single-crystal film with $\theta = 0$, phenomena regarding polarization domain nucleation and wall propagation are well described by the Kolmogorov–Avrami–Ishibashi theory. Since the electric fields are time-dependent in FeFET operations and the θ values are distributed in the polycrystalline film, the model in this paper forms an extended Kolmogorov–Avrami–Ishibashi (EKAI) model. Under a low electric field, the nucleation and domain propagation proceed according to thermally activated processes, meaning that switching the time scale of a grain with the angle θ is proportional to an exponential form as $\exp(\text{const.}/E_z \cos \theta)$ [E_z : the film-normal electric field]. Wide θ distribution makes the time response quite broad even on the logarithmic scale, which relates well with the broad switching time experimentally shown by FeFETs. The EKAI model is physics based and need not assume non-physical distribution functions in it.

Keywords: ferroelectric; dynamic model; polarization switching; domain wall; ferroelectric field-effect transistor; polycrystal; polarization reversal; memory



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1. Introduction

1.1. Necessity of a Physics-Based Model for Ferroelectric Device Dynamics

Ferroelectric-gate field-effect transistors (FeFETs) have attracted attention not only because of their potential functionality [1,2] such as being compact, non-volatile, and non-destructive-read memory cells, but also due to recent rich accumulations of experimental data. FeFETs have been characterized by various measurements. Quasi-static characteristics of drain current (I_d) vs. gate voltage (V_g) are measured with slow V_g sweeping by a semiconductor parameter analyzer. Also, Q_m vs. V_g are measured by a quasi-static procedure with the slow V_g sweeping by a ferroelectric tester. The Q_m is the metal-gate charge density induced by ferroelectric layer polarization. Dynamic time-dependent properties of FeFETs are characterized by a pulse-write-and- V_{th} -read (PWVR; see Figure A3) or pulse-write-and- I_d -read (PWIR) method. The pulse-write (PW) is done by a pulse generator. In a FeFET, while a positive or negative V_g pulse is given with the V_g height of V_h (>0) or V_l (<0), ferroelectric polarization responds dynamically as a function of pulse height (V_h or $-V_l$) and time width (t_w). After ceasing PW, considerable amounts of ferroelectric polarization are retained due to ferroelectricity. This retained polarization is a function of V_h , V_l , and t_w . A read operation is done after PW, where V_g of the transistor is swept in a narrow voltage range slowly compared to the PW time scale.

A threshold voltage (V_{th}) is read for PWVR, and the drain current (I_d) is read at a fixed V_g for PWIR. A threshold voltage difference (ΔV_{th}) for PWVR or a current ratio between the high- and low- I_d -current states for PWIR can be derived for a pair of the write voltages; V_h and V_l . ΔV_{th} by PWVR or the I_d ratio by PWIR is a performance indicator of an FeFET as a nonvolatile memory transistor.

A lot of experimental results by PWVR and PWIR are available to investigate dynamic polarization switching in metal ferroelectric insulator-semiconductor (MFIS) type FeFETs, whose ferroelectric is $\text{SrBi}_2\text{Ta}_2\text{O}_9$ or $(\text{Sr}_{1-x}\text{Ca}_x)\text{Bi}_2\text{Ta}_2\text{O}_9$ [3–5]. The former and the latter are abbreviated as SBT and CSBT, respectively. The SBT and CSBT belong to a family of the Bi-layered perovskite oxides with similar electrical properties. The coercive field of CSBT for $x = 0.1$ – 0.2 is 10% larger than that of SBT. Hereafter, FeFETs comprising SBT or CSBT in the ferroelectric layers are called SBT-FeFETs. The electric properties of SBT-FeFETs are suitable for model verification because they are reproducible with high switching endurance due to negligibly small charge injection and trapping in the FeFET gate stacks.

Despite the many experimental works of PWVR and PWIR reported in detail, there have been no correct theories based on physics for simulating them. As one of the existing models, a phenomenological Landau–Ginzburg–Devonshire (LGD) theory in ferroelectrics constructs a Gibbs free energy for the ferroelectrics where the primary energy term is expressed as a polynomial expansion form of polarization as an order parameter [6–8]. By minimizing the free energy, equilibrium or quasi-static properties are derived. The LGD theory described the transition between the paraelectric and ferroelectric phases with temperature variation across the Curie temperature [7]. It also described phase transitions between the tetragonal and orthorhombic and between the orthorhombic and rhombohedral in BaTiO_3 , a cubic-based ferroelectric material [6]. In the Gibbs free energy, the spatial differentiation term brought non-homogeneity, by which domain patterns were described [9,10]. The Gibbs energy for ferroelectrics can include the elastic energy term and the coupling terms of elasticity and polarization since the polarization accompanies lattice displacement of crystals. In the case that the ferroelectric layers are divided into LGD segments, the LGD theories are called phase field models [11,12]. The models showed coexistence of 180° - and non- 180° domains under constraints of substrates [11] and polycrystalline grain growth [13].

The LGD theory has its own representation of time dependence. In the case that the electric properties without elastic terms are matters of concern, the description of time dependence is sometimes called the Landau–Khalatnikov (LK) equation [14–16]. In the phase-field models, it is called the time-dependent Ginzburg–Landau (TDGL) equation [11,17]. LK and TDGL are essentially the same. A Lagrangian function, which includes a simple viscosity term of classical mechanics [18], may help us comprehensively understand the origin of the time-dependent polarization switching. The Gibbs free energy for the ferroelectrics replaces the potential term in the Lagrangian. In deriving equations of motion, the inertia term is usually neglected for polarization reversal problems, and the LK and TDGL equations are obtained [19]. Overdamped (i.e., strong viscosity) cases in the Lagrangian may allow us to omit the inertia term in the equation of motion. As is obvious from the derivation of these time-dependent equations, however, the LK and TDGL equations are deterministic and do not have thermal activation forms in them. As indicated by previous papers [20–22], nucleation and domain-wall propagation under an electric field occur via thermally activated steps. Thus, the LK and TDGL equations are not suitable (at least quantitatively). Additions of Gaussian white-noise terms to these equations are necessary for describing the thermal activation steps, and in fact the effect of the noise term was demonstrated for a small segment number case [23]. However, since the LDG segments should be finer than the domain-wall width and the wall width size is one crystal lattice or a few times of it [24,25], the number of the LDG segments for general objects including polycrystalline films becomes so huge that we cannot make calculations within a realistic time scale.

This paper proposes a physical model for describing polarization variation with time in a ferroelectric film and for calculating electronic device operations of FeFETs, metal-ferroelectric-metal (MFM) capacitors, and metal-ferroelectric-insulator-metal (MFIM) capacitors. In the model, the ferroelectric film can be a polycrystalline one, and to each grain, an angle θ is assigned where θ is the angle between the film normal and the direction along the spontaneous polarization. The θ distribution in the polycrystalline film is given by experiments. In fact, for SBT-based FeFETs, the angle distribution was derived by an electron backscattering diffraction (EBSD) patterns technique [26].

In each grain having θ , it is also assumed that, under an electric field, a seed for polarization reversal grows along the spontaneous direction and forms a narrow columnar 180° reversed domain, which is expanded along the sidewise direction, because 180° switching and $\pm 180^\circ$ domain formation are subjected to occur in SBT and CSBT ferroelectrics [27–29]. Experimental observations of the 180° switching and 180° domain-wall moving for $\theta \neq 0$ cases are found in [30,31].

The Kolmogorov–Avrami–Ishibashi (KAI) model [32–36] fits the physical picture mentioned above (i.e., 180° domain nucleation and domain wall propagation). The KAI model provides mathematical functions of the $\theta = 0$ case describing domain expansion with time under a constant electric field. As for epitaxial thin films, many papers indicated good agreement of the KAI model with experiments [37,38], but for polycrystalline films, the KAI model is asserted to be unsuitable [39]. This complicated issue concerning polycrystal films will be overcome in our present paper by introducing θ terms in grains. In order to explain wide-range $\log(t)$ distributions of polarization switching times that Pt/Pb(Zr,Ti)O₃/Pt capacitors showed, the inhomogeneous field mechanism (IFM) model [40] and the nucleation-limited switching (NSL) model [41] are proposed. Although switching reversal experiments in polycrystalline films were explained [42,43] using the IFM, the model assumed inhomogeneous electric-field distribution of a Gaussian type, which was not physics based. The NLS is a non-KAI model. A (111)-oriented Pb(Zr,Ti)O₃ was used. The waiting times of elementary regions are stochastic. By giving an exponentially broad distribution of the waiting time, the switching phenomena across a wide $\log(t)$ scale were described. Since the distribution function is assumed so that the numerical results reproduce the experimental ones, understanding the physics of the distribution function is not easy. If we infer a possible inclusion of grains with other crystal orientation in the film, physics in the wide $\log(t)$ characteristics might be explained by an effect of the orientation distribution. A HfO₂-based FeFET is reported to be consistent with the NLS [44]. The paper indicates that the grain size is ≈ 20 nm and the field for creating a nucleus is ≈ 1 MV/cm. This suggests that the nucleation size is already the same as the grain size, and thus there is no space left for the created nucleus to induce a wall expansion supposed in the KAI model.

Herein we propose an extended KAI (EKAI) model, which is applicable to represent characteristics of FeFETs with polycrystalline ferroelectrics under time-dependent electric fields. In the EKAI model, KAI-like pictures are adopted only inside individual grains. The EKAI describes 180° switching and $\pm 180^\circ$ domain wall propagations in every grain separately. No wall motions are assumed to propagate across adjacent grains. There are two fundamental premises of the EKAI. One is that only the electric field component along the spontaneous polarization works for the polarization switching. The other is that we pick up only the film-normal component of the switched polarization because the film-normal component is the important response to the externally applied potential. The in-plane components of the switching polarization are expected to be randomly distributed among grains. The effect of the in-plane components is thought to be weak because of the random distribution, and thus the boundary conditions between neighboring grains are ignored in the present EKAI model. The polarization of the KAI model is an averaged quantity where the polarization is represented by the average of the volume fraction of $\pm 180^\circ$ domain regions. The EKAI has a distinct perspective on ferroelectrics from the phase-field model in which the ferroelectrics are divided into small segments connected by strict boundary

conditions according to the idea of the LGD. The EKAI has a much shorter computation time than the phase-field model because it ignores the grain boundary conditions and averages the ferroelectric polarizations in grains. The PWVR and PWIR data show a wide time range of polarization switching characteristics from 50 ns to 10 ms [3–5]. We suppose that these rather slow and wide-ranged time responses are attributed to ferroelectric polycrystals consisting of grains that have broad distributions in the crystal orientations. The response times of the paraelectric components in the ferroelectric grains and the dielectrics in the insulator are supposed to be much shorter than those of the polarization-switching components. The potential formation time in the semiconductor is also supposed to be shorter. Therefore, the EKAI model in this paper assumes that the parameters except for the polarization switching in the ferroelectric grains vary instantaneously. Correctness of the EKAI model is supported by good agreement with experimental results of quasi-static I_d – V_g , Q_m – V_g , and PWVR for SBT-based FeFETs as discussed later in Section 4. The EKAI model in this paper assumes no free charges existing in the gate insulator and ferroelectric; thus the EKAI is not directly applicable to HfO₂-based FeFETs in which the ferroelectric polarization switching is always accompanied by charge injection currents [45–49].

1.2. Presentation of the KAI with the Characteristic Times for the EKAI Model

Let us write some equations of the original KAI model, because they are necessary in the succeeding section for the EKAI derivation. In the original KAI, polarization switching nucleation is instantaneous in comparison with domain growth motion. A constant electric field and the domain wall velocity (v_{wall}) depending on this constant field are assumed. As shown in Figure 1, the ferroelectric volume is constituted by domain regions. The switching polarizations in the downward and upward regions are P_s and $-P_s$, respectively. P_s is the spontaneous polarization. The polarization direction is parallel to the z -axis. The downward (or upward) domain regions expand with time under a positive (or negative) field, after application of step function with a constant positive field, E_{z+} . Consider a case that at the initial ($t < 0$) the volume is occupied fully by the upward regions, and a step function with a constant positive field, E_{z+} is applied at $t = 0$. Then, the volume fraction of the downward domain ($R_{dn||z}$) is varied with time for $t \geq 0$ under a constant E_{z+} as

$$R_{dn||z} = c(t), \quad (1)$$

with

$$c(t) = 1 - \exp\left(-\left(\frac{t}{t_0}\right)^n\right). \quad (2)$$

t_0 is the characteristic time for the polarization switching and is a function of the constant field E_{z+} . The power exponent, n , is a parameter relating to the domain growth dimension. The volume fraction of the upward domain ($R_{up||z}$) is

$$R_{up||z} = 1 - c(t). \quad (3)$$

The switching polarization ($\overline{P_z}$) averaged over the ferroelectric volume is

$$\overline{P_z} = R_{dn||z}P_s + R_{up||z}(-P_s) = P_s(2c(t) - 1). \quad (4)$$

Similarly, in the case that at the initial ($t < 0$) the volume is occupied fully by the downward regions, and step function with a constant negative field, E_{z-} is applied at $t = 0$, the volume fraction of the upward domain ($R_{up||z}$) is for $t \geq 0$ under a constant E_{z-} :

$$R_{up||z} = c(t). \quad (5)$$

t_0 in Equation (2) is a function of the constant field E_{z-} . The switching polarization ($\overline{P_z}$) averaged over the ferroelectric volume is

$$\overline{P_z} = -P_s(2c(t) - 1). \quad (6)$$

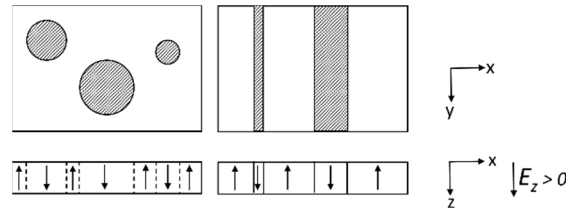


Figure 1. KAI schematic drawing of domain nucleation and growth in a film under an electric field parallel to the z -axis ($E_z > 0$). The uppers and lowers are top and side views, respectively. The lefts and rights represent two- and one-dimensional nucleation and growth manners, respectively. The shaded areas are on the way to expansion. An analytical function of the KAI model (Equation (2)) describes the volume fraction increase of the downward (upward) domain with time under a constant positive (negative) E_z .

According to Ishibashi and Takagi [36] and Ishibashi [50], in category 1, domain nucleation occurs with a fixed probability, and $n = 3$ when the wall shape is two-dimensional (i.e., circular) and $n = 2$ when the wall shape is one-dimensional (i.e., straight line). In category 2, there exist latent nuclei, and no new nucleation appears. In category 2, $n = 2$ when the shape is two-dimensional, and $n = 1$ when it is one-dimensional. In real materials, domain nucleation may occur, and latent nuclei may also exist. Some parts are two-dimensional and others are one-dimensional-like. Hence the value n is not an integer of the range $1 \leq n \leq 3$. When t_o is small in Equation (2), the transient time of the polarization reversal is short, and when t_o is large, it is long. That is, t_o is a characteristic time that gives a time scale of the polarization variation. t_o has a relationship with v_{wall} .

For category 1,

$$t_o = \gamma_1 (v_{wall})^{(1-n)/n}. \quad (7a)$$

For category 2,

$$t_o = \gamma_2 v_{wall}^{-1}. \quad (7b)$$

In Equation (7), γ_1 and γ_2 are constants.

The KAI model did not show explicit mathematical forms of t_o . The wall velocity v_{wall} as a function of the applied film-normal electric field (E_z) has been investigated mainly by switching current measurement of single crystals [51,52] and by piezoresponse force microscopy (PFM) of epitaxial thin films including random disorder by defects [21,53,54]. A consensus view in the case of films including the disorder is that v_{wall} under high electric fields quickly increases in linear equation whereas it creeps up in reciprocal exponential at low fields [52,55]. In the case of ferroelectric films including defects, v_{wall} under high field is expressed as $v_{wall} \propto E_z$ for $E_z \gg E_{dpin}$, where E_{dpin} is a critical field over which depinning of wall motions occurs at 0 K [55,56]. In an intermediate E_z region, v_{wall} is expressed using a power exponent τ' as

$$v_{wall} \propto (E_z - E_{dpin})^{\tau'} \quad (8a)$$

and in a low- E_z creep region, v_{wall} is expressed at finite temperature as

$$v_{wall} \propto \exp\left[-\frac{U'}{k_B T} \left(\frac{E_{dpin}}{E_z}\right)^\sigma\right], \quad (8b)$$

where U' is a scale of energy barrier and σ is a power exponent originated from random disorder defects in ferroelectric films [55,56] (k_B : the Boltzmann constant and T : the absolute temperature).

From Equations (7) and (8), the v_{wall} expressions are changed to t_o expressions. Using a renormalized constant τ , Equation (8a) is, irrespective of the category 1 or 2,

$$t_o \propto (E_z - E_{dpin})^{-\tau} \quad (9a)$$

Similarly, irrespective of the categories, Equation (8b) is converted to t_o , using a renormalized constant U , as

$$t_o = t_{inf} \exp\left[\frac{U}{k_B T} \left(\frac{E_{dpin}}{E_z}\right)^\sigma\right], \quad (9b)$$

where t_{inf} is a constant.

In the present work, experimental results of SBT-based FeFETs are used in order to demonstrate the EKAI model's credibility. High endurance of the SBT FeFETs can be realized on small or at least moderate write-voltage conditions where the charge injection and trapping in the gate stack are suppressed [2,57]. Since a small or moderate write voltage brings a low electric field in the ferroelectric, we adopt Equation (9b) rather than Equation (9a) hereafter in this paper; i.e., Equation (9b) will be used in calculations shown later. Further, since the separate determination of U and E_{dpin} is difficult, we have the following equation for t_o in this paper:

$$t_o = t_{inf} \exp\left[\left(\frac{E_{act}}{|E_z|}\right)^\sigma\right], \quad (10)$$

with an activation field constant $E_{act} \left(= (U/k_B T)^{-\sigma} E_{dpin}\right)$. To include E_z negative cases, $|E_z|$ instead of E_z , is used in Equation (10).

2. EKAI Model

Let us consider a ferroelectric polycrystal film as shown in Figure 2a. The thickness of the film is d_f . The film is divided into plural grains labeled l from one to l_{max} . All grains have the common thickness d_f . Grain boundaries are along the film normal, i.e., the z -axis. The area of grain l is A_l . The direction of the spontaneous polarization of grain l is parallel to the u_l axis. The angle between the u_l axis and the z -axis is θ_l . The range of θ_l is defined as $0 \leq \theta_l \leq 90^\circ$. All grains have a same spontaneous polarization, P_s or $-P_s$. The polarization of the direction of the u_l axis is defined as P_s .

In Section 4, the EKAI model will be compared to the experimental results of MFIS FeFETs, where the ferroelectric layers consist of ferroelectric polycrystals. Experimental FeFETs with 135 nm thick ferroelectric SBT layers are available for discussion in the present EKAI model. Averaged in-plane diameters of the SBT grains are about 200 nm, which is larger than the ferroelectric layer thickness in the FeFETs. Therefore, we shall assume a single grain occupation along the z -direction or the film normal in the SBT FeFETs. Each grain stands as a pillar with a constant cross-section from the film top to the bottom.

Figure 2b is an expanded schematic picture of grain l . The grain consists of upward domain regions and downward domain regions. In the downward (or upward) domain regions, the spontaneous polarization P_s (or $-P_s$) is parallel (or anti-parallel) to the u_l axis. Figure 2c is a schematic picture focusing on a cylindrical-shape downward domain existing in the grain. The EKAI model in this section describes polarization variation in one grain. In the model, there are two fundamental assumptions (described in Sections 2.1 and 2.2) prior to the significant description (Section 2.3) of the polarization dynamics under a varying electric field with time. Section 3 provides calculation schemes for the following specific devices including ferroelectric polycrystal: (1) MFM capacitors, (2) MFIM capacitors, and (3) MFIS FeFETs.

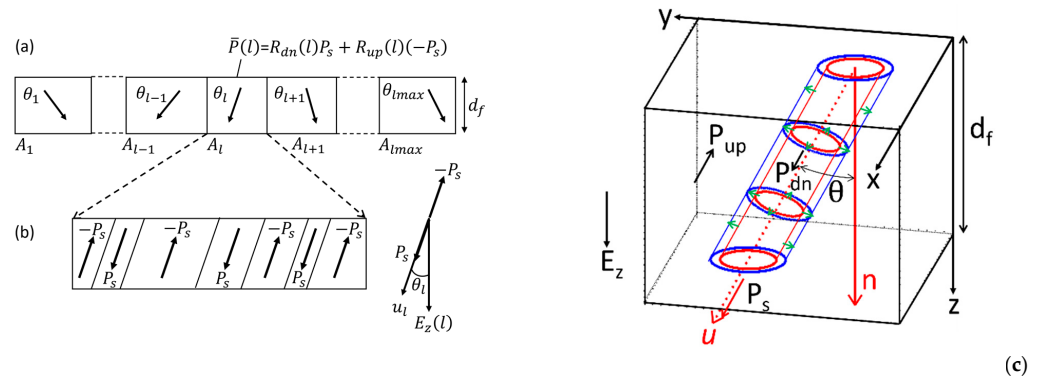


Figure 2. (a) EKA schematic picture of a ferroelectric film constituted by polycrystal grains. Grain l has an orientation angle θ_l and area A_l . θ_l is the angle between the z -axis and the u_l axis. The u_l axis is parallel to the spontaneous polarization P_s . (b) Grain l consists of downward (P_s) and upward ($-P_s$) domain regions. The P_s direction in the upward (downward) domains is parallel (anti-parallel) to the u_l axis. (c) A scheme of the EKA model. A polarization nucleus is formed along the u -direction and the domain wall spreads laterally to the u -direction.

2.1. Polarization Variation under a Constant Electric Field

In grain l , the polarization direction is tilted from the z -axis by θ_l . Nevertheless, it is assumed that, under a constant field, E_z , the wall-motion equations are formally the same as Equations (1)–(6) of the KAI model.

Consider a case that a positive constant field E_{z+} as a step function is applied at $t = 0$. At $t < 0$, the volume is occupied fully by the upward regions. Then, the volume fraction of the downward domain ($R_{dn}(l)$) is varied with time for $t \geq 0$ as

$$R_{dn}(l) = c(t), \quad (11)$$

The volume fraction of the upward domain ($R_{up}(l)$) is

$$R_{up}(l) = 1 - c(t). \quad (12)$$

The switching polarization ($\bar{P}_z(l)$) averaged over the volume of grain l is

$$\bar{P}_z(l) = R_{dn}(l)P_s + R_{up}(l)(-P_s) = P_s(2c(t) - 1). \quad (13)$$

Consider the opposite case that a negative constant field E_{z-} as a step function is applied at $t = 0$. At $t < 0$, the volume is occupied fully by the downward regions. Then, the volume fraction of the upward domain ($R_{up}(l)$) is varied with time for $t \geq 0$ as

$$R_{up}(l) = c(t), \quad (14)$$

The switching polarization ($\bar{P}_z(l)$) averaged over the volume of grain l is

$$\bar{P}_z(l) = -P_s(2c(t) - 1). \quad (15)$$

2.2. Effect of the Spontaneous Polarization Direction Different from the Z-Axis

The function $c(t)$ in Equations (11)–(15) is $1 - \exp(-(t/t_o)^n)$, which is the same as Equation (2). However, the u_l axis is tilted from the z -axis by θ_l . In the EKA model, the characteristic time for the polarization switching t_o is assumed to be

$$t_o = t_{inf} \exp \left[\left(\frac{E_{act}}{|E_z| \cos(\theta_l)} \right)^\sigma \right] \quad (16)$$

i.e., $|E_z| \cos(\theta_l)$ replaces $|E_z|$ in Equation (10).

2.3. Switching Polarization under Time-Dependent Electric Fields

Let us consider switching polarization evolution in grain l in the case that the electric field varies with time. Using the information of $(R_{dn}(l))_{now}$, $(R_{up}(l))_{now}$, and $(E_z(l))_{now}$, $(R_{dn}(l))_{next}$ and $(R_{up}(l))_{next}$ are derived by the method of this subsection, where $t_{next} = t_{now} + \Delta t$ (Δt : a small time-increment), and $(\dots)_{now}$ or $(\dots)_{next}$ means the amounts of $(\dots)$ at $t = t_{now}$ or $t = t_{next}$, respectively.

The EKAI model assumes that the polarization varies during a short period Δt as if the polarization varies under a constant field $(E_z(l))_{now}$. Note, however, that we must consider two cases, i.e., the cases of $(E_z(l))_{now} > 0$ and $(E_z(l))_{now} < 0$.

Figure 3 shows an explanation for the case $(E_z(l))_{now} > 0$. Let us consider a case in grain l that, at $t = t_{now}$, $R_{dn}(l)$ is $(R_{dn}(l))_{now}$ under $E_z(l) = (E_z(l))_{now}$. This status is point A in the graph. Draw a curve of the EKAI function (Equation (11)) at a constant field, $E_z(l) = (E_z(l))_{now}$, as the blue solid line $c(t)$. Note that $c(t)$ always starts from the origin of the graph (i.e., $R_{dn}(l) = 0$ at $Time = 0$.) The line $c(t)$ has $(R_{dn}(l))_{now}$ at point B. The time at point B is $(t_{Kdn})_{now}$, which is obtained by solving the $c(t)$ (Equation (2)) as

$$(t_{Kdn})_{now} = (t_o)_{now} \{-\ln[1 - (R_{dn}(l))_{now}]\}^{\frac{1}{n}} \quad (17)$$

with

$$(t_o)_{now} = t_{inf} \exp\left(\left(\frac{E_{act}}{|(E_z(l))_{now} \cos \theta_l|}\right)^\sigma\right). \quad (18)$$

We assume that the growth of $(R_{dn}(l))_{now}$ from $t = t_{now}$ to $t = t_{now} + \Delta t = t_{next}$ under $E_z(l) = (E_z(l))_{now}$ at point A is the same as the growth of $(R_{dn}(l))_{now}$ at point B under the same constant field $(E_z(l))_{now}$. The distance between points A and B is $t_{now} - (t_{Kdn})_{now}$. The $R_{dn}(l)$ growth during Δt at the point A can thus be calculated by a parallel-shifted function, $c(t - t_{now} + (t_{Kdn})_{now})$, and thus $(R_{dn}(l))_{next}$ in the case of $(E_z(l))_{now} > 0$ is obtained as

$$(R_{dn}(l))_{next} = 1 - \exp\left(-\left(\frac{(t_{Kdn})_{now} + \Delta t}{(t_o)_{now}}\right)^n\right). \quad (19)$$

The volume fraction of the upward domain and the z-axis component of the switching polarization averaged over grain l are

$$(R_{up}(l))_{next} = 1 - (R_{dn}(l))_{next} \quad (20)$$

and

$$\begin{aligned} (\overline{P_z}(l))_{next} &= (R_{dn}(l))_{next} P_s \cos \theta_l + (R_{up}(l))_{next} (-P_s \cos \theta_l) \\ &= (2(R_{dn}(l))_{next} - 1) P_s \cos \theta_l. \end{aligned} \quad (21)$$

Quite similarly, we derive the following equations in the case of $(E_z(l))_{now} < 0$. The volume fractions of the upward domains and the downward domains are

$$(R_{up}(l))_{next} = 1 - \exp\left(-\left(\frac{(t_{Kup})_{now} + \Delta t}{(t_o)_{now}}\right)^n\right), \quad (22)$$

and

$$(R_{dn}(l))_{next} = 1 - (R_{up}(l))_{next}, \quad (23)$$

with

$$(t_{Kup})_{now} = (t_o)_{now} \{-\ln[1 + (R_{up}(l))_{now}]\}^{\frac{1}{n}}. \quad (24)$$

The z-axis component of the switching polarization averaged over grain l is

$$(\overline{P_z}(l))_{next} = -(2(R_{up}(l))_{next} - 1) P_s \cos \theta_l. \quad (25)$$

The electric field $(E_z(l))_{next}$ can be obtained using the obtained $(\overline{P}_z(l))_{next}$ (Equation (21) or Equation (25)) and the electrostatic equation, which depends on the device structure considered. See the next section. Once $(E_z(l))_{next}$ is obtained, we know now $(R_{dn}(l))_{next}$, $(R_{up}(l))_{next}$, and $(E_z(l))_{next}$. Then, the quantities of $(\dots)_{next}$ are regarded as the quantities at $t = t_{now}$ of $(\dots)_{now}$; we can repeat calculation.

When Δt is infinitesimally small, Equations (19) and (22) can be expressed as a differential style of $R_{dn}(l)$ and $R_{up}(l)$, that is, for $(E_z(l))_{now} > 0$,

$$\left(\frac{dR_{dn}(l)}{dt}\right)_{now} = (1 - (R_{dn}(l))_{now}) \frac{n}{((t_o)_{now})^n} [(t_{Kdn})_{now}]^{n-1}, \quad (26)$$

and for $(E_z(l))_{now} < 0$,

$$\left(\frac{dR_{up}(l)}{dt}\right)_{now} = (1 - (R_{up}(l))_{now}) \frac{n}{((t_o)_{now})^n} [(t_{Kup})_{now}]^{n-1}. \quad (27)$$

The physical meaning of Equations (26) and (27) is that the differential of $c(t - t_{now} + (t_{Kdn})_{now})$ at point A in Figure 3 equals the differential of $c(t)$ at point B.

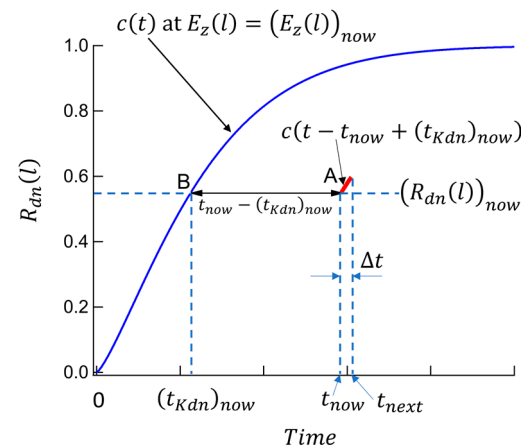


Figure 3. Concept of the EKAI model when the electric field changes with time. In the case of E_z varying with time, let us consider a case in grain l that, at $t = t_{now}$, $R_{dn}(l)$ is $(R_{dn}(l))_{now}$ under $E_z(l) = (E_z(l))_{now}$. This status is point A in the graph. Draw a curve of the EKAI function (Equation (11)) at a constant field, $E_z(l) = (E_z)_{now}$, as the blue solid line $c(t)$ (Equations (2) and (11)). The point on the curve $c(t)$ at $R_{dn}(l) = (R_{dn}(l))_{now}$ is B, and the time at point B is $(t_{Kdn})_{now}$. We assume that the growth of $(R_{dn}(l))_{now}$ from $t = t_{now}$ to $t = t_{now} + \Delta t = t_{next}$ with $E_z(l) = (E_z(l))_{now}$ at point A is the same as the growth of $(R_{dn}(l))_{now}$ at point B under the same constant field $(E_z(l))_{now}$. The $R_{dn}(l)$ growth during Δt at point A can thus be calculated by a parallel-shifted function, $c(t - t_{now} + (t_{Kdn})_{now})$, and $(R_{dn}(l))_{next}$ is obtained as Equation (19). At $t = t_{next} + \Delta t$ the same procedure is repeated under a varied new- $E_z(l)$, and we obtain $R_{dn}(l)$ at $t = t_{next} + \Delta t$. The same is performed for $R_{up}(l)$ in the case of $E_z(l) < 0$, and $(R_{up}(l))_{next}$ is derived as Equation (22).

3. Total Calculation Scheme for Describing Time-Varying Switching Polarizations of Specific Devices

Figure 4 shows a schematic drawing of (a) an MFM capacitor, (b) an MFIM capacitor, and (c) an MFIS FeFET. As stated before, the ferroelectric film consists of poly-crystal grains indexed by l with $l = 1, 2, \dots, l_{max}$. We apply a time-dependent voltage, V_g , to the top metal electrode of the MFM and MFIM capacitors and to the gate metal electrode of the MFIS FeFET. We provide the ground voltage, 0 V, to the bottom metal electrode of the MFM and MFIM capacitors and to the semiconductor substrate terminal.

Following the EKAI model in the previous section, we derived, at a moment, the z-axis component of the switching polarization $\overline{P}_z(l)$ averaged in the volume of grain l .

We assume that the paraelectric component of the ferroelectric is isotropic. The electric displacement $\overline{D}_z(l)$ averaged in the volume of grain l is represented as

$$\overline{D}_z(l) = \varepsilon_0 \varepsilon_{fdi} E_z(l) + \overline{P}_z(l), \quad (28)$$

where ε_0 is the permittivity in vacuum and ε_{fdi} is the dielectric constant of the paraelectric component of the ferroelectric.

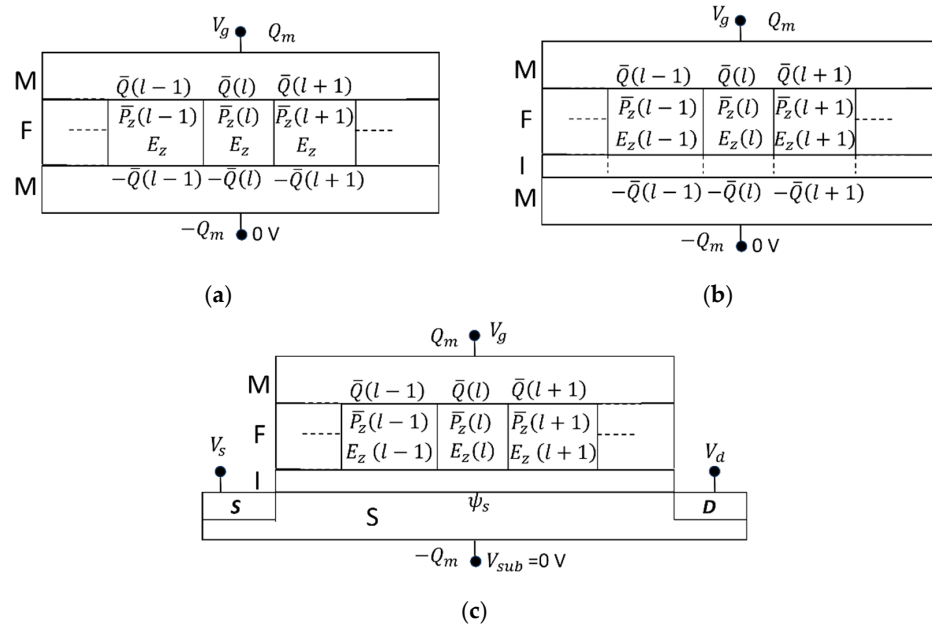


Figure 4. Total calculation scheme for specific devices. (a) an MFM capacitor; (b) an MFIM capacitor; (c) an MFIS FeFET. The EKAI model under a varying field E_z with time provides $\overline{P}_z(l)$, $R_{dn}(l)$, and $R_{up}(l)$ at $t = t_{next}$ using $R_{dn}(l)$, $R_{up}(l)$, and $E_z(l)$ at $t = t_{now}$. To repeat the calculation, it is necessary to obtain $E_z(l)$ at $t = t_{next}$. Depending on the structure of the specific devices, the method of deriving $E_z(l)$ is different. For an MFM capacitor case (a), $E_z(l)$ does not depend on l , and E_z at $t = t_{next}$ is obtained by Equation (33). For an MFIM capacitor case (b), the induced charges of the bottom electrode of grain l , $-\overline{Q}(l)$ is a good approximation. $E_z(l)$ depends on l . $Q(l)$ at $t = t_{next}$ and is derived by Equation (38). Then $E_z(l)$ at $t = t_{next}$ is obtained by Equation (37). For an MFIS FeFET case (c), D_z at the top surface of the insulator is averaged over all the grains due to a transitional thin layer between the ferroelectric and the insulator (see Figure 5). The surface potential ψ_s of the semiconductor is assumed to be uniform because of insufficient acceptor density N_A . The uniform D_z and ψ_s lead to a grain-independent field E_z [$E_z(l) = E_z$ for all l]. ψ_s at $t = t_{next}$ is derived by Equation (42). Then, Q_m is obtained from Equation (44), and E_z is obtained from Equation (40).

The metal electrodes of all the three devices are assumed to have large free carrier densities. At the metal electrode surfaces facing the ferroelectric or insulator, the electric-field penetrations are negligibly small, and thus no potential variations inside the metal can be assumed. The potential in the metal is uniformly V_g . Following Equation (28) and Gauss's law, the induced charge per unit area facing the grain l is

$$\overline{Q}(l) = \overline{D}_z(l) \quad (29)$$

Because of the averaged value of $\overline{D}_z(l)$, $\overline{Q}(l)$ is also averaged in the volume of grain l . The total induced charges of the top metal electrode of the potential, V_g , is the summation of the induced charge $\overline{Q}(l)$ over all the grains. The total induced charges are defined as the charge per unit area, Q_m , which is

$$Q_m = \frac{1}{A_{tot}} \sum_{l=1}^{l_{max}} A_l \overline{Q}(l), \quad (30)$$

where A_l is the area that grain l faces the electrode and $A_{tot} = \sum_{l=1}^{l_{max}} A_l$. This Q_m is the quantities obtained experimentally in $Q_m - V_g$ measurements, which are explained in (2) in Appendix A. The switching polarization (i.e., not including the paraelectric polarization) averaged over the entire ferroelectric, P_z , is as

$$P_z = \frac{1}{A_{tot}} \sum_{l=1}^{l_{max}} A_l \overline{P_z}(l). \quad (31)$$

Using the EKAI and electrostatic equations across MFM, MFIM, and MFIS stacks, calculation steps are expressed as follows.

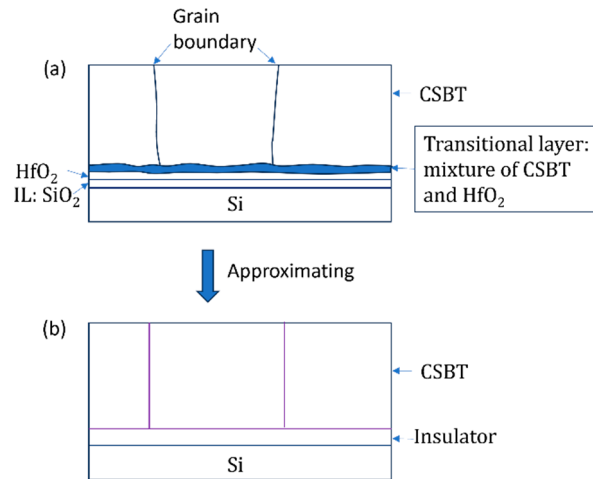


Figure 5. (a) Schematic cross-section of the experimental MFIS FeFETs. (b) The approximate structure assumed in the EKAI. In the experiment, the insulator is the bilayer of a 4 nm thick HfO₂ layer and a 2.6 nm thick IL (SiO₂) layer. The ferroelectric CSBT is 135 nm thick. A transitional layer exists at the interface between the CSBT and HfO₂ layers. A photo of a cross-section TEM confirmed this layer presence [58]. The transitional layer (≈ 5 nm thick) is constituted by fine grains. The TEM photo contrast indicates that the main atom elements are of the CSBT. Since a CSBT-originated high permittivity can be assumed, $D_z(l)$ is expected to be averaged of this transitional layer. Therefore, we can approximate the structure as (b) in this figure. D_z is averaged over all the grains at the top surface of the insulator.

3.1. MFM Capacitor

The electrostatic equation of the MFM capacitor is

$$V_g - V_{fb} = V_f, \quad (32)$$

where V_f is the voltage across the ferroelectric layer. The flat band voltage, V_{fb} , is the work function difference between the metal top electrode and the metal bottom electrode. Since V_f does not depend on the grains, the electric field is also independent of l as

$$E_z(l) = E_z = (V_g - V_{fb}) / d_f. \quad (33)$$

We have Equation (30) as

$$Q_m = \epsilon_0 \epsilon_{fdi} E_z + \frac{1}{A_{tot}} \sum_{l=1}^{l_{max}} A_l \overline{P_z}(l). \quad (34)$$

The second term of Equation (34) is the switching polarization averaged over the entire ferroelectric, P_z (Equation (31)).

Equations (21) and (25) of the EKAI model in the proceeding section can give us the $\overline{P_z}(l)$ (for $l = 1 \dots l_{max}$) at $t = t_{next}$. We also know V_g at $t = t_{next}$, because V_g is externally

applied. Then, E_z and Q_m at $t = t_{next}$ are obtained by Equation (33) and Equation (34), respectively. We know the behavior of the MFM capacitor at $t = t_{next}$.

$R_{dn}(l)$, $R_{up}(l)$, and $E_z(l)$ at $t = t_{next}$ are regarded as those at $t = t_{now}$. The EKAI model provides $R_{dn}(l)$ and $R_{up}(l)$, and $\bar{P}_z(l)$ at $t = t_{next}$. Equation (33) gives us $E_z(l)$ at $t = t_{next}$. We repeat these procedures and obtain fully the time-dependent solution of the MFM capacitor.

3.2. MFIM Capacitor

Charges appear at the top surface of the bottom electrode. We shall extend the z-axis-orientated boundaries between the adjacent grains into the insulator. We have the potential and E_z relationships for each grain; i.e., we have the following for $l = 1, 2, \dots, l_{max}$:

$$V_g - V_{fb} = V_f(l) + V_i(l), \quad (35a)$$

and

$$E_z(l) = V_f(l)/d_f. \quad (35b)$$

Here, $V_f(l)$ is the voltage across the grain l . $V_i(l)$ is the voltage across the region in the insulator belonging to grain l . At the top surface of the bottom electrode corresponding to grain l , the induced charge is $-Q(l)$, and we have for $l = 1, 2, \dots, l_{max}$:

$$V_i(l) = \bar{Q}(l)/C_i, \quad (36a)$$

with the insulator capacitance, C_i :

$$C_i = \frac{\epsilon_o \epsilon_i}{d_i}, \quad (36b)$$

and

$$\bar{Q}(l) = \epsilon_o \epsilon_{fdi} E_z(l) + \bar{P}_z(l). \quad (37)$$

We eliminate $E_z(l)$ from Equations (35)–(37). Then, we derive

$$\bar{Q}(l) = \frac{C_i C_{fdi}}{C_i + C_{fdi}} \left[V_g - V_{fb} + \frac{\bar{P}_z(l)}{C_{fdi}} \right], \quad (38)$$

with C_{fdi} is the paraelectric component capacitance of the ferroelectric as

$$C_{fdi} = \frac{\epsilon_o \epsilon_{fdi}}{d_f}. \quad (39)$$

The EKAI model provides $R_{dn}(l)$ and $R_{up}(l)$, and $\bar{P}_z(l)$ at $t = t_{next}$. We also know V_g at $t = t_{next}$, because V_g is externally applied. Equation (38) leads to $\bar{Q}(l)$ at $t = t_{next}$ for all l , and Equation (37) gives us $E_z(l)$ at $t = t_{next}$, using the obtained $\bar{Q}(l)$ for all l . All physical quantities are derived at $t = t_{next}$. Then, similarly to the case of the MFM capacitor, we can return the EKAI model calculation, and consequently we derive the time-dependent numerical solution for the MFIM capacitor.

3.3. MFIS FET

Figure 6 summarizes the total calculation scheme for MFIS FeFETs. Regarding the semiconductor, in the MFIS stack, the acceptor concentration (N_A) and carrier density in the semiconductor are much smaller than the carrier density in the metal layer. Thus, the electric field penetration into the semiconductor inevitably occurs so that the semiconductor surface potential ψ_s is different from the substrate potential ($V_{sub} = 0$). Imagine further a surface case where a region of an inversion state adjoins a region of an accumulation state. The surface potential cannot change abruptly on the surface. A good measure of the potential variation on the surface is the maximum depletion width, $W_m = 2\sqrt{\epsilon_o \epsilon_s \ln(N_A/n_i)/(e_o N_A \zeta)}$, where ϵ_s is the relative permittivity of the semiconductor, n_i the intrinsic carrier concen-

tration, $\zeta = e_o / (k_B T)$, and e_o the elementary charge [56]. For example, $W_m \cong 300$ nm when $N_A = 10^{16} \text{ cm}^{-3}$, $T = 300$ K using $\epsilon_s = 11.9$ and $n_i = 1.45 \times 10^{10} \text{ cm}^{-3}$ for Si. If the size of ferroelectric grains is smaller than W_m , a uniform surface potential ψ_s over all the grains is a good approximation (Figure 4c). Figure 5 shows a schematic drawing of a ferroelectric-insulator-semiconductor (FIS) as part of the experimental MFIS FeFETs. As shown in Appendix A, the gate stack of the experimental FeFETs is Ir/CSBT/HfO₂/Si. Via the crystallization annealing of the CSBT, a 2.6 nm thick SiO₂ interfacial layer (IL) was formed between HfO₂ and Si. The HfO₂ and CSBT layers are 4 nm thick and 135 nm thick, respectively. The bilayer of the HfO₂ and IL forms the insulator in the MFIS. Transmission electron microscope photos confirmed a thin (about 5 nm thick) transitional layer as shown in Figure 5a [58]. The transitional layer is constituted by fine grains (≈ 5 nm) whose main elements are originated from the ferroelectric CSBT. Due to the fine sizes, these grains may be non-ferroelectric but work as a high permittivity material. The dielectric constants of this transitional layer, the HfO₂ layer, and the SiO₂ IL are typically 180, 25, and 3.9, respectively. The different values of $\bar{P}_z(l)$ (Equation (28)) at the bottom of the ferroelectric among the grains are averaged via the in-plane pass in the transitional layer (Figure 5b). Therefore, the switching polarization at the interface between the CSBT and the insulator consisting of the bilayer of HfO₂ and IL can be reasonably assumed to equal the z-axis component of the polarization $\bar{P}_z(l)$ averaged over all the grains, P_z , that is already defined in Equation (31). Since P_z at the top surface of the insulator and ψ_s at the bottom of it are uniform laterally, the electric field E_i along the z-axis in the insulator and the potential V_i across the insulator are also laterally uniform, which leads to a grain-independent field E_z [$E_z(l) = E_z$ for all l] in the ferroelectric and a grain-independent potential $V_f = E_z d_f$ across the ferroelectric. The z-axis component of the electric displacement D_z averaged over all the grains as well as Q_m from Equations (28)–(30) is

$$Q_m = D_z = \epsilon_o \epsilon_{fdi} E_z + \frac{1}{A_{tot}} \sum_{l=1}^{l_{max}} A_l \bar{P}_z(l). \quad (40)$$

FeFETs have the gate, source, drain, and substrate terminals. Let us consider the case where the gate voltage V_g is generally varied with time and other terminals are grounded ($V_s = V_d = V_{sub} = 0$). Here V_s , V_d , and V_{sub} are the voltages applied on the source, drain, and substrate, respectively. The electrostatic equation across the MFIS stack is

$$V_g - V_{fb} = V_f + V_i + \psi_s, \quad (41)$$

where V_{fb} is the flat-band voltage, i.e., the difference between the metal work function and semiconductor fermi level. By eliminating E_z from Equations (40) and (41) and using Gauss's law while noticing the capacitance definition of Equations (36b) and (39), we have

$$V_g - V_{fb} + \frac{1}{A_{tot}} \sum_{l=1}^{l_{max}} A_l \bar{P}_z(l) = Q_m \left(\frac{1}{C_f} + \frac{1}{C_i} \right) + \psi_s. \quad (42)$$

If there is no interface state density between the insulator and semiconductor, the induced charge density, Q_s , in the semiconductor surface region has the same magnitude as Q_m with the opposite polarity ($Q_m = -Q_s$). Q_s is a function of semiconductor surface potential ψ_s as follows [59]:

$$Q_s = \mathcal{F}(\psi_s) = \mp \frac{\sqrt{2\epsilon_o \epsilon_s}}{\zeta L_D} \left[e^{-\zeta \psi_s} + \zeta \psi_s - 1 + \frac{n_{po}}{p_{po}} \left(e^{\zeta \psi_s} - \zeta \psi_s - 1 \right) \right]^{\frac{1}{2}}, \quad (43)$$

with a negative sign for $\psi_s > 0$. This equation is for n -channel FeFETs formed in p -type substrates. The equation for p -channel FeFETs can be rewritten appropriately. The Debye length is $L_D = \sqrt{\epsilon_o \epsilon_s / e_o p_{po} \zeta}$ with $p_{po} = \left(N_A - N_D + \left((N_A - N_D)^2 + 4n_i^2 \right)^{1/2} \right) / 2$ and

$n_{po} = n_i^2 / N_A$. The donor, acceptor, and intrinsic carrier densities in the semiconductor are N_D , N_A , and n_i , respectively, and p_{po} and n_{po} are the equilibrium densities of holes and electrons, respectively.

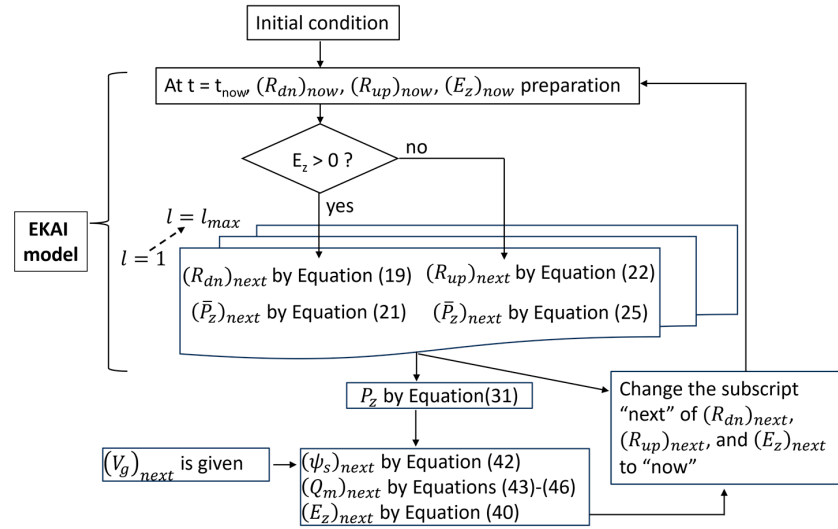


Figure 6. Calculation scheme of MFIS-type FeFETs. The core part of the scheme is the EKAI model.

In the case that the interface states between the semiconductor and insulator are considered, the equation $Q_m = -Q_s$ is modified as

$$Q_m = -Q_s - Q_{it}, \quad (44)$$

where Q_{it} is the trapped charge at the interface per area that is expressed as

$$Q_{it} = -e_0 \int N_{it}(\mathcal{E}) F_{SA}(\mathcal{E} - e_0 \psi_s) d\mathcal{E}. \quad (45)$$

Here, $\mathcal{E}$ is an electron-energy variable, $N_{it}(\mathcal{E})$ is the area density of interface-states per electron energy, and F_{SA} is the Fermi–Dirac distribution function for acceptors [59].

In the case that $N_{it}(\mathcal{E})$ is approximated as a constant D_{it} [$V^{-1} \text{cm}^{-2}$] with respect to the energy, Q_{it} can be approximated as

$$Q_{it} = -e_0 D_{it} \psi_s. \quad (46)$$

For convenience of numerical root-finding calculations, we emphasize that Q_s (Equation (43)) monotonically decreases with the increase of ψ_s , and Q_{it} (Equation (45) or Equation (46)) also has the same monotonical property. Equation (44) shows that Q_m is a monotonically increasing function of ψ_s .

See Equation (42). The right-hand side quantity is a monotonically increasing function of ψ_s . At $t = t_{next}$ in the previous section, we derived $\bar{P}_z(l)$ for all l by either Equation (21) or Equation (25). V_g at $t = t_{next}$ is given by an external voltage source. Thus, the left-hand side of Equation (42) is a known constant at $t = t_{next}$. The right-hand side of Equation (42) consists of only one variable ψ_s and is a monotonically increasing function of ψ_s . Hence, ψ_s can be uniquely determined at $t = t_{next}$. Once ψ_s is determined, we derive Q_m from Equations (43)–(46), and E_z from Equation (40) at $t = t_{next}$.

We now have E_z at $t = t_{next}$, and, in the previous section, we have $R_{dn}(l)$ and $R_{up}(l)$ at $t = t_{next}$ for all l . The set of E_z , $R_{dn}(l)$, and $R_{up}(l)$ at $t = t_{next}$ replaces a set of E_z , $R_{dn}(l)$, and $R_{up}(l)$ at $t = t_{now}$. If $E_z > 0$, $R_{dn}(l)$ and $R_{up}(l)$ at $t = t_{next}$ are obtained by Equations (19) and (20). If $E_z < 0$, $R_{up}(l)$ and $R_{dn}(l)$ at $t = t_{next}$ are obtained by Equations (22) and (23). The procedure of this section gives us E_z at $t = t_{next}$. Repeating these procedures provides the dynamics of the MFIS FeFETs.

The status of the polarization in ferroelectric or the electric displacement can be monitored by the drain current, I_d , of the sub-threshold region, which is represented as functions of the drain voltage V_d and the surface potential ψ_s by [59]:

$$I_d = \frac{\mu k_B T}{e_0} \sqrt{\frac{\epsilon_0 \epsilon_s p_{po} k_B T}{2}} \left(\frac{n_i}{N_A} \right)^2 (1 - e^{-\zeta V_d}) e^{\zeta \psi_s} (\zeta \psi_s)^{-1/2} \quad (47)$$

In this paper, all numerical results of FeFETs are obtained on the premise of $V_s = V_d = V_{sub} = 0$, whereas the practical I_d measurements of n -channel FeFETs are usually on the condition of $V_d = 0.1$ V and $V_s = V_{sub} = 0$. Such a small difference in V_d condition does not affect the validity of comparing results from the calculations and the measurements.

The EKAI, the formulae from Equations (11)–(27), and the total calculation scheme for MFIS FeFETs, those from Equations (28)–(31) and from Equations (40)–(47), describe the general transient response of MFIS FeFETs under time-dependent V_g conditions. The formulae also cover slowly changing phenomena. There is a so-called data retention mode, in which all the quantities such as Q_m , E_z , $R_{dn}(l)$, and $R_{up}(l)$ vary very slowly, and the Δt values in Equations (19) and (22) can be chosen flexibly with minimal changes of those quantities; thus, retention results of the period of days and years are obtained in a practical computation time.

4. Calculation Results of FeFETs and Comparison to the Experimental

4.1. Parameters Being Able to Be Assigned

The EKAI model and the total calculation scheme of this paper are verified using experimental data of FeFETs consisting of MFIS gate stacks of Ir/CSBT/HfO₂/IL/Si. The experimental details are reviewed in Appendix A. An insulator in the modeled MFIS FeFET corresponds to the bilayer of IL and HfO₂ in a real CSBT FeFET. Capacitance of the insulator (C_i) was evaluated as $C_i = 0.99$ $\mu\text{F}/\text{cm}^2$. Regarding the ferroelectric, the dielectric constant ϵ_{fdi} of the paraelectric component is determined by the Q_m – V_g curves at $V_g < 0$ or in the third quadrant of Figure A2 because the semiconductor depletion layer does not affect at $V_g < 0$. In the third quadrant, by taking the gradient of the curve of a V_g sweep amplitude, the combined capacitance of C_i and C_{fdi} (Equations (36b) and (39)) was 0.54 $\mu\text{F}/\text{cm}^2$. Since $C_i = 0.99$ $\mu\text{F}/\text{cm}^2$ and $d_f = 135$ nm, $\epsilon_{fdi} = 180$ at room temperature was obtained and used for calculation in the EKAI. The P_s direction of SBT and CSBT ferroelectrics is the a -axis direction of the crystal unit cell of SBT and CSBT [60,61].

With regard to the angle θ_l and the area A_l , the technique of EBSD patterns could characterize the crystal orientation and grain size. The bar graph plots in Figure 7 show the distribution function of grains with the orientation angle θ . The quantity of the vertical axis is the area of grains whose θ is in the range from θ to $\theta + \Delta\theta$ ($\Delta\theta$: the bar width). The scanning area of EBSD, ≈ 56 μm^2 , is not enough for statistical treatment, meaning that ΔV_{th} versus $\log(t_w)$ curves simulated by the EKAI model and the calculation scheme using the bare bar graph plots were not smooth. As shown in Figure A4, the experimental $\Delta V_{th} - \log(t_w)$ curves are very smooth. Therefore, we used a fitted smooth curve in Figure 7 instead of the bare data. Although the smoothed curve is used in the actual calculation, the curve is digitized at every 3° to save calculation time.

When we make quasi-static calculation of I_d – V_g and Q_m – V_g , a sinusoidal V_g function is provided as $V_g = V_{fb} + V_{amp} \sin(2\pi f_s t)$. The frequency f_s and the calculation time length are typically set as 10 Hz and 0.2 s, respectively. The time step $\Delta t = 1 \times 10^{-9}$ s is commonly used in the calculation of I_d – V_g , Q_m – V_g , and PWVR. Validity of the value Δt and accuracy of the calculated results were verified by confirming that calculations with $\Delta t = 0.5 \times 10^{-9}$ s gave the same results as those with $\Delta t = 1 \times 10^{-9}$ s.

Experimental I_d – V_g curves do not suggest any electron-energy dependence of $N_{it}(\mathcal{E})$ in Equation (45), and thus we use D_{it} and Equation (46) regarding the interface states between the insulator and semiconductor. Several series of I_d – V_g simulations with various V_{fb} and

D_{it} values were examined and compared to the experimentally obtained $I_d - V_g$. We found that $D_{it} = 4 \times 10^{12} \text{ V}^{-1} \text{ cm}^{-2}$ is a good value to fit the experiment. Regarding V_{fb} , the suitable range was between -0.8 V and -1.0 V , and thus we used $V_{fb} = -0.8 \text{ V}$ in this work.

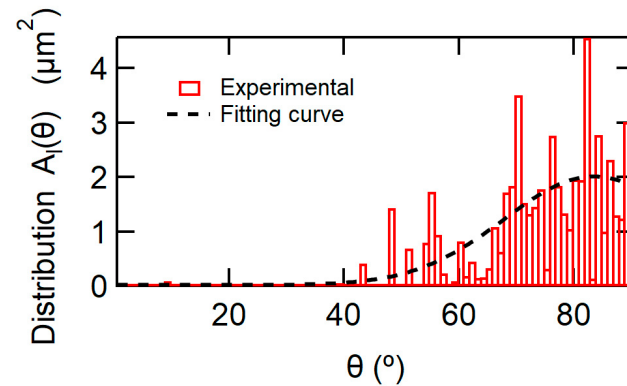


Figure 7. Area distribution vs. θ of CSBT crystal orientations. The EBSD technique derived the distribution in the polycrystalline ferroelectric CSBT layer, constituting the MFIS stack in the Ir/CSBT/I/Si FeFETs. The vertical quantity of the bar graph is the total area of the grains whose angle is in the range from θ to $\theta + \Delta\theta$ ($\Delta\theta$: the bar width). The dashed line is a smoothing curve of the bar graph used in the model calculation.

According to the PFM experiments and the analyses by phenomenological theories including random disorder potentials originated from imperfections in epitaxial films [53], the exponent σ of v_{wall} in Equation (8b) and that of t_0 in Equations (9b) and (10) are generally $\sigma \neq 1$. The magnitude of σ depends on materials and material preparation methods [62]. Some experiments indicated $\sigma \approx 0.5$ of BaTiO_3 [63], 0.5–0.6 in $\text{PbZr}_x\text{Ti}_{1-x}\text{O}_3$ (PZT) of $x = 0.2$ [64], and 0.20–0.28 of ferroelectric organic polymer [65]. In the case that the defect densities were intentionally increased, σ was decreased more [53]. However, other experiments showed $\sigma \approx 0.9$ and ≈ 1.0 for epitaxial PZT films [21,55]. Furthermore, the experiments switching current to single crystals of BaTiO_3 and triglycine sulfate showed an exponential relationship without the exponent σ [51,52]. The theory of wall propagation in a defect-free crystal by Miller and Weinreich [20] led to an exponential form like Equation (8b) but did not include σ . Molecular dynamics simulation for a defect-free domain interface also demonstrated v_{wall} as a form of Equation (8b) but without σ [22]. Zhao et al. [66] showed that polarization switching times of ferroelectric organic polymer films obeyed simply the Merz exponential law [51]. We did not use a method for intentionally introducing defects during annealing processes for ferroelectric layer crystallization of MFIS FeFETs [3–5]. Like these, there is no reason to choose $\sigma \neq 1$ in the following calculations for the SBT-based FeFETs. $\sigma = 1$ is assumed in simulations shown later in this paper, but σ as the mathematical expression is maintained. The σ appears in Section 5.2. later.

We adopted $n = 1.3$, which is a value derived experimentally for less than 200 kV/cm for an epitaxial PZT film [37] and which is also close to the average value, 1.25, of the n range, 1.0–1.5, reported for polymer ferroelectric films [66]. Note also that the calculated results were insensitive to the n variation from 1 to 3. The acceptor density was also not sensitive to the results, and $N_a = 1 \times 10^{16} \text{ cm}^{-2}$ is used for calculation.

4.2. Method for Determining Significant Three Parameters

The remaining parameters, E_{act} , t_{inf} , and P_s can be determined by curve fitting of numerical results to the experimental about the ΔV_{th} vs. t_w in PWVR. The experimental results of ΔV_{th} vs. t_w are found in Figure A4 in Appendix A. Regarding the numerical results, PWVR simulations with varying E_{act} , t_{inf} , and P_s are introduced in Figure 8a, Figure 8b and Figure 8c, respectively. Every marker corresponds to a calculated point of ΔV_{th} vs. t_w . Using the cases of Figure 8, we show how uniquely three parameters, E_{act} , t_{inf} , and P_s , are determined. We present a reference curve (the blue solid line with filled square markers

in Figure 8a, Figure 8b and Figure 8c, respectively), which was a numerical solution for well simulating an experimentally obtained ΔV_{th} vs. t_w . The reference curve was drawn using a set of parameters $E_{act} = E_o$, $t_{inf} = t_1$, and $P_s = P_o$ with $V_h = -V_l = 4$ V. The E_o , t_1 , and P_o are constants for the sake of explanation. The E_{act} and t_{inf} are deeply involved in ferroelectric polarization dynamics. The P_s is an inherent parameter of the ferroelectric. As shown in Figure 8a, if E_{act} is as large as $1.7 E_o$, the increase of ΔV_{th} with t_w is very slow, and the curve is far from the reference curve in a realistic t_w range of the experimental. If E_{act} is as small as $0.43 E_o$, rapidly increasing ΔV_{th} approaches a saturated value. This is far from the log-linear styles. An appropriate ΔV_{th} can draw a log-linear curve like the reference curve at $E_{act} = E_o$. As shown in Figure 8b, t_{inf} determines a quantity of the ΔV_{th} vs. $\log(t_w)$ curve shift in parallel along the $\log(t_w)$ axis. The polarization growth in Equation (21) or Equation (25) is proportional to P_s , meaning that if P_s is larger, the separation between a ΔV_{th} vs. $\log(t_w)$ curve written by pulses of $V_h (= -V_l)$ and the neighboring curve written by $V_h \pm 1V (= -V_l \mp 1V)$ is wider. See Figure 8c, where the curves are drawn in the case of $P_s = P_o$ and $1.7P_o$, respectively. The role of P_s is to adjust this separation distance to fit the experimental results. By experiencing these processes, E_{act} , t_{inf} , and P_s are uniquely determined under a fixed σ . Here, “uniquely determined” means that no solutions having a new parameter set exist far from the derived parameter set.

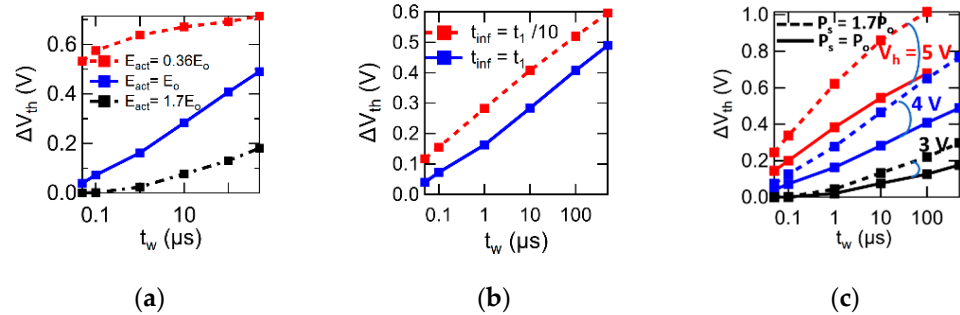


Figure 8. Graphs explaining how the parameters, E_{act} , t_{inf} , and P_s , are determined when we compare the model calculations to experimental PWVR data. (a–c) Show E_{act} , t_{inf} , and P_s dependences of ΔV_{th} vs. t_w curves, respectively. As shown in (a), if E_{act} is not optimized, the log-linear relation of ΔV_{th} vs. t_w cannot be derived across the t_w wide range from 50 ns to 1 ms. (b) indicates that t_{inf} variation brings a parallel shift of ΔV_{th} vs. $\log(t_w)$ curves. (c) indicates that the separation of ΔV_{th} vs. t_w lines at $V_h = -V_l = 3$ V, 4 V, and 5 V is very sensitive to P_s . The line separation by the dashed lines is larger than the solid lines, where the former P_s is 1.7 times larger than the latter. E_o in (a), t_1 in (b), and P_o in (c) are example constants for explanation convenience.

Remember that E_{act} has a meaning of an activation- or a threshold-field for domain wall motions as Equations (9b) and (10) indicate. The domain wall energy is affected by elastic and electric-dipole contributions in atomic scales. Theoretical works [20,24,25,53,67] indicated that the domain wall energy included a power exponent of P_s , indicating that the E_{act} may also be a function of P_s . Since the treated temperature is only room temperature, three parameters, P_s , E_{act} , and t_{inf} , can be searched independently to fit the experimental data. In the case that temperature is varied, P_s is also changed with temperature. We must consider that E_{act} is a function of P_s via the domain wall energy in addition to the thermally activation term $(k_B T)^{-1}$ (Equation (9b)).

4.3. Calculation Using Optimized Parameters and Comparison with the Experimental Data

Figure 9 shows a fitting result of PWVR where the calculated curves compared to the experimental data at $V_h = 3$ V, 4 V, 5 V, and 6 V. Markers represent the calculated points of ΔV_{th} vs. t_w using an optimum parameter set of $E_{act} = 828$ kV/cm, $t_{inf} = 8.30 \times 10^{-12}$ s, and $P_s = 3.0$ $\mu C/cm^2$. Solid lines mean the experimental results of Figure A4 introduced in Appendix A. The calculation well simulated the experimental ΔV_{th} vs. $\log(t_w)$ throughout

the wide t_w range from 50 ns to 0.5 ms. Other parameters for the calculation are summarized as follows: $\sigma = 1$, $n = 1.3$, $V_{fb} = -0.8$ V, $D_{it} = 4 \times 10^{12}$ V⁻¹cm⁻², $N_A = 1 \times 10^{16}$ /cm³, $d_f = 135$ nm, $\epsilon_{fdi} = 180$, $d_i = 3.5$ nm, and $\epsilon_i = 3.9$.

Using the same values of parameters as those solved for fitting PWVR (Figure 9), other correlations were simulated that were quasi-static characteristics of I_d - V_g (Figure 10) and Q_m - V_g (Figure 11) with various V_g sweep amplitude. The calculated results are drawn with thick and red-colored lines. The experimental results are expressed by thin lines colored in black. In the calculations, V_{th} was defined as V_g at which the semiconductor surface potential ψ_s was equal to 85% of $2\psi_B$, the surface strong inversion condition (i.e., $\psi_s = 2\psi_B \times 0.85$ where $\psi_B = (1/\zeta)\ln(N_A/n_i)$ [59]). Figures 10 and 11 show moderate agreements of the calculated results with the experimental results. However, high curvature of Q_m - V_g around $V_g = 0$ V seems more emphasized in the calculated than in the experimental results as shown in Figure 11. As an effort of the Q_m - V_g matching, for example, D_{it} may be raised for decreasing the nonlinearity of Q_m - V_g . But the attempt enhances another mismatch in I_d - V_g as shown in Figure 10. The reason for the inconsistency is not clear now. Despite having some numerical mismatch remaining in the curve fitting, the EKAI model and the calculation scheme qualitatively and comprehensively well simulate FeFET characteristics such as dynamic PWVR and quasi-static I_d - V_g and Q_m - V_g .

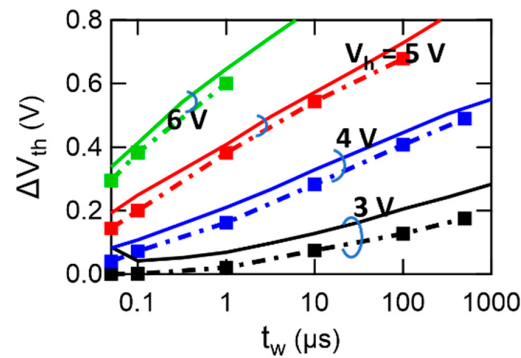


Figure 9. Model calculation compared to the experimental data regarding PWVR. Dash-and-dot lines are the results of the calculation. Solid lines are the results of the experiment (Figure A4). The points at the filled square markers on the ΔV_{th} vs. t_w plane are the actual calculation points. Write pulse height conditions are $V_h = -V_l = 3, 4, 5$, and 6 V. The calculation results agree fairly well with the experimental ones. In particular, the calculation reproduces the log-linear characteristics well. The significant three parameters are $E_{act} = 828$ kV/cm, $t_{inf} = 8.30 \times 10^{-12}$ s, and $P_s = 3.0$ μ C/cm². Other parameters used for the calculation is summarized as $\sigma = 1$, $n = 1.3$, $V_{fb} = -0.8$ V, $d_f = 135$ nm, $\epsilon_{fdi} = 180$, $d_i = 3.5$ nm, $\epsilon_i = 3.9$, $D_{it} = 4 \times 10^{12}$ /Vcm², $N_A = 1 \times 10^{16}$ /cm³, $\epsilon_s = 11.9$, $n_i = 1.45 \times 10^{10}$ cm⁻³, and $T = 300$ K.

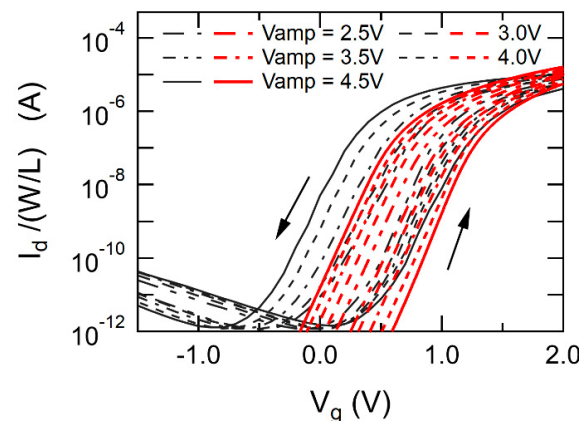


Figure 10. Model calculation with the experiment (Figure A1) of quasi-static I_d vs. V_g measurements for various V_g sweep amplitude. Red lines and dark grey lines are the calculation and experiment results, respectively. We used the same parameters as those for PWVR calculation in Figure 9.

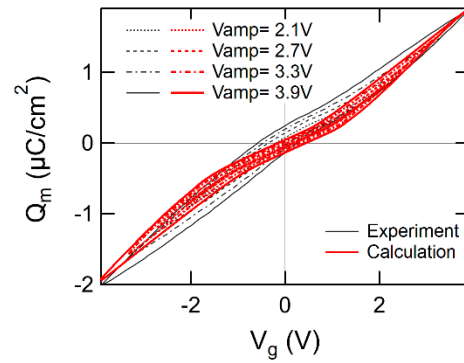


Figure 11. Model calculation with the experiment (Figure A2) of quasi-static Q_m vs. V_g measurements for various V_g sweep amplitude. Thicker red lines and dark grey lines are the results of calculation and experiment, respectively. The same parameters as those for PWVR, I_d vs. V_g calculations in Figures 9 and 10 were used.

5. Discussion

5.1. Insight Regarding FeFET Dynamics

5.1.1. Details of PWVR Operations Using Q_m vs. E_z Domains

In the EKAI model, a Q_m vs. E_z correlation is calculated along a hysteresis loop as shown in Figure 12a. The drawing sequence is explained by corresponding V_g variations with checkpoints as shown in Figure 12b, which are, **a**, **b**, **c**, **d**, **g**, **g'**, **d'**, **e**, **f**, **a**, **h**, **h'** and back to **a**, repeated cyclically in this order. A positive pulse writing (PPW) draws a trajectory connecting **a**, **b**, **c**, and **d**. A negative pulse writing (NPW) draws a trajectory connecting **d'**, **e**, **f**, and **a**. As stated in the introduction, we assume in this paper that the parameters except for the polarization switching varies instantaneously. On the Q_m – E_z curve, points instantaneously move from **a'** to **b**, from **c** to **d**, from **d'** to **e**, and from **f** to **a**. These curves can be written as

$$Q_m = \epsilon_0 \epsilon_{fdi} E_z + P_{zconst}, \quad (48)$$

where P_{zconst} is a constant that each straight line has and P_{zconst} equals P_{zb} , P_{zc} , P_{ze} , and P_{zf} for the line **a**–**b**, **c**–**d**, **d'**–**e**, **f**–**a**, respectively.

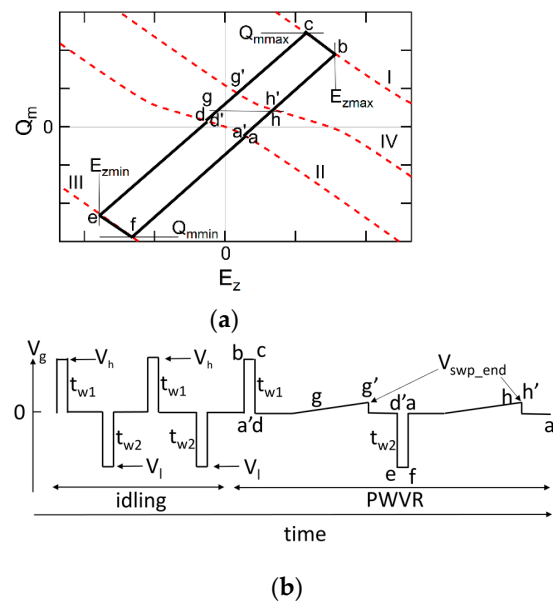


Figure 12. (a) Solid-line loop is the trajectory on the Q_m – E_z plane during a PWVR operation and (b) V_g variation diagram for explanation. Letters from **a** to **h** with **a'**, **d'**, **g'**, and **h'** are checkpoints commonly found in (a,b). When a point indexed by a letter represents a state on the V_g vs. time diagram in (b), the ferroelectric state takes the state on the point indexed by the same letter in the solid-line

loop in (a). For a step-function-like abrupt change of V_g such as **a'-b**, **c-d**, **d'-e**, or **f-a**, Q_m varies instantaneously on a line whose gradient is $\varepsilon_0 \varepsilon_{fdi}$. During a constant V_g application like **b-c** or **e-f**, the Q_m - E_z trajectory follows the load line I or III, $Q_m = -C_i d_f (E_z - (V_g - V_{fb} - \psi_s) / d_f)$. $R_{dn}(l)$ grows on **b-c** according to Equation (19), and $R_{up}(l)$ grows on **e-f** according to Equation (22) by the EKAI. The line **d-g-g'-d'** or **a-h-h'-a'** corresponds to data retention (or holding) and V_{th} read stage. At the read end, Q_m rises to **g'** or **h'**. At the retention stage the trajectory also exists on the load line II, $Q_m = -C_i d_f (E_z - V_{fb} - \psi_s) / d_f$. Due to the presence of an electric field, the polarization may be decreased, i.e., **d** (or **a**) may move to an inside point **d'** (or **a'**) on the load line at $V_g = 0$. The decreasing extent depends on E_{act} , E_z , $\cos(\theta_l)$, and the time length between **d** and **d'** (or **a** and **a'**). Q_m rising to **h'** for the read operation may also decrease the polarization.

As discussed in Section 3.3, the electrostatic potential equation across the MFIS stack (Equation (41)) is valid at any moment where $V_f = E_z d_f$ and $V_i = Q_m / C_i$. The Q_m is a function of ψ_s by a discussion at Equations (43)–(46). Consequently, at any time, Q_m - E_z satisfies the following equation:

$$Q_m = -C_i d_f \left(E_z - (V_g - V_{fb} - \psi_s) / d_f \right) \quad (49)$$

Curves described by Equation (49) are called load lines in this paper. Four load lines I, II, III, and IV appear in Figure 12a. The load lines I, II, III, and IV are the lines when V_g in Equation (49) equals V_h , 0, V_l , and V_{swp_end} , respectively. Equation (49) indicates that a solution point (E_z, Q_m) locates at any moment (t_a) on a load line having the V_g value at $t = t_a$. The EKAI model decides which point on the load line is really the solution point.

The point **b**, **d**, **e**, and **a** are decided by that Equations (48) and (49) are simultaneously satisfied. From **b** to **c** in PPW, the EKAI model describes a P_z increase from P_{zb} to P_{zc} during the period t_{w1} of V_h application (Equation (19)). Similarly, from **e** to **f** in NPW, the model describes a P_z decrease from P_{ze} to P_{zf} during the period t_{w2} of V_l application (Equation (22)).

Initially, idling write cycles are executed that consist of PPW and NPW without a V_{th} reading (VR). The idling cycles have the role of making the Q_m - E_z trajectory converge into the steady loop shown in Figure 12a. The simulation can be started from the coordinate origin at $t = 0$, where $E_z = 0$, $Q_m = 0$, and $R_{dn}(l) = R_{up}(l) = 1/2$ for all l . The Q_m - E_z trajectory changes during the idling write cycles and is converged into a steady state loop after experiencing plural cycles. Then the PWVR operation starts. After one PPW is executed, a VR draws a trajectory connecting **d**, **g**, **g'**, and **d'**. After one NPW is executed, another VR draws a trajectory connecting **a**, **h**, **h'**, and **a'**. At read, V_g is swept to V_{swp_end} (i.e., V_g at point **g'** and **h'**). When $V_g = V_{swp_end}$, **g'** and **h'** are on the load line IV. V_{th} values are decided at a reference level of Q_m , i.e., at points **g** and **h**. Q_m and ψ_s have a single-valued function relationship with each other via Equations (43)–(45). The reference level of ψ_s (ψ_{th}) can replace the reference of Q_m . The ψ_{th} is chosen in a sub-threshold region of the FeFETs so that $\psi_B \leq \psi_{th} \leq 2\psi_B$. The EKAI model simulation indicates that, during a V_g sweeping after NPW, there is a tendency that P_z increases (i.e., the stored negative P_{zf} decreases). If this is a visible case, point **a'** separates from **a** and shifts to the E_z smaller direction on load line II. The EKAI model works during all the period **d-g-g'-d'** and **a-h-h'-a'**, which means that this period is also in a data-retention stage. If the depolarization electric field is not small, Q_m shifts to the $|Q_m|$ decreasing direction on load line II. In this sense, **d'** and **a'** differ from **d** and **a**, respectively. The decrease amounts depend on the relationship among E_{act} , E_z , and $\cos(\theta_l)$, as shown in Equation (16).

5.1.2. Strategy to Reduce Charge Injections into FeFET Gate Stacks

Note that, in drawing the loop in Figure 12a, it passes through two points: the maximum induced charge (Q_{mmax}) and the minimum one (Q_{mmin}) (i.e., the negative maximum one). The Q_{mmax} and $-Q_{mmin}$ decide the amount of an undesirable current of the direct tunneling type or the electric-field-assisted (Fowler-Northeim, FN) tunneling type. At

$Q_m = Q_{mmax} = Q_{mmin}$, $|V_{imax}| = Q_{mmax}/C_i = -Q_{mmin}/C_i$ is defined where the V_{imax} is the maximum voltage drop across the insulator. If $Q_{mmax} = 2.0 \mu\text{C}/\text{cm}^2$ and the insulator is 1.6-nm-thick SiO_2 , then $V_{imax} = 0.93 \text{ V}$ and the corresponding field maximum of the insulator, $E_{imax} = 5.8 \text{ MV}/\text{cm}$. Let us estimate gate leakage currents thorough the insulator. Using a high permittivity insulator or a combination of such insulators weakens the field a little, but the field is still high enough to induce the leakage currents. Investigations of the tunneling current of polysilicon/ SiO_2/Si [68,69] are good references to know the impact of the charge injection for the MFIS stacks where the semiconductor is Si. The charge injection is mainly caused by the tunneling current through the IL (i.e., SiO_2). We propose a significant guideline in investigating ferroelectric FETs. Imagine what happens at $Q_m = Q_{mmax} = 2.0 \mu\text{C}/\text{cm}^2$. At this moment, the charge injection is the highest. According to Ref. [68], in the case that SiO_2 was about 1.6 nm thick, the tunneling current was $\approx 10 \text{ A}/\text{cm}^2$ at the 5.8 MV/cm whereas it was $\approx 10^{-5} \text{ A}/\text{cm}^2$ in the case of about 3.2 nm thick SiO_2 , at the same field. The voltage drops across the SiO_2 layer, Q_m/C_{SiO_2} , [C_{SiO_2} : the SiO_2 layer capacitance] at $Q_m = 2.0 \mu\text{C}/\text{cm}^2$ are 0.93 V and 1.85 V for the 1.6 nm thick and 3.2 nm thick SiO_2 layers, respectively. By choosing this twice thick insulator SiO_2 , the tunneling current decreases $\approx 10^{-6}$ times, and the V_g for writing increases only about 0.9 V. As this quantitative consideration indicates, there seems no way to avoid the tunneling current except for increasing the thickness for SiO_2 . To preserve the nonvolatile device reliabilities, the IL SiO_2 should be moderately thick enough to avoid charge injection caused by the tunneling current. A strategy of thinning SiO_2 is logically failed.

If charge injections are not negligible, a scenario is as follows: In PPW, electrons are injected from the silicon. The electrons may mostly arrive at the metal electrode and be absorbed. However, some of them are trapped in the ferroelectric layer, the insulator, and the interface between the ferroelectric layer and insulator. The trapped ones near the silicon side may return to the semiconductor by tunneling back after PPW [45], but other trapped electrons remain trapped, leading to the increase of V_{th} of n -channel FeFETs, while NPW holes are injected from the silicon. Similarly, some holes are stably trapped, leading to the decrease of V_{th} of n -channel FeFETs. Since the number of trapped electrons after PPW and that of trapped holes after NPW are not the same, unintended V_{th} shifts appear with increasing the cycle of PPW and NPW in endurance tests.

5.1.3. Short Consideration in Negative-Capacitance-Transistors

On load lines I, II, III, and IV mentioned above, P_z - and Q_m -increase accompanies E_z decrease, meaning that a capacitance dQ_m/dE_z is negative. Note that, as described in the EKAI model and the total calculation scheme, the time response of the linear dielectric part is instantaneous, but P_z variation needs time. Thus, while V_g is swept back and forth between negative and positive voltages, the derived Q_m - V_g and I_d - V_g curves inevitably draw hysteresis loops. The EKAI model does not realize the idea discussed in Ref. [70] regarding steep-slope non-hysteresis transistors during on-off operation for back-and-forth voltage sweeping.

5.2. Coercive Field in the EKAI Model

Although the coercive fields can be read in the Q_m - V_g hysteresis curves derived by the calculation of this model, the EKAI model of this paper does not contain the coercive field (E_c^*) as an explicit parameter. Let us find the relationship between the model and E_c^* for a case of a single grain ferroelectric indexed by θ . To take Q_m vs. E_z curves, a triangular shape E_z as a function of time, like Figure 13b, whose linear slope is K , is supplied to an MFM capacitor. Figure 13a shows a P_z vs. E_z curve. During E_z increasing with time, R_{dn} varies from 0 to 1, like Figure 13c. Since $E_z = K \text{ time} + \text{constant}$, R_{dn} vs. time is converted to R_{dn} vs. E_z . At a narrow region of E_z , R_{dn} increases rapidly, as shown in Figure 13c. The R_{dn} rapid increase corresponds to P_z increase of the right-side branch of the hysteretic loop in Figure 13a, indicating that an E_z at which the R_{dn} rapid increase occurs is regarded as a coercive field. Since the R_{dn} increase is rapid within a narrow range of E_z , a defined coercive

field well approximates E_c^* which is defined as the field at $Q_m = 0$ (Figure 13a). The E_z representing this narrow range field can be decided by the E_z (E_{cm}) at which dP_{dn}/dE_z takes a maximum (Figure 13d). E_{cm} is the coercive field derived analytically in the EKAI model. Exactly speaking, E_{cm} approximates E_c^* , but E_{cm} is not equal to E_c^* .

By starting from Equation (26) with the use of $dE_z = Kdt$ and by calculating the second derivative, $d^2R_{dn}/dE_z^2 = 0$, we have, without any approximation,

$$\exp \left[- \left(\frac{E_{act}}{E_z \cos \theta} \right)^\sigma \right] - \frac{\sigma K \cos \theta}{E_{act}} \frac{t_{inf}}{g(n)} \left(\frac{E_{act}}{E_z \cos \theta} \right)^{\sigma+1} = 0 \quad (50)$$

with $g(n) = n[-\ln(1 - R_{dn})]^{(n-1)/n} - (n-1)[- \ln(1 - R_{dn})]^{-1/n}$.

In Equation (50), K is the sweep slope, and E_{act} , t_{inf} and σ are the model simulation parameters. In $g(n)$, n is the model parameters. Although $g(n)$ contains R_{dn} , $g(n)$ weakly depends on R_{dn} variation. This means $g(n)$ can be regarded as a constant. (In the case of $n = 1$, $g(n)$ equals 1, and Equation (50) does not contain the dimension parameter, n .) Hence, Equation (50) can be solved for E_z , and the root of it is E_{cm} .

Equation (50) is a finding-root problem of $x_e = E_{act}/E_z \cos \theta$ on the condition of $g(n) = 1$. Since E_{act} is included in x_e , E_{cm} is changed rapidly with E_{act} . Since K appears only in the coefficient in Equation (50), the coercive field E_{cm} varies slowly with K . The solid curve in the inset of Figure 13e is the solution of Equation (50), where K is varied with the constants of $\sigma = 1$, $E_{act} = 828$ kV/cm, and $t_{inf} = 8.30 \times 10^{-12}$ s. The filled-circle markers are the results of the full simulation of the EKAI model with MFM capacitor structures. Good agreement is confirmed between the solid line and the filled circles. The obtained E_{cm} values that vary with K are about 50 kV/cm. This value agrees well with the experimentally known value of SBT. In fact, the Q_m - V_g curve of an MFM with a (100)/(010)-oriented SBT thin film [71] showed $E_c^* = 48$ kV/cm when the swing amplitude and frequency were 225 kV/cm and 20 Hz that corresponds to $K = 1.8 \times 10^4$ (kV/cm)/s. This point is added in the inset graph of Figure 13e as the filled square, indicating good agreement with the solid curve by Equation (50).

Slower sweeping cases are also solved by Equation (50) as shown in the solid curve of Figure 13e. E_{cm} decreases very slowly with the decrease of $\log(K)$. The figure shows $E_{cm} = 48$ kV/cm and 20 kV/cm at $K = 1.8 \times 10^4$ (kV/cm)/s and 5.5×10^{-8} (kV/cm)/s, respectively. This means that E_{cm} is 20 kV/cm when the field is swept with a cycle period of 1.6×10^{10} s (≈ 500 years) with sweeping ± 225 kV/cm. That is to say, although the model does not have a coercive field as an explicit parameter, the derived results assure nonvolatile performance.

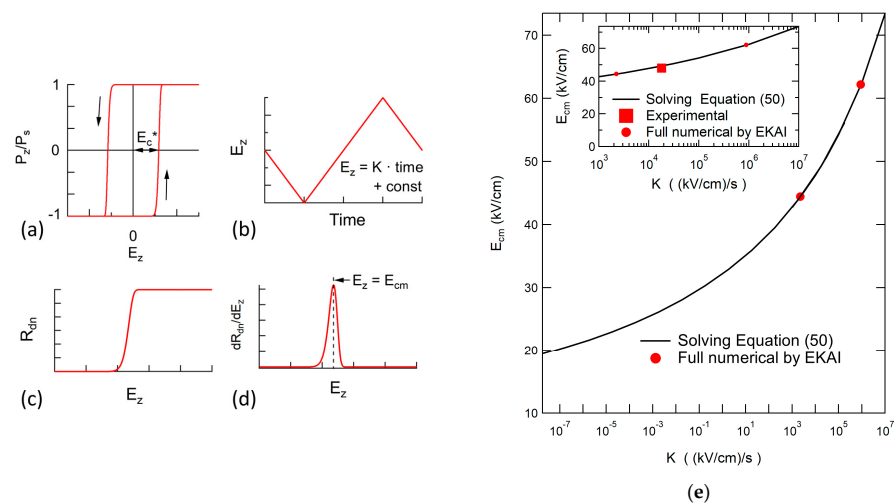


Figure 13. Semi-analytical discussion of a quantity equivalent to a coercive field in the EKAI model. For an MFM with a single grain ferroelectric, schematic curves of (a) P_z/P_s vs. E_z , (b) triangular waveform

$E_z(t)$, (c) R_{dn} vs. E_z , and (d) dR_{dn}/dE_z vs. E_z . The slope, dE_z/dt , is $\pm K$. Since the field (E_{cm}) at which dR_{dn}/dE_z takes a maximum is very close to the coercive field (E_c^*) defined as the field at $Q_m = 0$, E_{cm} can be regarded as a coercive field. An analytical equation, Equation (50), is derived, the root of which is E_{cm} . The solid lines in (e) and the inset of (e) are the root curve of Equation (50) as a function of K . The inset in (e) is the graph in the range of $10^3 < K < 10^7$. For usual Q_m - E_z measurement, K is within this range. The filled circles are the E_c^* values obtained by the full numerical calculation of the EKAI and scheme (Figure 6), and the filled square mark in the inset is the experimental result of SBT [71]. The solid line in (e) indicates that E_{cm} is maintained as about 20 kV/cm under an ultraslow rate $K = 5.5 \times 10^{-8}$ (kV/cm)/s, which corresponds to the case that E_z of ± 225 kV/cm sweeping is executed by spending 8×10^9 s.

6. Conclusions

An extended KAI (EKAI) model for describing the electrical properties of ferroelectric-gate field effect transistors was proposed. The model is physics based and was validated via comparison with rich experimental data of metal-ferroelectric-insulator-semiconductor type FeFETs where the ferroelectric was of SBT or CSBT in the Bi-layered-perovskite oxides. The model features and the results of comparison with the experimental data are summarized as follows.

6.1. The EKAI Model and the Calculation Scheme for FeFETs

The orientation angle θ of each grain in the ferroelectric film and its size is assigned, where θ is the angle between the film normal and the spontaneous polarization direction. In each grain, polarization reversed domain nucleation occurs along the spontaneous polarization direction, and the domain wall expands to the lateral direction of the P_s direction. In the case of large θ , the time scale of transient phenomena under an electric field is much larger than that in the $\theta = 0$ case. This is the essential cause that the ΔV_{th} vs. t_w of PWVR indicates log-linear relationships.

Since the ferroelectric thickness of experimental FeFETs compared to the model is 135 nm, which is comparable with the average size of grains, we assumed a single grain occupation along the z-direction in the SBT-based FeFETs. Each grain is supposed to have a pillar shape with a constant area from the film top to the bottom.

The electrostatic condition of the MFIS stacked structure renders a time-varying electric field in each grain in the ferroelectric film. The KAI equation about the time evolution of polarization is presented on a condition of a fixed electric field. The EKAI model represents polarization variation under the time-varying field as follows: At $t = t_{now}$, let grain l have the volume fraction of the downward polarization domain $(R_{dn}(l))_{now}$ at a positive field $(E_z)_{now}$. The polarization changes from t_{now} to $t_{next} = t_{now} + \Delta t$ as if the $(R_{dn}(l))_{now}$ would change under a constant $(E_z)_{now}$. In the case of negative $(E_z)_{now}$, the volume fraction variation of the downward domain $(R_{up}(l))_{now}$ is calculated similarly. At $t = t_{next}$, using obtained $(R_{dn}(l))_{next}$ or $(R_{dn}(l))_{next}$ and the external gate voltage, the electrostatic equations of MFIS stack derives the electric field $(E_z)_{next}$. By repeating this procedure from t_{now} to t_{next} , the time-dependent behavior of FeFETs can be derived.

The characteristic time $t_o \propto \exp(\text{const.}/E_z \cos \theta)$ in the EKAI model is a measure of switching time of respective grains. Wide distribution of θ makes the time FeFET response quite broad on the $\log(t)$ scale. Regarding the connection of the ferroelectric to the insulator and semiconductor, the polarization is averaged over the area at the bottom of the ferroelectric film. This average procedure can be accepted because semiconductors have a much smaller ability to shield polarization than metals and the transitional layer at the bottom of the ferroelectric works for averaging the polarization variation among the grains.

6.2. Comparison with Experimental Data and Discussion

The parameters, P_s , E_{act} , and t_{inf} can be uniquely determined in comparison with experimental data as $P_s = 3 \mu\text{C}/\text{cm}^2$, $E_{act} = 828 \text{ kV}/\text{cm}$, $t_{inf} = 8.30 \times 10^{-12} \text{ s}$. Using these

parameters, I_d vs. V_g , Q_m vs. V_g , and PWVR were calculated. The calculation results were explained consistently and entirely by the corresponding experimental data.

Transient behavior can well be understood using Q_m vs. E_z planes. The paraelectric component in Q_m ($=D_z$) of Equation (40) instantaneously follows the electric field variation $Q_m = \epsilon_0 \epsilon_{fdi} E_z + P_{zconst}$ (Equation (48)). Q_m always moves on the load line $Q_m = -C_i d_f (E_z - (V_g - V_{fb} - \psi_s) / d_f)$. On the PWVR measurement, V_g is set to equal V_h or V_l , at the pulse write (PW) stage and is swept in a small voltage range to find the V_{th} at the V_{th} read (VR) stage. At the PW stages, P_z and Q_m grow via the EKAI model during the pulse width t_w and finally reach the maximum or the negative maximum of Q_m .

In order to suppress the effect of charge trapping in the FeFET operations, there should be restrictions on the values of Q_{mmax} and $-Q_{mmin}$. The guideline was proposed for avoiding the charge injection. For preserving the nonvolatile reliabilities, the IL SiO_2 should be moderately thick enough to avoid charge injection caused by the tunneling current.

On the load line mentioned above, the increase in P_z and Q_m accompanies the decrease in E_z , meaning that a capacitance dP_z/dE_z is negative. In our model, linear dielectric response is instantaneous, but P_z variation needs time, and thus, during back-and-forth sweeping of V_g , the derived curves of Q_m – V_g and I_d – V_g always draw hysteresis loops.

The EKAI model and the calculation scheme do not explicitly have a coercive electric field (E_c^*). When a triangular waveform field is given across the ferroelectric film for a metal-ferroelectric-metal capacitor, a simple equation (Equation (50)) is derived, containing the field increasing rate, K , as well as E_{act} , and t_{inf} . The root of Equation (50) gives an electric field E_{cm} that approximates E_c^* . E_{cm} decreases with the decrease of K , but even if a very slow K corresponding to a time scale of more than 100 years is chosen, a sufficient E_{cm} remains. This means that the EKAI model assures a non-volatile memory function that the ferroelectrics hold.

The EKAI model of this paper described polarization variation based on 180° polarization switching. The model is applicable to materials showing 180° or nearly 180° polarization switching such as $\text{SrBi}_2\text{Nb}_2\text{O}_9$, $\text{Bi}_4\text{Ti}_3\text{O}_{12}$, $\text{Bi}_{4-x}\text{Ln}_x\text{Ti}_3\text{O}_{12}$ ($\text{Ln} = \text{La}, \text{Nd}, \text{Sm}$), LiTaO_3 , and LiNaO_3 [72–78].

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Appendix A. Summary of Experimental Results of FeFETs

The proposed EKAI model and calculation scheme for MFIS FeFETs are verified via comparison with experimental data of MFIS FeFETs with the gate stack of $\text{Ir}/\text{CSBT}/\text{HfO}_2/\text{IL}/\text{Si}$. Manufacturing details of the FeFETs were explained in, for example, [58]. The thicknesses of CSBT and HfO_2 were 135 nm and 4 nm, respectively. The interfacial layer (IL) was formed on the silicon substrate surface during the crystallization annealing by which the ferroelectricity appeared in the CSBT. The IL was an amorphous SiO_2 with the thickness of 2.6 nm according to the cross-sectional observation by transmission electron microscopy. The insulator layer of the MFIS was composed of double layers of the HfO_2 and the IL. Since the dielectric constants of SiO_2 and HfO_2 are 3.9 and about 20, respectively,

the insulator layer is characterized by $d_i = 3.5$ nm, $\varepsilon_i = 3.9$, and $C_i = 0.99$ $\mu\text{F}/\text{cm}^2$ in the calculation scheme. Gate metal length L_m was 10 μm . Channel length L was 8 μm as a distance between the source and drain edges, implying that the overlap lengths were 1 μm for both gate-and-drain and gate-and-source. The gate widths (W) were in the range from 10 μm to 200 μm .

To achieve thin ILs, FeFETs were annealed for the CSBT crystallization in an N_2 main gas mixed with a small amount of O_2 . We found that this mixing ratio of the ambient gas during the annealing changed the CSBT crystal-orientation distribution. The EBSD characterization showed the crystal-orientation distribution as a function of θ . The distribution was mostly flat in O_2 annealed FeFETs [26], but not so in N_2 dominant annealed FeFETs. The FeFETs adopted in the present work are the ones annealed in the N_2 dominant, where the orientation is unevenly distributed. Major grains have $\theta \geq 65^\circ$ [79] as shown in Figure 7.

Three kinds of experimental data are compared to numerical results by the EKAI model calculations, i.e.,

- (1) drain current (I_d) versus gate voltage (V_g),
 - (2) Induced charge Q_m in the metal gate versus V_g , and
 - (3) V_g -pulse-write-and- V_{th} read, i.e., PWVR.
- (1) Experimental I_d - V_g

I_d - V_g curves were obtained using a semiconductor parameter analyzer (4156C, Keysight Technologies, Santa Rosa, CA, USA), in which the V_g sweeping was quasi-statically slow. The experimental curves of an n -channel FeFET are shown in Figure A1. The source voltage V_s and the substrate voltage V_{sub} were 0 V, and the drain voltage $V_d = 0.1$ V. The I_d was normalized by W/L , and V_{th} was defined as the V_g at $I_d = 10^{-8}$ A. The memory window V_w was defined by $V_{thr} - V_{thl}$, where the threshold voltage V_{thr} (V_{thl}) is on the right- (left-) side on the I_d - V_g hysteresis curve. With increasing the V_g sweep amplitude, V_w was increased (the inset of Figure A1) due to increased polarization switching. By using Ir [80] or Pt [3] as a gate metal, SBT or CSBT FeFETs could have long retention and high endurance [3,80]. Since the work functions of Pt and Ir [81] are larger than the fermi level of p -type Si substrates, SBT or CSBT FeFETs originally have a larger V_{thl} than 1 V [3,82]. Practically, FeFETs with nearly 0 V for $(V_{thr} + V_{thl})/2$ were preferred, and thus the surface potentials of the channel were controlled by n -type shallow doping in the Si channel [58,83]. By adjusting the dose and energy of the dopants, V_{thl} and V_{thr} can be shifted to negative by more than 1 V at the cost of increase in off-state I_d . In the I_d - V_g curves as shown in Figure A1, a high off-state current of 10^{-12} A order is due to the channel surface doping. In the calculation scheme of this paper, this surface doping effect is treated as an adjustment of the flat-band voltage V_{fb} with negative values. Presence of a large surface state density, D_{it} , in the channel is suggested by large SS (subthreshold swing) values of 140 mV/decade at around $I_d = 10^{-9}$ A. As shown in Figure A1, I_d increases with decreasing V_g below about -1 V. This is the gate-induced drain leakage (GIDL) current [3,84]. Due to the overlapped large area of the gate and drain, a p -type inversion layer is formed at the surface of the drain beneath the gate metal, when a negative V_g is applied. This p -inversion forms a reverse-biased $p-n$ junction in the n -drain region. Since the impurity concentration is heavy in the drain, the reverse-biased junction easily accompanies a tunnel current. The GIDL is closed in the substrate and related neither to the gate ferroelectric defects nor the gate leakage current between the gate and silicon. If one chooses a structure with negligible gate-and-drain overlapping, the GIDL current can be diminished. When we used a self-aligned gate structure, this current was indeed decreased [2,5].

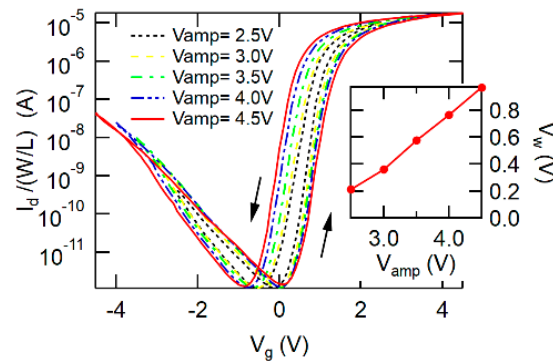


Figure A1. Experimental I_d vs. V_g characteristics of an Ir/CSBT/I/Si FeFET at various V_{amp} . V_g was swept between $\pm V_{amp}$ with $V_d = 0.1$ V. Insulator I is the bilayer of HfO₂ layer and SiO₂-like IL layer. The thickness is 135 nm, 5 nm, and 2.6 nm for CSBT, HfO₂, and IL, respectively. The I_d that is normalized to W/L is shown in the figure. $L = 10$ μ m and $W = 80$ μ m. The small window in the figure shows in the figure V_w vs. V_{amp} , where $V_w = V_{thr} - V_{thl}$, and V_{thr} (V_{thl}) is the V_g value at $I_d/(W/L) = 10^{-8}$ A of the right- (left-) side branch of the hysteresis curves.

(2) Experimental Q_m - V_g

Q_m vs. V_g curves were obtained using a ferroelectric test system (RT6000S, Radiant Technologies, Albuquerque, NM, USA). The gate is connected to one terminal of the system, and the substrate, source, and drain are connected to the other terminal. The measurement time between the neighboring two points is 1.16 ms, meaning that if 200 measurement points are assigned for one loop, it takes 0.23 s to measure one loop. The experimentally obtained Q_m vs. V_g curves with several V_g sweep amplitudes are shown in Figure A2. Because of the MFIS structure if we fix Q_m and assume no charge injection, V_g is the summation of the voltages across the ferroelectric and across the insulator, and the surface potential of the silicon channel. The curves in the first quadrant of the Q_m - V_g coordinates include the depletion state of the semiconductor surface side, and those in the third quadrant do not include it. Hence, the curves are asymmetric for the origin of the coordinate. Despite the semiconductor surface depletion, the curve variation with changing V_g in Figure A2 is smoother than expected. This smoother phenomenon can be explained by charge occupation and release in a rather high interface state density presented at the silicon channel surface. The gradient of the curves in the third quadrant can be utilized to decide the permittivity of the linear paraelectric component, ϵ_{fdi} , of the ferroelectric because the depletion state is not included in this side.

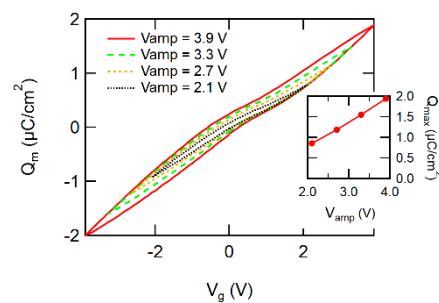


Figure A2. Experimental Q_m vs. V_g characteristics for Ir/CSBT/I/Si FeFET for various V_{amp} . V_g was swept between $\pm V_{amp}$. The stack material and thickness of each layer are the same as those of the FeFET in Figure A1. $Q_m = Q_{max}$ at $V_g = V_{amp}$, and $Q_m = Q_{min}$ at $V_g = -V_{amp}$. $Q_{max} \cong -Q_{min}$. Q_{max} vs. V_{amp} is shown in the small window on the right side.

(3) Experimental PWVR

ΔV_{th} versus t_w with various V_h and V_l of (PWVR) were obtained experimentally. According to the schematic chart (Figure A3), the measurement was performed. In the case of

FeFETs we usually cannot use a fully saturated state like that all grains are in their saturated polarization states. If we intend to make the fully saturated state, we must apply large V_g , that leads to charge injection and traps as discussed in Section 5.1.2. This means that there are no well-defined reference voltages as the threshold voltage. Therefore, regarding ΔV_{th} , we do not take the difference from a well-defined reference voltage level. Instead, in order to derive ΔV_{th} , we take the write voltages of a pair, (V_h, t_w) and $(-V_h, t_w)$. $V_l = -V_h$. That is, the pair has the same volage height but the opposite polarity with the same pulse width. Idling pulse cycles of this pair were given plural times before performing the read operation. The role of this idling-cycles is, regardless of the history of previous operations, to obtain the threshold voltages of writing by the pair. In this experiment the idling cycles were repeated twice. During the write and the idling, $V_d = V_s = V_{sub} = 0$. After the write by a positive pulse and a negative pulse, respectively, V_g was swept in narrow range from V_{swp_start} to V_{swp_end} with $V_d = 0.1$ V, and $V_s = V_{sub} = 0$. Time length of the read by sweeping V_g was of the order of 1 s. V_g was applied by a pulse generator (81110A, Keysight Technologies, Santa Rosa, CA, USA), and I_d was measured by the semiconductor parameter analyzer (4156C). Our homemade program codes [5] controlled these machines. Figure A4 shows the experimental results of PWVR. The figure shows that ΔV_{th} varies linearly with $\log(t_w)$. These log-linear properties have been commonly obtained for SBT- FeFETs [85] and CSBT- FeFETs [2,5] reported previously. In writing, t_w was changed from 100 ns to 1 ms, with $V_h = 3$ V, 4 V, 5 V, 6 V. In reading, $V_{swp_start} = 0$ V, $V_{swp_end} = 1.4$ V, and $V_d = 0.1$ V. Write pulses with combinations of long t_w and high $V_h = -V_l = 5$ V and 6 V were not applied to avoid charge injection and trap in the FeFET.

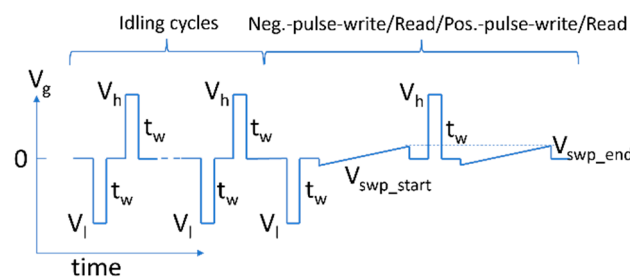


Figure A3. Diagram of V_g vs. time used for the experimental PWVR measurement. For a set of V_h , V_l , and t_w , after plural times repeating the idling cycle by the (V_l, t_w) and (V_h, t_w) pulses, the procedure of V_l (<0) pulse write, V_{th} read, V_h pulse write, and V_{th} read was performed.

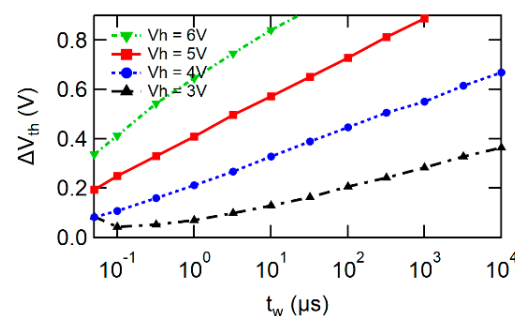


Figure A4. ΔV_{th} vs. t_w for the experimental Ir/CSBT/I/Si FeFET. The stack material and thickness of each layer are the same as those of the FeFET in Figures A1 and A2. t_w was changed from 50 ns to 10 ms, with $V_h = -V_l = 3$ V, 4 V, 5 V, 6 V for writing. $V_{swp_start} = 0$ V, $V_{swp_end} = 1.4$ V, and $V_d = 0.1$ V for reading. The markers in the graph are to show measured results. The lines connecting the markers show log-linear relationships of ΔV_{th} and t_w . In particular, the line for $V_h = 4$ V indicates the log-linear line across more than five orders of t_w .

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