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Factors for the polarization lifetime in metal–ferroelectric–insulator–semiconductor capacitors

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ABSTRACT

Depolarization field in metal–ferroelectric–insulator–semiconductor (MFIS) capacitors with a ferroelectric–electrode interface layer was derived theoretically in this work. The polarization relaxation characteristics were investigated in details based on Lou's polarization retention model. It is found that the retention time of ferroelectric field-effect transistors (FETs) can be affected significantly by the dielectric constant and the thickness of ferroelectric thin film, and by the interface layer thickness. The results may provide some insights into the design and the retention property improvement of MFIS–FET as nonvolatile memory.

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1. Introduction

Single-transistor ferroelectric-gate field effect transistor (FeFET) has been widely studied as a candidate for nonvolatile memory in the past decades [1–5] due to its attractive properties such as non-destructive readout operation, low power consumption, and high switching speed. However, the commercialization of FeFET as nonvolatile memory has not been realized yet because of the short retention time of FeFET. The relatively short retention time is attributed to two major causes: gate leakage current and depolarization field [6,7]. It is known that the gate leakage current and the trapping of carriers in gate dielectric stack can lead to local charge compensation in ferroelectric, and gradually diminish the polarization [8]. On the other hand, the depolarization field induced by imperfect screening at the electrode-film interface causes polarization loss via backswitching [9]. Recently, the effect of depolarization field on ferroelectric polarization has been widely investigated using experimental methods. For example, Black et al. [10] successfully controlled the strength of the depolarization field in ferroelectric by systematically adjusting the amount of charge available to compensate the polarization. Kim et al. [11] and Jo et al. [12] determined the depolarization field from an applied external field to stop the polarization relaxation and demonstrated that a large E_d inside the ultrathin ferroelectric layer could cause severe polarization relaxation. Some other research groups have focused on the problem of retention loss at different time scales and have fitted their data using different empirical functions, such as linear-log [13–15], power-law [11,12,16], and a stretched exponential relation [14,15,17,18]. However, the microscopic mechanism that dominates the problem of retention loss at both short and long time scales in ferroelectric thin film is still poorly understood. The customary way to obtain the retention properties of a ferroelectric capacitor in the literature is to empirically extrapolate the data measured over a shorter period of time (up to 10^6 s) to 10 years without any physical justifications. In this paper, by theoretically deriving the depolarization field in the MFIS capacitor (shown in Fig. 1a), we investigated the dependences of polarization retention loss on some critical physical parameters, including the linear ferroelectric dielectric constant, the thicknesses of the ferroelectric and metal–ferroelectric interface layer, as well as the remnant polarization.

2. Device model and theoretical calculation

As shown in Fig. 1b, the gate stack of the MFIS field-effect transistor with a ferroelectric–electrode interface layer (or a dead

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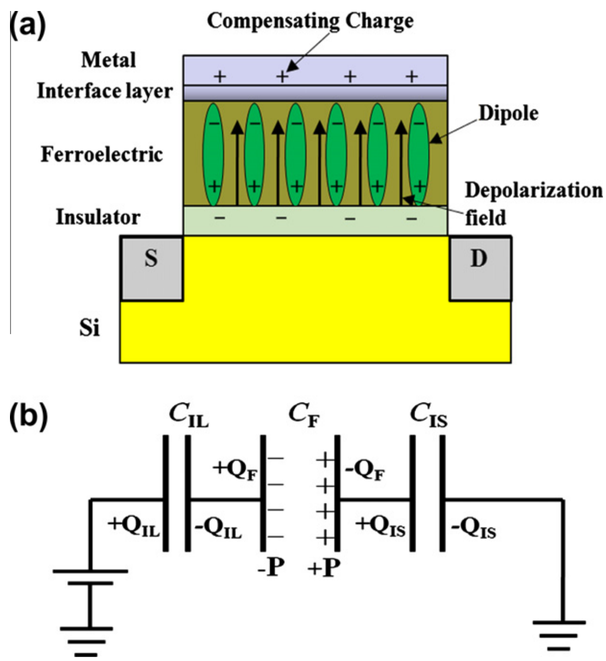

Fig. 1. (a) Schematic MFIS structure in which the ferroelectric layer is polarized and the incomplete charge compensation gives rise to the depolarization filed. (b) Gate stack of the MFIS transistor is modeled by a ferroelectric capacitance C_F in series with an interface layer capacitance C_{IL} and a semiconductor capacitance C_{IS}, where C_{IS} represents the series combination of an insulating buffer layer on the top of the semiconductor. A gate voltage V induces a polarization P, a voltage V_{IL} across C_{IL} and a voltage V_{IS} across C_{IS}.

layer) was modeled by a ferroelectric capacitance (C_F) in series with an interface layer capacitance (C_{IL}), an insulator layer capacitance (C_I), and a semiconductor capacitance (C_S). For convenience, we use C_{IS} to represent the series combination of the insulating buffer layer on the top of the semiconductor. A given gate voltage V could induce a polarization P and a voltage drop of V_F across the ferroelectric such that

$$V_F = \frac{C_{IL}C_{IS}V}{C_{IL}C_{IS} + C_{IL}C_F + C_F C_{IS}} - \frac{(C_{IL} + C_{IS})P}{C_{IL}C_{IS} + C_{IL}C_F + C_F C_{IS}} \tag{1}$$

when V goes to zero, we have

$$V = V_{IL} + V_F + V_{IS} = 0 \tag{2}$$

this is to say

$$\frac{Q_{IL}}{C_{IL}} + \frac{Q_F - P}{C_F} + \frac{Q_{IS}}{C_{IS}} = 0 \tag{3}$$

Solving Eq. (3) yields to

$$Q_F = \frac{C_{IL}C_{IS}P}{C_{IL}C_{IS} + C_{IL}C_F + C_F C_{IS}} \tag{4}$$

The depolarization field can be written as

$$E_d = \frac{P(C_{IL}C_F + C_F C_{IS})}{\varepsilon_0 \varepsilon_F (C_{IL}C_{IS} + C_{IL}C_F + C_F C_{IS})} \tag{5}$$

where ε_F is the relative dielectric constant of the ferroelectric thin film, C_{IL}, C_F, and C_{IS} are unit-area capacitances of the interface layer, ferroelectric layer and series combination of the insulating buffer layer, and are defined as $\varepsilon_0\varepsilon_{IL}/t_{IL}$, $\varepsilon_0\varepsilon_F/t_F$ and $\varepsilon_0\varepsilon_I\varepsilon_S/(t_I\varepsilon_S + t_S\varepsilon_I)$, respectively. We then assume that backswitching causes the polarization loss with time via polarization switching driven purely by a time-dependent depolarization field represented by

$$E_d(t) = \frac{P(t)(C_{IL}C_F + C_F C_{IS})}{\varepsilon_0 \varepsilon_F (C_{IL}C_{IS} + C_{IL}C_F + C_F C_{IS})} \tag{6}$$

Now let us call Lou's model and consider a fully poled ferroelectric capacitor in which the total surface area is divided uniformly into M_0 ($M_0 \gg 1$, an integer) parts. It is assumed that the capacitor backswitches in a part-by-part or region-by-region manner due to the hindering effects of grain boundaries [19], defect planes/dislocations, and/or 90° domain walls [20], which is consistent with the observation found in the ferroelectric thin film [19–21]. In other words, the backswitch occurs via nucleation of opposite domain, followed by relatively quick forward and sideways growth of domain until it reaches the boundary of this part. This means that the domain wall motion is only allowed within each part/region in our current model. Note that both $P(t)$ and $E_d(t)$ relax with time (see Eq. (6)), which indicates a feedback mechanism for $E_d(t)$ is included in our model. Indeed we will consider a feedback loop of the depolarization field corrected by the updated retained polarization at each time point, where one more part has just switched.

We further assume a fully poled ferroelectric capacitor with retained polarization P_{M0} at $t = t_0 = 0\text{–}10^{-13}$ s (the period of soft mode) when the external field is just removed. This is followed by the assumption that $1/\zeta(t_N)$ ($\zeta \gg 1$) is the backswitching probability for one of the retained parts after t_c from the time point where the Nth part has just backswitched. Let t_N denotes the time interval that the Nth part takes to backswitch. Note that t_c is a characteristic time and can be chosen arbitrarily as long as it ensures $1/\zeta(t_N) \ll 1$ for any t_N. Therefore, the probability that one part will retain its polarization after t_c from time t_0 can be written as $[1 - 1/\zeta(t_0)]$. The probability that this part will survive from backswitching after $t_1 (t_1 \gg t_c)$ from time t_0 is $[1 - 1/\zeta(t_0)]^{t_1/t_c}$. According to the definition of t_1, the time interval that the first part takes to switch, the total number of the parts that survive from backswitching after t_1 can be written as

$$M_0 - 1 = M_0 \left(1 - \frac{1}{\zeta(t_0)}\right)^{t_1/t_c} \tag{7}$$

Rearrangement yields to

$$\frac{M_0 - 1}{M_0} = \left(1 - \frac{1}{\zeta(t_0)}\right)^{t_1/t_c} \tag{8}$$

Taking natural logarithm on both sides of Eq. (8), we have

$$\ln \frac{M_0 - 1}{M_0} = \frac{t_1}{t_c} \ln\left(1 - \frac{1}{\zeta(t_0)}\right) = \frac{t_1}{t_c}\left[-\frac{1}{\zeta(t_0)} - \frac{1}{2}\left(\frac{1}{\zeta^2(t_0)}\right) + \cdots\right] \tag{9}$$

Because $\zeta(t_0) \gg 1$, all the higher-order terms can be neglected. Thus we obtain

$$\frac{M_0 - 1}{M_0} = \exp\left(-\frac{t_1}{t_c \zeta(t_0)}\right) \tag{10}$$

Consider Merz's law [22], which has been used to fit the switching data in both bulk and thin-film ferroelectrics [22–25]

$$t_{sw} = t_\infty \times \exp\left(+\frac{\alpha}{E}\right) \tag{11}$$

where t_{sw} and t_∞ are the switching time for E and an infinite field, respectively. α is the activation field for switching and is dependent on temperature T and film thickness d [22,23]. The value of α was reported ranging from 200 to 800 kV/cm for ferroelectric thin films in the literature [24–26]. Recalling the meaning of $1/\zeta(t_0)$ defined above, we have

$$\frac{1}{\zeta(t_0)} = \frac{t_c}{t_{sw}(t_0)} = \frac{t_c}{t_\infty} \times \exp\left(-\frac{\alpha}{E_d(t_0)}\right). \tag{12}$$

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