Effect of Grain Orientation on NBTI Variation and Recovery in Emerging Metal-Gate Devices

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***Abstract*—This letter identifies and investigates the effect of grain orientation (GO) on negative-bias temperature instability (NBTI) characteristics of emerging metal-gate devices. A modified reaction–diffusion model is presented for estimating the effect of GO on NBTI. It is shown that neglecting the GO effect leads to substantial underestimation of the impact of the gate-oxide electric field (E_{OX}) on the threshold voltage degradation (ΔV_{TH}). Moreover, GO results in significant fluctuation in E_{OX} and, hence, fluctuation in NBTI for ultrascaled CMOS devices. In addition, in FinFETs, stand-alone GO-induced gate-oxide electric field not only results in ΔV_{TH} fluctuation but also decelerates the recovery process.**

***Index Terms*—Grain orientation (GO), metal gate, negative-bias temperature instability (NBTI), work-function (WF) variation (WFV).**

I. Introduction

METAL has become the primary gate material in all sub-65-nm CMOS technologies due to incompatibility of polysilicon with high-k dielectric materials. However, using metal as the gate material introduces a new source of random variation due to the dependence of its work function (WF) on the metal grain orientations (GOs) [1]. The GO-induced WF variation (WFV) has been modeled and experimentally verified as the dominant source of the threshold voltage variation in metal-gate CMOS devices [1]–[3]. In this letter, for the first time, the effect of GO on the negative-bias temperature instability (NBTI) characteristics of metal-gate devices is investigated and reported.

II. Effect of GO on NBTI

A. Effect of Oxide Electric Field on NBTI Characteristics

NBTI is an important reliability concern in p-type MOSFETs that increases their threshold voltage and consequently lowers their ON current. There are several approaches to model the NBTI degradation and recovery processes [4]–[7]. In all these approaches, the threshold voltage degradation (ΔV_{TH}) is a strong function of the bias conditions and, hence, of the gate-oxide electric field (E_{OX}). In this letter, without loss of generality, the reaction–diffusion (R–D) model is used, where the impact of E_{OX} on ΔV_{TH} is given by (1) and (2) [7], [8]

$$\Delta V_{\mathrm{TH}}(t) = \frac{qN_{\mathrm{IT}}(t)}{C_{\mathrm{ox}}} = f_{\mathrm{AC}}(S_P) \times K_{\mathrm{DC}} \times t^s \qquad (1)$$

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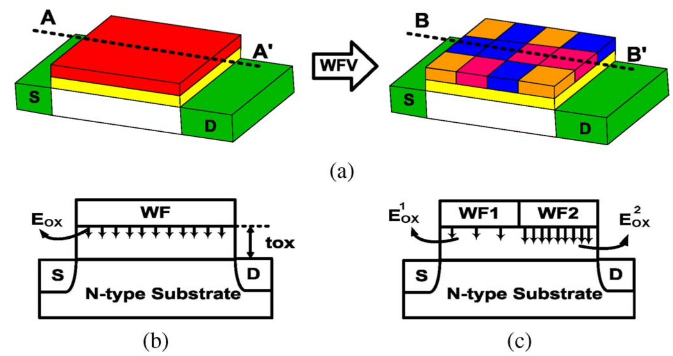


Fig. 1. (a) Metal-gate PMOS transistor (left) without and (right) with considering the GO effect. The different area colors represent grains with different orientations. (b) Cross-sectional view along $\mathrm{A}-\mathrm{A}'$. Neglecting the impact of the GO results in uniform vertical gate-oxide electric field (E_{OX}). (c) Cross-sectional view along $\mathrm{B}-\mathrm{B}'$. Considering the GO effect results in nonuniform E_{OX} across the gate.

where N_{IT}, C_{ox}, S_p, f_{AC}, q, and t are the density of interfacial traps, gate-oxide capacitance, effective ON time of the transistor, ac dependency function, electron charge, and time, respectively. s is the process- (which depends on hydrogen species) and experimental-setup-dependent parameter. K_{DC} is expressed as follows [7], [8]:

$$K_{\mathrm{DC}} \cong \beta \times E_{\mathrm{OX}}^{\frac{2}{3}} \times e^{\frac{2}{3}F_{\mathrm{acc}}E_{\mathrm{OX}}} \times e^{-\frac{E_A}{v_T}} \qquad (2)$$

where β, E_{ox}, E_A, F_{acc}, and v_T are the constant factor, effective vertical oxide field, activation energy, field acceleration factor, and thermal voltage (kT/q), respectively. Moreover, the recovery process has also been shown to depend on the bias voltage applied to the gate during the recovery [5].

B. Modeling of the Effect of GO on Oxide Electric Field

In order to consider the effect of GOs, as shown in Fig. 1(a), using a 3-D device simulator from Silvaco (ATLAS) [9], the gate area is divided into several segments. The area of each segment is determined based on the average size of the grains in a specific gate material (for instance, 17 nm for MoN) [10]. Then, the WF of each segment is randomly assigned based on the probabilities of the GOs and corresponding WFs [1]. As an example, a MoN metal gate consists of two types of grains, namely, grains in $\langle 110\rangle$ orientation $(WF = 5.0\ \mathrm{eV})$ and grains in $\langle 112\rangle$ orientation $(WF = 4.4\ \mathrm{eV})$. The probabilities of these grains are 0.6 and 0.4, respectively. Hence, the mean value of the WF (when the gate is composed of a large number of grains) is given by

$$0.6 \times 5.0\ \mathrm{eV} + 0.4 \times 4.4\ \mathrm{eV} = 4.76\ \mathrm{eV}. \qquad (3)$$

The proposed NBTI models in the literature assume an average WF for the entire gate (4.76 eV for MoN) and neglect the impact of GO [Fig. 1(b)] on $E_{\rm ox}$. Assuming a MoN bulk PMOS, with a channel dopant concentration of 7×10^{17} cm^{-3} and an effective gate-oxide thickness of 1 nm, for $V_{\rm GS} = -0.9$ V, $E_{\rm OX}$ is 3.07 MV/cm. Assuming that $2/3F_{\rm acc} = 1/E_0$ [from (2)], where $E_0 = 2.0$ MV/cm, as is inferred from (1) and (2)

$$\Delta V_{TH} \propto E_{OX}^{\frac{2}{3}} \times e^{\frac{E_{OX}}{E_0}} = 3.07^{\frac{2}{3}} \times e^{\frac{3.07}{2}} = 9.8(\text{MV/cm})^{2/3}. \quad (4)$$

However, in a metal-gate device, the $E_{\rm OX}$ under the grains with different orientations is different [Fig. 1(c)]. For instance, for the aforementioned MoN PMOS, the $E_{\rm OX}$ values under the metal grains in $\langle 110 \rangle$ and $\langle 112 \rangle$ orientations are 4.66 and 1.41 MV/cm, respectively. In order to consider the GO effect, one can rewrite (1) and (2) as follows:

$$\Delta V_{\rm TH}(t) = \frac{qN_{\rm IT}(t)}{Cox} = \frac{\Delta Q(t)}{Cox} = \frac{1}{Cox}\sum_{i=1}^{n} \Delta Q^i(t)$$
$$= f_{\rm AC}(S_P) \times t^s \times \sum_{i=1}^{n} K_{\rm DC}^i \quad (5)$$

where n is the number of grains, $\Delta Q^i(t)$ is the trapped charge at the silicon/oxide interface (due to NBTI) under the ith grain, and $K_{\rm DC}^i$ represents $K_{\rm DC}$ related to the ith grain, as given by

$$K_{\rm DC}^i \cong \frac{\beta}{n} \times \left(E_{\rm OX}^i\right)^{\frac{2}{3}} \times e^{\frac{2}{3}F_{\rm acc}E_{\rm OX}^i} \times e^{-\frac{E_A}{vT}} \quad (6)$$

where $E_{\rm OX}^i$ is the $E_{\rm OX}$ under the ith grain. Subsequently, for a large number of grains in a metal-gate device, we have

$$\Delta V_{\rm TH} \propto \sum_{j=1}^{m} p_j \times \left(E_{\rm OX}^j\right)^{\frac{2}{3}} \times e^{\frac{2}{3}F_{\rm acc}E_{\rm OX}^j} \quad (7)$$

where m is the number of different types of grains ($m = 2$ for MoN), p_j is the probability of the jth type of the grain (in MoN, 0.4 for $\langle 112 \rangle$ grains and 0.6 for $\langle 110 \rangle$ grains), and $E_{\rm OX}^j$ is the $E_{\rm OX}$ under the jth type of grain (in MoN, 1.41 MV/cm for $\langle 112 \rangle$ grains and 4.66 MV/cm for $\langle 110 \rangle$ gains). As a result, we have

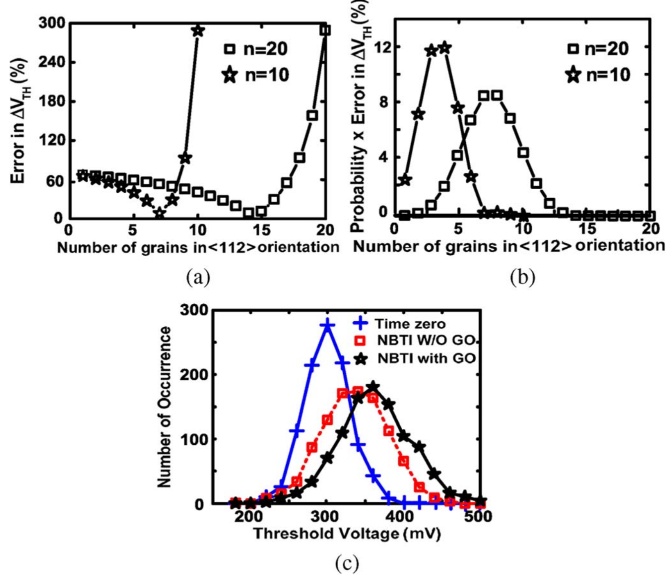
$$\Delta V_{\rm TH} \propto 0.4 \times 1.41^{\frac{2}{3}} \times e^{\frac{1.41}{2}} + 0.6 \times 4.66^{\frac{2}{3}}$$
$$\times e^{\frac{4.66}{2}} = 18.2\ (\text{MV/cm})^{2/3}. \quad (8)$$

Comparing (4) and (8) reveals that the impact of the $E_{\rm OX}$ is underestimated by approximately 46% compared to the case where the impact of GO is considered. This error has not been detected in reported measurement data because this underestimation of the impact of the $E_{\rm OX}$ is compensated by fitting parameters (β in (2)), which, however, does not provide any physical insight. Moreover, as discussed in the following section, GO results in $\Delta V_{\rm TH}$ fluctuation, which can not be explained if GO effect is neglected.

III. Influence of GO on NBTI Variation and Recovery

A. GO-Induced Fluctuation in $V_{\rm th}$ Degradation

The R–D-based model discussed in Section II-A assumes nominal $V_{\rm TH}$ degradation ($\Delta V_{\rm TH}$) without considering $\Delta V_{\rm TH}$ fluctuation [11]. However, in metal-gate devices, different combinations of the grains result in $V_{\rm TH}$ variation [1]–[3]. In addition, GO results in $E_{\rm OX}$ fluctuation and, hence, fluctuation in $V_{\rm TH}$ degradation [from (5) and (6)], as shown in Fig. 2(a)–(c). Fig. 2(a) shows the error in $V_{\rm TH}$ degradation if the GO effect is neglected, while Fig. 2(b) shows the "$error \times probability$" for different combinations of the grains. As can be observed, different combinations of the grains (with different GOs) result in $\Delta V_{\rm TH}$ fluctuation. Moreover, the GO effect becomes more severe for lower numbers of grains (shorter channel-length devices). Fig. 2(c) shows the fluctuation in threshold voltage for three cases: time zero (no negative bias is applied), NBTI without GO effect, and NBTI with GO effect. Monte Carlo simulations were performed with 1000 samples, and it is assumed that the mean value of the threshold voltage is increased by 10% due to NBTI without GO effect. As can be observed, GO significantly increases the fluctuation in threshold voltages.



(a) (b) (c)

Fig. 2. (a) Estimated error in $\Delta V_{\rm TH}$ when GO effect is neglected (uniform $E_{\rm OX}$ is assumed across the gate) compared to the case where GO impact is considered for different grain combinations in a MoN PMOS device. n represents the total number of grains. (b) $Probability \times error$ in $\Delta V_{\rm TH}$ for different grain combinations. (c) GO significantly increases the fluctuation in the threshold voltage degradation. Note that the results for the case labeled "NBTI W/O GO" include the effect of all other parameter variations.

It is worth noting that the hydrogen diffusion coefficient (which plays an important role in determining the NBTI characteristics) in a pure metal crystal also depends on the metal surface orientation [12]. However, in polycrystalline thin metal films consisting of several grains, hydrogen diffusion is dominated by grain boundary diffusion [12]. Moreover, as shown in [13], the timescale over which the differences in the temporal evolution of diffusion along various crystal orientations disappear is on the order of several hundred minutes, which is negligible compared to the typical timescales over which NBTI degradation takes effect. Hence, variation in GOs is expected to have negligible effect on hydrogen diffusion in the metal gate.

It is perhaps relevant to mention that the WFV is less important in polysilicon gates than that in metal-gate devices [2]. The WF of the polysilicon gate changes only at the grain boundaries (which are typically < 1 nm in width [14]), since the Fermi levels of the grains themselves are pinned above

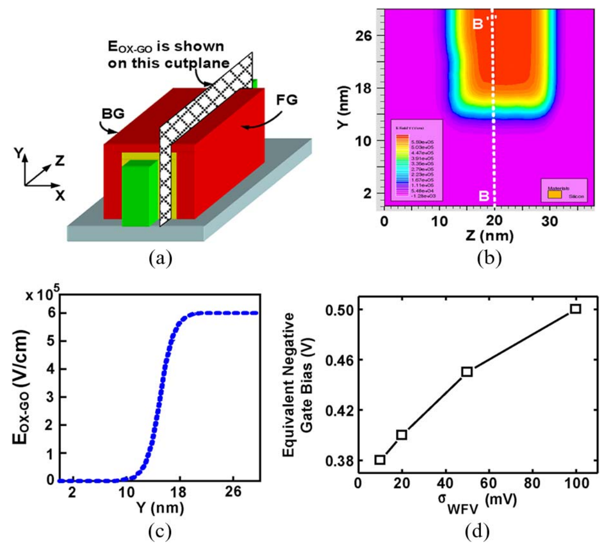


Fig. 3. (a) FinFET structure. FG and BG denote the front and back gates. (b) $E_{\mathrm{OX-GO}}$ (along the x-direction), when one grain in FG has a different WF compared to those of other grains in the gate. (c) $E_{\mathrm{OX-GO}}$ along $\mathrm{B-B'}$. (d) Equivalent negative gate voltage for various standard deviations (σ) of WFV in the gate (both FG and BG).

the conduction band due to heavy doping. Hence, (considering the technology nodes where polysilicon is used as the gate material) the nonuniformity in WF occurs over a very small fraction of the gate area, leading to negligible impact on NBTI characteristics.

B. Impact of GO on NBTI Recovery in FinFETs

GO results in an exclusive phenomenon in FinFET devices. Grains in FG and BG [Fig. 3(a)] can have different orientations, which result in a stand-alone oxide electric field, as given by

$$E_{\mathrm{OX\_GO}} = \frac{\varepsilon_{\mathrm{si}}}{\varepsilon_{\mathrm{ox}}} \times \frac{V_{\mathrm{FBf}} - V_{\mathrm{FBb}}}{\frac{\varepsilon_{\mathrm{si}}}{\varepsilon_{\mathrm{ox}}}(t_{\mathrm{ox}f} + t_{\mathrm{ox}b}) + T_{\mathrm{si}}} \tag{9}$$

where $E_{\mathrm{OX\_GO}}$ is the GO-induced electric field, and V_{FBf} and V_{FBb} are the flatband voltages of the FG and BG, respectively. T_{si}, $t_{\mathrm{ox}f}$, and $t_{\mathrm{ox}b}$ are the channel thickness and oxide thicknesses of the FG and BG, respectively. $\varepsilon_{\mathrm{ox}}$ and $\varepsilon_{\mathrm{si}}$ are the permittivities of the gate oxide and silicon, respectively. In bulk devices, the body thickness is large (which can be treated as a thick T_{si}), and in SOI devices, the back-gate oxide (t_{oxb}) is thick. In both cases, as can be observed from (9), $E_{\mathrm{OX\_GO}}$ is small. However, in FinFETs (for 22-nm technology node and beyond), the fin thickness is less than 10 nm to suppress the short-channel effects. Consequently, different GOs in FG and BG result in significantly high $E_{\mathrm{OX_{GO}}}$. Assuming that $V_{\mathrm{GS}} = 0$ V, Fig. 3(b) and (c) shows the $E_{\mathrm{OX\_GO}}$ for the case where only one grain in FG has different orientation than the other grains in the gate. This GO-induced electric field not only affects the E_{OX} (which is created by the gate–source bias) but also decelerates the recovery process when the gate–source bias is removed. It is worth noting that the existence of this stand-alone electric field does not imply that the FinFET device is under degradation all the time. The reason is that the degradation only happens when the hole concentration is high enough (device should operate in the inversion regime). This situation occurs only when a negative gate–source bias is applied.

As mentioned earlier, the recovery process strongly depends on the bias condition. In Fig. 3(d), the equivalent negative gate voltage corresponding to the various WFV standard deviations in FG and BG is shown. As an example (assuming that the WF of the gate is 4.5 eV), a standard deviation of WFV of 50 meV is equivalent to applying a -0.45 V bias to the gate of the device during the recovery process.

IV. Conclusion

The impact of GO on the NBTI characteristics of metal-gate devices has been investigated and reported for the first time in this letter. Using a modified R–D model, the impact of gate-oxide electric field on the V_{TH} degradation is shown to be underestimated by nearly 50% if the GO effect is neglected. Moreover, GO results in a significant fluctuation in threshold voltage degradation due to temperature instability. In addition, the GO in FinFETs creates a stand-alone electric field $(E_{\mathrm{OX\_GO}})$, which not only results in fluctuation in the V_{TH} degradation but also decelerates the recovery process when the negative gate–source bias is removed. Since, in all NBTI models, oxide electric field significantly affects the degradation and recovery of the threshold voltage, in order to accurately characterize NBTI effects, the GO effect must be considered in emerging metal-gate devices.

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