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A Vacancy-Interstitial Defect Pair Model for Positive-Bias Temperature Stress-Induced Electron Trapping Transformation in the High-$k$ Gate n-MOSFET

Chenjie Gu, Diing Shenp Ang, Yuan Gao, Renyuan Gu, Ziqi Zhao, and Chao Zhu

Abstract—Recent device reliability studies have observed the shallow-to-deep transformation of electron-trap states under positive-bias temperature stressing. Being two typical types of defects in the high-$k$ oxide, the oxygen vacancy and oxygen interstitial have been investigated in many simulations, but results have indicated that the corresponding defect levels are either too shallow or too deep and fail to explain the experimental observation. Here, we propose a vacancy-interstitial ($V_O$-$O_i$) model. By tuning the relative positions of $V_O$ and $O_i$, we show that the charge trap level of the defect pair can be adjusted continuously within the HfO$_2$ bandgap. This allows us to depict a possible atomic picture for understanding the shallow-to-deep transformation of electron trapping.

Index Terms—CMOS reliability, dynamic bias temperature instability (BTI), high-$k$ dielectric, oxide traps, $V_O$-$O_i$ defect pair.

I. INTRODUCTION

The replacement of the polysilicon/oxynitride gate-stack by the metal/high-$k$ gate-stack is one of the most significant moves made by the semiconductor industry. Although the latter has enabled the further downscaling of equivalent oxide thickness (EOT) and suppression of gate leakage current [1]–[3], it has also brought along a new set of challenges [4]–[6]. Among these, the bias temperature instability (BTI) is believed to be an extremely critical one, which manifests itself as time-dependent drifts of key performance parameters such as threshold voltage, drain current, etc. [7], [8]. While negative-BTI (NBTI) was already a serious concern for the polysilicon/oxynitride gate p-MOSFET [9] before the changeover was made, the metal/high-$k$ gate-stack suffers from an additional positive-BTI (PBTI) problem, which severely impacts the performance of the n-MOSFET [10], [11]. Therefore, there has been considerable effort made in recent years to understand the underlying mechanisms governing the BTI issues in the metal/high-$k$ gate-stack [12]–[16].

To-date, a good level of consistency has been attained in terms of the experimental behaviors of the BTI problem. Broadly, BTI induced parametric shift may be divided into two parts: 1) a recoverable part typically characterized by a rapid relaxation transient that sets in upon removal of the applied stress and 2) a relatively permanent part that builds up steadily over time and accounts for the long-term parametric shift. In early studies on NBTI, these two parts were assumed to originate from different mechanisms [17], [18]. Recent works [19] have, however, consistently revealed a link between them, whereby part of the recoverable portion may be transformed into a more permanent form as the stressing continues. More recent studies on small-area transistors have unambiguously demonstrated such a recoverable-to-permanent transformation behavior of individual oxide trap [20], [21]. Meanwhile, atomistic simulation studies have provided a microscopic picture of the degradation mechanism [22], [23]. In [24], a discussion on the vacancy-interstitial ($V_O$-$O_i$) defect pair reveals its capability to act as either a shallow or deep trap level, depending on the specific $V_O$-$O_i$ structure. However, knowledge on the defect pair dynamics and the corresponding electrical behaviors under stress is still not available.

In this paper, we observe, through continuous defect structure relaxation, that the electron-trap state of a $V_O$-$O_i$ defect pair could vary across the entire bandgap of HfO$_2$, depending on the relative positions of $V_O$ and $O_i$. This allows us to conclude that the $V_O$-$O_i$ defect pair is a promising candidate for the shallow-to-deep electron-trap state transformation observed during PBTI testing.

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Fig. 1. (a) Evolution of threshold voltage shift \( \Delta V_t \) during PBTI stressing followed by relaxation. Initial oxide stress field was 7 MV/cm, [estimated based on \( (V_{o,x} - V_d)/\text{EOT} \), where \( V_{o,x} \) is gate stress voltage and \( V_d \) is prestress threshold voltage]; relaxation was carried out at \( V_g = 0 \) V for \( 1 \times 10^3 \) s, followed by \(-1\) V for another \( 1 \times 10^3 \) s. The temperature was 100 °C. (b) Compared with the prestress transconductance curve, the curve after PBTI stress is laterally shifted toward more positive \( V_g \) without reduction in the peak value. This test device was stressed with a 1-MHz \( V_g \) pulse alternating between \( +1.9 \) V (\(~7\) MV/cm) and 0 V for \( 5 \times 10^3 \) s.

II. SHALLOW-TO-DEEP ELECTRON-TRAP STATE TRANSFORMATION

In this section, we review recent experimental results showing the transformation of electron trapping from shallow-to-deep energy levels during PBTI stressing [25].

A. Deep-Level Electron Trapping

The test devices were n-MOSFETs with 0.25- and 10 - \( \mu \)m drawn channel length and width, respectively. The gate-stack consisted of a 3-nm atomic-layer-deposited HfO\(_2\) and a 0.9-nm SiO\(_x\) interfacial layer, with an EOT of 1.4 nm. Fig. 1 shows the threshold voltage shift \( (\Delta V_t) \) in a typical PBTI stress/relax cycle obtained through the ultrafast-switching method [26]. The relaxation curve shows that besides the shallow-level electron trapping responsible for the fast recovery transient [27], a nonnegligible \( \Delta V_t \) stems from electrons trapped at deep energy states. This is evident from the second abrupt decrease of \( \Delta V_t \) that occurred during the \(-1\) V recovery, applied upon the prior 0 V recovery reaching a quasi-saturation level. Since a negative gate voltage \( (V_g) \) will further bring down the Fermi level toward the Si valence band, the second abrupt \( \Delta V_t \) decrease may be ascribed to the emission of electrons trapped at deeper energy states in the HfO\(_2\) bandgap. After the \(-1\) V recovery, the remnant \( \Delta V_t \) is \(~0\), which implies that the electrons trapped in deep energy states were almost fully detrapped, i.e., nearly the entire \( \Delta V_t \) was due to electron trapping. This is also apparent in another test device, whose transconductance curve is shifted laterally toward more positive \( V_g \) after PBTI stress, without any apparent decrease in the peak value [Fig. 2(b)], indicating that electron trapping is the dominant degradation mechanism for PBTI [28].

B. Conversion of Shallow-to-Deep-Level Electron Trapping

As can be seen from the \( \Delta V_t \) evolution in a single stress/relax cycle [Fig. 1(a)], PBTI stress leads to electron trapping in a broad range of trap states in the HfO\(_2\) bandgap. For a given relax interval, electrons trapped at relatively shallow-level states are able to emit, whereas those trapped at deeper states can be emitted only with the aid of a negative \( V_g \). These deep states may include those originally deep ones generated by the stress or shallow ones, which were converted quickly into deeper ones when the stress was applied (i.e., the conversion time constants are much shorter than the stress interval). To differentiate the part of deep-level electron trapping which results from shallow-level traps having longer time constants, multiple stress/relax cycles are needed. The conversion of these shallow-level traps may be inferred from the decrease of \( R_0 \) (Fig. 2) as explained in the following [19].

Fig. 2(a) shows typical \( \Delta V_t \) change over selected cycles, for a device stressed at an oxide field at the beginning of PBTI cycle and 0 V relaxation over selected stress/relax cycles. (b) \( \Delta V_t \) recovery per 0 V \( (R_0) \) or \(-1\) V \( (R_{-1}) \) relaxation interval as a function of the number of stress/relax cycles applied. (c) \( \delta \Delta V_t^{\text{rel}} = \Delta V_t^{\text{rel}}(n\text{th cycle}) - \Delta V_t^{\text{rel}}(1\text{st cycle}) \) (right axis) and \( \delta \Delta V_t^{\text{ecl}} = \Delta V_t^{\text{ecl}}(n\text{th cycle}) - \Delta V_t^{\text{ecl}}(1\text{st}) \) (left axis) as a function of the number of stress/relax cycles applied for the case of 0 V relaxation.

\( 1 \)Oxide field here refers in particular to the oxide field at the beginning of the PBTI cycle, the same definition is used for the rest of this paper.
remains nearly constant as in the case of the 5.5-MV/cm stress.

Fig. 2(c), wherein the evolution of $\Delta V_{t}^{\text{eo}}$ and $\Delta V_{t}^{\text{e}}$ (with respect to the first cycle) is compared, offers an insight into the progressive decrease of $R_{0}$ seen at the higher 7-MV/cm stress. $\Delta V_{t}^{\text{eo}}$, taken at the end of each stress interval [Fig. 2(a)], reflects the total electron trapping prior to the start of relaxation. On the other hand, $\Delta V_{t}^{\text{e}}$, taken at the end of each relax interval, gives the remnant electron trapping, i.e., electrons trapped at deep energy states and were unable to emit during the relax interval. Under the 5.5-MV/cm stress, the steady increase of $\Delta V_{t}^{\text{eo}}$ means that in each stress interval, besides the retracting of electrons at shallow trap states “emptied” in the previous relax interval, there was additional trapping of electrons at deep trap states. The similar rise in $\Delta V_{t}^{\text{e}}$ implies that these trapped electrons were unable to emit at the end of the following relax cycle, resulting in a gradual accumulation of deep-level electron trapping. For the 7-MV/cm stress, $\Delta V_{t}^{\text{eo}}$ increases at a similar rate as that of the 5.5 MV/cm, indicating that the incremental electron trapping at deep trap states after each stress interval is comparable under both oxide stress fields. However, $\Delta V_{t}^{\text{e}}$ increases at a faster rate than that of the 5.5-MV/cm stress. This means that at the end of each relax interval, the remnant electron trapping, i.e., electrons trapped at deep energy states, increases more quickly under the 7-MV/cm stress. Given that the incremental electron trapping at deep trap states per stress interval is similar for both oxide stress fields, the results thus imply that the gradual reduction in $R_{0}$ under the 7-MV/cm stress is due to some of the formerly shallow trap states being transformed into deeper ones as stressing is continuously applied. We speculate that such transformation may involve the transition from a metastable shallow trap state to a deeper trap state [29], facilitated by oxide-field-induced lowering of the energy barrier.

To check the above-mentioned conclusion, stressing was carried out under the same oxide stress field of 7 MV/cm but with a relaxation voltage of $-1 \text{ V}$. Since electron emissions from deep trap states can also occur, the decrease in $R_{0}$ or emissions from shallow trap states (due to the conversion of some of these states to deeper levels) seen under the 0 V relaxation should be suppressed under the $-1 \text{ V}$ relaxation. This is because even if a shallow trap state has changed into a deeper one, emission from the resultant trap state may still occur under the $-1 \text{ V}$ relaxation [see Fig. 1(a)]. This inference is indeed borne out by the evolution of $R_{-1}$ [Fig. 2(c)]. Other than the expected increase in $R_{-1}$ over $R_{0}$, the reduction in $R_{0}$ is not observed in $R_{-1}$. The nearly constant $R_{-1}$ result supports our conclusion that the decrease in $R_{0}$ stems from shallow-to-deep trap state transformation.

III. DEFECT MODEL AND SIMULATION METHOD

The relatively high density of defects in low-temperature deposited high-κ oxides (as compared with the thermally grown SiO2) has attracted considerable attention. Electron spin resonance studies on high-κ oxides have shown the existence of both oxygen vacancy ($V_{O}$) and oxygen interstitial ($O_{i}$) defects [30]. Ab-initio simulation has found that the electron-trap state associated with $V_{O}$ is rather shallow ($\sim 1 \text{ eV}$ below the HfO2 conduction band edge), whereas that linked to $O_{i}$ is very deep (near to the valence band edge) [31]. Therefore, neither $V_{O}$ nor $O_{i}$ is able to explain the above experimental phenomenon. In view that high-κ oxides are generally oxygen deficient, the presence of $O_{i}$ alone is unlikely. Moreover, being transition metal oxides, the metal–oxygen bonds have a partial ionic character. In HfO2, the $Hf-O$ bond has $\sim 70\%$ ionic character [32]. Under an applied electric field, weak $Hf-O$ bonds in the amorphous oxide may tend to break. In view of the above-mentioned considerations, the presence of $O_{i}$ near a $V_{O}$ is a likely scenario. Therefore, in the following simulation work, we focus on the $V_{O}$-$O_{i}$ defect pair; evolution of the defect level with a change in the relative positions of $V_{O}$ and $O_{i}$ is investigated in detail.

First principles simulation was performed by Vienna Ab initio Simulation Package [33–36], which employed the plane wave pseudopotential methods within the density functional theory [37]. The ultrasoft pseudopotential was used to represent the interactions between the ion core and the valence electrons. The exchange correlation energies were treated within the generalized gradient approximation of Perdew et al. [38]. In all calculations, the cutoff energy and points were tested. For structure optimization, the conjugate gradient method was used and the ion positions were optimized until the residual force was less than 0.01 eV/Å. The hybrid scheme was used here to correct the bandgap so that the trap level could be precisely determined [39]. The formation energy $E_f$ of a defect in HfO2 was calculated from the total energy $E$ of the defective supercell per the following formula [40]:

$$E_f(\alpha, q) = E(\alpha, q) - (E_0^\alpha + n_{Hf}\mu_{Hf} + n_{0}\mu_{0})$$

$$+ q(\epsilon_F + E_{\text{VBM}})$$

(1)

where $E_0^\alpha$ is the system energy of the defect-free supercell and $E_{\text{VBM}}$ is the valence band maximum of HfO2. For a defect $\alpha$ in charge state $q$, $E_f$ is a function of the Fermi level $\epsilon_F$ and the respective chemical potential of $Hf$ and $O$ denoted by $\mu_{Hf}$ and $\mu_{O}$. The terms $n_{Hf}$ and $n_{O}$ represent the corresponding number of $Hf$ and $O$ atom(s) added/removed from the supercell to form the defect. The charge transition level (CTL) for negative-to-neutral ($-0$) state transition of the defect is also calculated and is given by $\epsilon_F$, which corresponds to $E_f(\alpha, q) = 0$. The CTL, measured with respect to $E_{\text{VBM}}$, is akin to the trap level of the defect in the HfO2 bandgap [41]. The supercell used in our simulation study was amorphous HfO2, which was generated from a crystalline HfO2, via molecular dynamics, following the melt-and-quench scheme [42]. It consisted of 48 Hf atoms and 96 O atoms, with a density of 9.68 g/cm$^3$.

To introduce a $V_{O}$-$O_{i}$ defect pair into the amorphous HfO2 supercell, a lattice oxygen atom ($O_L$) was manually moved to a nearby lattice vacancy position (Fig. 3). However, as this initial structure might be energetically unfavorable, it was subjected to full structure relaxation under a negative charged environment until the structure reached the stable state ($S0$). In subsequent study on the $V_{O}$-$O_{i}$ defect pair, we fixed the
position of VO and moved the Oi to the other neighboring lattice vacancy positions, thus changing the relative positions of VO and Oi. Structure relaxation was performed after each Oi position change until the new structure reached a stable state. The minimum energy path (MEP) for the transformation between the consecutive two defect structures was calculated by the nudged elastic band method [43]. Meanwhile, the CTL change during the defect transformation process was extracted.

We investigated a total of ten VO-Oi defect pairs based on the amorphous HfO2 supercell. Here, we discuss two cases showing characteristics that support the shallow-level electron trapping and shallow-to-deep defect transformation phenomenon evidenced in our experimental work. The other cases show either stable switching or fixed charging characteristics, and will be discussed elsewhere.

IV. SIMULATION RESULTS DISCUSSION

We give a full picture of the MEP and CTL results pertaining to the evolution of the first VO-Oi defect pair (D1) in Fig. 4. As aforementioned, the VO-Oi defect was generated by moving one Oi to an arbitrary lattice vacancy position. It was not a stable defect initially. This is evident in the phase I of Fig. 4, which shows a steep drop in the system energy during the structural relaxation step. After this, the supercell with the D1 defect reached a stable state and is named D1_S0 [Fig. 5(a)]. As guided by the arrows on Fig. 5(a), there are four possible paths (1–4) along which Oi may migrate to get to a new position, one lattice vacancy away from VO. Therefore, we manually moved the Oi to each of the four lattice vacancies, thus creating four new defect structures. These four structures were then subjected to structural relaxation until they each reached a final stable state (S1). The resultant defect structures, D1_S1_A, D1_S1_B, D1_S1_C, and D1_S1_D, corresponding to Oi migration along paths 1–4, are shown in Fig. 5(b)–(e), respectively. The MEP and CTL (for a total of 18 intermediate atomic structures or transition coordinates) were also calculated for each of the four models, and the results are shown in the phase II of Fig. 4. From MEP results, the energy barriers $E_B$ for the transformation from S0 to each of the four S1 states (A, B, C, and D) is 1.16, 1, 1.77, and 1.68 eV, respectively. At temperature $T = 100$ °C, the corresponding time constant $\tau (=\tau_0 \cdot \exp(E_B/\kappa T); \tau_0 = 10^{-13}$ s; $\kappa$ is Boltzmann’s constant [44]) for the transformation are $\sim 470$, $3$, $8 \times 10^{10}$, and $5 \times 10^3$ s. Thus, upon the application of stress, D1_S0 may readily be transformed into D1_S1_B. The CTL of D1_S0 is $\sim 3.1$ eV, near the middle of the Si bandgap, which shows that D0_S1 is a shallow electron-trap state. After the transformation, the CTL is relatively unchanged (in fact it becomes slightly shallower). D1_S1_B remains a shallow electron-trap state and the transformation is not detectable from the $\Delta V_t$ relaxation characteristic.

Results for the second VO-Oi defect pair (D2) are shown in Figs. 6 and 7. The first step of structure relaxation brought it to a more stable state (D2_S0), as manifested by the decrease in system energy (phase I of Fig. 6). The CTL of D2_S0 is $\sim 3.4$ eV, which is also around the middle of the silicon

![Fig. 3](image-url) VO-Oi defect is created by moving the lattice oxygen (OL) to a neighboring lattice vacancy (Oi). This initial structure was then subjected to fully structure relaxation until it reached the stable state (S0).

![Fig. 4](image-url) Change in system energy along the MEP for (I) initial structural relaxation toward a stable state S0, following the creation of a VO-Oi defect pair (D1) by manual relocation of a lattice oxygen atom to a nearby lattice vacancy position. (II) Further evolution of D1_S0 toward four new stable defect structures (D1_S0_A, D1_S0_B, D1_S1_C, and D1_S1_D), via Oi relocation along four possible paths to other nearby lattice vacancies. Change in the charge trap level is also shown.

![Fig. 5](image-url) (a) Atomic structure of the D1 defect (Fig. 3) following full structural relaxation. Arrows show four possible paths along which Oi may migrate to a new lattice vacancy position, leading to a further evolution of D1_S0. Stable defect structures obtained after Oi migration to a new lattice vacancy along paths 1–4 are denoted as (b) D1_S1_A, (c) D1_S1_B, (d) D1_S1_C, and (e) D1_S1_D, respectively.
shows three available migration paths (1–3) for \( \text{Oi} \) compared with the other two cases. These results imply that accompanied by a much larger decrease in system energy as shown in Fig. 6. The minimum energy barrier is 1.28 eV, which corresponds to a \( \tau \) of \( 1.9 \times 10^4 \) s, much longer than the stress interval of \( 1 \times 10^3 \) s. Moreover, there is no lowering of the system energy in the \( S_2 \) state. It is also worth mentioning that the energy barrier for the change from \( D_2 S_1 A \) back to \( D_2 S_0 \) is rather large (\( \sim 3.8 \) eV). These findings imply that \( D_2 S_1 A \) would tend to remain in the local “energy valley” of its current state and is not likely to revert to \( D_2 S_0 \) even under a moderate negative \( V_g \) or further transformed under stressing for fixed stress and relax intervals. This relative stability of \( D_2 S_1 \) with stress/relaxation cycling can still be observed (not shown), indicating a gradual build-up of deep-level electron trapping, although the rate of increase is lesser than the case of \( 0 - V \) relaxation (Fig. 2).

We have also examined the trajectory of \( \text{Oi} \) during the migration process. It is found that \( \text{Oi} \) moves by a “swapping” method, as shown in Fig. 8 and elaborated in the following. \( \text{Oi} \) represents the initial position of the interstitial oxygen.
of a $V_{O}O_{1}$ defect pair. With the help of the local electric field or high temperature, $O_{11}$ moves toward a lattice oxygen denoted as $O_{L}$. Meanwhile, $O_{2}$ moves away from its original lattice position toward the destination lattice vacancy position, labeled as $O_{22}$. In the end, $O_{11}$ takes the place of $O_{1}$, with $O_{L}$ being relocated to $O_{22}$. Through this swapping method, the migration of $O_{1}$ can occur throughout the whole HfO$_{2}$ network.

V. Conclusion

Experimental results from PBTI stress/relaxation cycling have indicated that electron trapping may change from an initial shallow trap state to a deeper trap state. Here, we present a $V_{O}O_{1}$ defect pair model, which may satisfactorily explain such a transformation. It is found that a $V_{O}O_{1}$ defect pair may evolve into a much more stable state, with the $O_{1}$ migrating from its original location to a different lattice vacancy position, as marked by a substantial decrease in the system energy at the end of the $O_{1}$ migration process. This evolution is shown in some cases to correspond to a shift in the electron-trap state to a deeper energy level. This atomic model could explain not only the shallow-to-deep electron-trap state transformation, but also long-term PBTI recovery involving the reverse transformation of an electron-trap state from a deep to a shallower level with the concurrent emission of the trapped electron. This paper provides a possible atomic picture of the underlying mechanisms governing the dynamics of the PBTI reliability issue in high-κ/metal gate-stack.

REFERENCES


Authors’ photographs and biographies not available at the time of publication.