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ABSTRACT

Current understanding of the bias temperature instability degradation usually comprises two parts: (1) shallow-level component that can recover within a short time and (2) deep level traps that the emission time of the trapped carrier is extremely long. Previous studies of the positive bias temperature instability degradation in the high- κ n -MOSFET indicate that oxygen vacancy (V_O) is the dominant defect type that responds for the shallow electron trapping. However, recent experimental results reveal that the V_O defect density required to accommodate the experimental measured recoverable threshold voltage degradation (ΔV_{th}) is much higher than that of the reasonable atomic structure in the amorphous HfO_2 . On the other hand, investigations on the disordered Hf-O-Hf network in the amorphous HfO_2 reveal their capabilities as charge trapping centers; therefore, in this work, atomic simulation work is performed, and our results show that the disordered Hf-O-Hf networks can act as effective electron capture centers with shallow levels near the Si conduction band. Moreover, the high density of the stretched Hf-O-Hf networks in the amorphous HfO_2 also significantly enriches the shallow electron traps in the oxide.

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I. INTRODUCTION

Electron trapping under a moderate positive stress condition in the HfO_2 n -MOSFET, named as positive bias temperature instability (PBTI), has been intensively studied since the invoking of high- κ era.^{1–11} Presently, a prevailing understanding of the stress-induced bias temperature instability (BTI) degradation comprises two components: (1) shallow traps typically identified by short detrapping time once the stress is removed and (2) relatively deep traps that take much more time to recover after removing the stress.^{12,13} Since the trap level position in the oxide bandgap, which determines the time constant of charge trapping/detrapping, closely related to the defect morphologies in the material, therefore seeking the proper defect types, by both atomic simulation and experimental characterization, that can respond for the device degradation becomes one of the most challenging tasks in the bias temperature instability study.

Physical characterizations, e.g., electron spin resonance (ESR) or optical absorption methods, conducted on the HfO_2 gate stack, indicate that the oxygen vacancies (V_O) are the dominant defect type in the high- κ gate stack and electron trapping most likely happens on them; also, the characterizations evidence that the electron trap levels induced by the V_O defects are near the Si conduction band (CB) edge, which holds the shallow characteristics.^{14–16} Meanwhile, numerous electrical measurement data obtained through conventional PBTI characterization methods reveal that the majority of the electrons trapped in the gate oxide are shallow and will recover within a relatively short period.^{5,17} Additionally, experimental results obtained through dynamic PBTI measurement reveal that a greater number of the defect centers in the oxide could be repetitively charged/discharged under the low stress field without further degradation, which could be observed on both large and small dimension devices;

however, this balance will be broken if the stress condition is changed to harsher parameter.^{18–20} Up to now, a well-established understanding for the above device degradation behaviors is ascribed to the broad spatial spreading of the V_O defects in the gate stack and the shallow-level characteristics of them under the PBTI stress. And the trapping/de-trapping of the electrons happened in the defects depends on the nonradiative multiphonon assisted trapping, two steps are included in the procedure: (1) the resonant tunneling of the electrons into the near interface pre-existing defects that responds for the fast trapping/detrapping and (2) further migration of the trapped carrier toward deeper unoccupied traps accounted for the slower trapping/detrapping.^{5,21} Meanwhile, first-principles simulation, as one of the most effective and precise methods to investigate the specific defect characteristics in the material, is also extensively implemented in the BTI study.^{22–24} A plethora of modeling and simulation works are performed to investigate the V_O characteristics under the PBTI stress. The results obtained from these studies support the inference that V_O is a shallow electron trap center and could be an effective electron capturing point under the PBTI stress.^{25–27}

In spite of the great success of the V_O defect model in explaining the recoverable component of the PBTI degradation, recent experimental results obtained through PBTI recovery studies in the high- κ n -MOSFET showed some discrepancies. As it is illustrated in a typical stress and recovery measurement [Fig. 1(a)], electrons are injected into the oxide during the stress phase, inducing significant V_{th} degradation. In the recovery phase, it shows that, within the measurement window, the ΔV_{th} right after the stress cycle is ~ 150 mV (R_0) (similar ΔV_{th} could also be found in Refs. 13 and 28).⁶ Considering the 1.4-nm EOT of the high- κ gate oxide, the defect density can be calculated and is in the order of

$\sim 10^{19}/\text{cm}^3$ (see the Appendix). For the HfO_2 material, the typical volume density of the oxygen atoms is $\sim 10^{22}/\text{cm}^3$, this gives us the fact that there is one V_O defect within every thousand oxygen atoms. Similar conclusions are also reported in Refs. 29–31. However, the defect density mentioned above is far more than that of the reasonable atomic structure, which impedes the V_O as the sole defect morphology to explain the significant recoverable component of the PBTI degradation. Nevertheless, recent defect modeling work in SiO_2 reports that the hydrogen species related defect pairs in the SiO_2 have multiple characteristics under different stress situation.^{32–34} This suggests that a similar degradation mechanism may exist in the HfO_2 oxide. Furthermore, simulation studies on amorphous HfO_2 networks report that disordered atomic structures in the dielectric (e.g., stretched Hf-O-Hf bond) could be an inherent relatively deep polarons.³⁵ However, unanimous understandings of the structure properties of the above defect precursors as well as their corresponding defect-level dynamics under the PBTI stressing conditions are still unavailable.

In this paper, we perform continuous defect structure relaxation simulations to investigate the electron trapping mechanism under the PBTI stress. We have focused on the stretched Hf-O-Hf networks in the oxide, by tracing the structure dynamics of the Hf-O-Hf networks after capturing the electron. Our simulation results reveal that stretched Hf-O-Hf networks could be an effective shallow electron trap center. Moreover, the trap level under the PBTI stress condition will continuously evolve with the change of the defect structure. These observations allow us to depict an important physical picture for the shallow electron trapping in the HfO_2 n -MOSFET under the PBTI stress.

II. DEFECT MODELING AND SIMULATION

Our simulation work was performed by Vienna Ab-initio Simulation Package (VASP).^{36–39} The ultra-soft pseudo-potential and plane-wave expansions of wave functions and potentials were implemented during the calculation.⁴⁰ The exchange correlation energies were treated within the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE).⁴¹ Based on the converging tests, the cut-off energy of 400 eV for the plane wave basis and κ -space grids of $5 \times 5 \times 5$ with the Monkhorst Pack scheme were used to calculate the total system energy. For structure optimization, the conjugate gradient method was used and the ion positions were optimized until the residual force was less than $0.01 \text{ eV}/\text{\AA}$. The hybrid density functionals that based on the semi-local PBE approximation were implemented by replacing 25% of PBE exchange with the exact exchange to correct the underestimated bandgap.^{42,43} However, since the energy levels of the localized defect were barely affected by the use of the hybrid functions, therefore the usual GGA functionals of PBE were kept for the system energy calculation.^{44,45} Other than that, the formation energy E_f of a defect in the HfO_2 was calculated by using the

FIG. 1. (a) Typical PBTI recovery curve of high- κ n -MOSFET after the stress phase. R_0 denotes the recoverable component. $R_{\infty} - R_0$ denotes the permanent components, which are extracted by applying negative voltage on the gate.⁶ (b) Schematic energy band diagrams for the device structure under stress and recovery conditions, showing the electron trap distribution in the gate oxide. (c) Schematic energy band diagrams for the device structure under the zero voltage recovery condition. The color shadow illustrates the trapped electron distribution.

following equation:⁴⁶

$$E_f(\alpha, q) = E(\alpha, q) - (E_0^0 + n_{\text{Hf}}\mu_{\text{Hf}} + n_{\text{O}}\mu_{\text{O}}) + q(\epsilon_F + E_{\text{VBM}} + \Delta V) + E_{\text{corr}}, \quad (1)$$

where E_0^0 is the system energy of the defect-free supercell and E_{VBM} is the valence band maximum of HfO_2 . For a defect α in charge state q , E_f is a function of the Fermi level ϵ_F and the respective chemical potential of Hf and O denoted by μ_{Hf} and μ_{O} , respectively. 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 the ϵ_F when $E_f(\alpha, q) = 0$.⁴⁵ The $-/0$ CTL, measured with respect to E_{VBM} , is akin to the trap level of the defect in the HfO_2 bandgap.

In this simulation work, amorphous HfO_2 supercell with 144 atoms was used. To generate the amorphous structures, a melt-quench scheme was implemented.⁴⁷ First, three groups of cubic HfO_2 supercells with the volumes of $1825.147 \text{ \AA}^3$ ($\rho = 9.2 \text{ g/cm}^3$), $1747.703 \text{ \AA}^3$ ($\rho = 9.68 \text{ g/cm}^3$), and $1605.899 \text{ \AA}^3$ ($\rho = 10.04 \text{ g/cm}^3$) were prepared, respectively. Then, they were “heated” to a temperature of 3500 K and maintained at this temperature for 4 ps to fully liquefy the system. After that, the material was annealed to 300 K in 1 ps to create the amorphous HfO_2 structure. As in the amorphous HfO_2 , stretched Hf-O-Hf networks were always expected, therefore we extracted the statistical distribution of bond length for these three HfO_2 materials with different densities, which is shown in Fig. 2.

It can be observed that the bond length of the HfO_2 with an ideal density of 9.68 g/cm^3 shows less scattering than those of the rest two, indicating that process induced stress or tension during the HfO_2 deposition will result in higher

number of stretched Hf-O-Hf bonds in the material. However, for the structure of 9.68 g/cm^3 , it also can be found that $> 18.8\%$ of the Hf-O-Hf bond is longer than the ideal one ($2.1 \text{ \AA}$),⁴⁸ and $\sim 5\%$ of them even are severely outstretched (bond length $> 2.7 \text{ \AA}$). Under the stress condition, these precursors will capture electrons and interact with the lattice phonon to compensate the energy increase.^{49,50} Therefore, in the subsequent work, we will focus on the amorphous HfO_2 with the density of 9.68 g/cm^3 and investigate the dynamic characteristics of the stretched Hf-O-Hf networks under the stress. Since fully structural relaxation will completely cure the stretched Hf-O-Hf bond in the supercell, a dynamic structure relaxation method is implemented in this work.^{8,21} First, the initial stretched Hf-O-Hf network is manually broken by moving the O atom to the neighboring lattice void, and then this structure is subjected to structure relaxation under the negative charged condition (-1 charge state) until it reaches the new stable structure. Thereafter, a *Nudged Elastic Band* (NEB) method is used to search the transition structures and meanwhile the corresponding minimum energy path (MEP); the corresponding CTLs are also calculated when the initial stretched Hf-O-Hf (s0) evolves into the obtained stable network (s5).⁵¹

III. RESULTS AND DISCUSSION

The amorphous HfO_2 features various Hf-O-Hf atomic networks that can be found in the supercell, and as revealed in the early studies, disorders of the atomic network typically induces electron traps, which is also evidenced in our simulation work.³⁴ In Fig. 3, it shows the localized partial electron density of the monoclinic and amorphous HfO_2 after they are negatively charged (-1), respectively. Obviously, we can find that the electron cloud density in the amorphous HfO_2 is more localized on certain disorder local networks,

FIG. 2. The histogram and cumulative probability plot of the bond length distribution for the amorphous HfO_2 with a density of (a) 9.2 g/cm^3 , (b) 9.68 g/cm^3 , and (c) 10.04 g/cm^3 , respectively.

FIG. 3. Partial charge analysis: charge iso-surface = 0.01, the light blue indicates the partial electron density that equals to the iso-surface value. (a) The monoclinic HfO_2 ; (b) the amorphous HfO_2 with a lot of stretched Hf-O bonds. As we can see that the electron cloud in (b) is strongly localized on a certain disordered network, which indicates that stretched Hf-O in the amorphous HfO_2 is an effective electron-capturing center. The Hf atoms are in yellow, and the O atoms are in red.

implying that imperfect oxide structure could be an effective electron-capturing body under the negatively charged condition.

In the subsequent discussions, three typical stretched Hf-O-Hf networks are investigated in detail. The first atomic structure of the stretched Hf-O-Hf network is shown in Fig. 4(a), in which oxygen atom— O_a denotes the initial position of the O atom in the Hf-O-Hf network and O_b denotes the stable position after structure relaxation. As it can be seen in Fig. 4(a) that the Hf-O bond in the initial state (s_0) is stretched by $\sim 34.8\%$ when compared to the ideal length of $2.1\text{\AA}$, and the CTL of this initial atomic configuration, as shown in Fig. 4(b), is 1.03 eV above the Si CB, which is extremely shallow. During the PBTI measurement, the electron will fill this disordered network once the Fermi level is raised up to it by the applied stress voltage. On the other hand, the electron trapped on this defect will be released immediately when the stress voltage is removed due to its

shallow characteristics. However, interaction with the lattice phonon is inevitable once the defect captures the electron, and therefore it will trigger the structure relaxation, although it takes time.³³ With the synergetic impact from the stress field, O_a tends to move toward O_b with the moving distance of $\sim 1.06\text{\AA}$ (Δd). The MEP for the above negatively charged structure transition and the corresponding CTL change is calculated and shown in Fig. 4(b). Totally, four transitional structures in-between s_0 and s_5 states are included, and two relatively low energy barriers with the barrier height of 0.45 eV and 0.16 eV can be observed in the MEP curve, which indicates that structure's transition are ready to happen under the stress period.⁵² Besides, it can be observed on the CTL curve that there is $\sim 1.27\text{ eV}$ change of the defect level position in accordance with the structure change, the final position of the CTL is $\sim 0.23\text{ eV}$ below the Si CB, which is slightly deeper than that at s_0 , but it is still considered as shallow defect level. Meanwhile, as it can be found in the MEP curve in Fig. 4(b) that the reverse barrier for the structure switching back from s_5 to s_0 at -1 charge state is 0.05 eV , whereas it change to 2.53 eV if it happens at the neutral state [Fig. 4(c)]. Since the electron trapped here is shallow, thus it can be expected that electron will be detrapped instantaneously once the stress voltage is removed, and for the disordered network in this case, the high reverse energy barrier at the neutral state will impedes the s_5 structure switching back to s_0 .

The second case is shown in Fig. 5(a), it can be found that Hf-O bond is outstretched by $\sim 28.1\%$ in the initial structure, and the CTL of the structure is 0.2 eV above the Si CB, implying that it is also a shallow defect network. Under the increased stress time and voltage, O_a tends to move toward O_b along the transitional path, and the CTL decreases with the O position changes. When the O_a finally reaches O_b position ($\Delta d = 0.676\text{\AA}$), it needs to overcome two energy barriers (0.71 eV and 0.23 eV) as indicated in Fig. 5(b). Meanwhile, for the CTL, 0.83 eV drops of the energy level between the initial and final stable structure can be observed and the final stable state is $\sim -0.6\text{ eV}$ below the Si CB. The above result suggests that the shallow characteristics of this stretched Hf-O-Hf network in this case is not stable. Under proper stress condition, the O atom can overcome the energy barrier ($0.71\text{ eV} + 0.23\text{ eV} < 1\text{ eV}$) and push the defect level from shallow to relatively deep position. On the other hand, as we look into the reverse energy barrier from s_5 to s_0 at negative state, it is 0.06 eV [Fig. 5(b)], whereas no energy barrier is found if it happens under the neutral state [Fig. 5(c)]. Considering the electrical measurement data as shown in Fig. 1(a), we can have the picture that, as a deep electron trap center for the structure in this case, when the bias is removed, the electron trapped here will be kept only when it is neutralized by a negative detrapping bias and then the defect structure will roll back to the initial s_0 state without energy barrier.

In the end, the atomic structure of the third stretched Hf-O-Hf network is shown in Fig. 6(a). Similarly, the Hf-O bond is stretched by $\sim 18.6\%$, and the initial CTL is 0.1 eV

FIG. 4. (a) Atomic structure of the first stretched Hf-O-Hf network. The length of the stretched Hf-O is 2.83 Å (referring to the ideal bond length 2.1 Å, it is stretched by ~34.8%). The single ended arrow indicates the moving direction of the O atom during the structure relaxation ($O_a \rightarrow O_b$), and the number on the arrow denotes the moving distance (0.634 Å); (b) the MEP curve and the CTL of the corresponding structures for the first Hf-O-Hf network. The total energy barrier for the structure transition from the initial to stable state is 0.45 eV + 0.16 eV. And the change of the structure will induce ~1.27 eV drops of the CTL; (c) the reverse energy barrier for the O_i at the neutral state.

above the Si CB, which is a shallow defect at this state. The structure relaxation brings ~1.06-Å change of the O position. However, as it can be observed from the MEP curve that the O_a needs to overcome ~1.33 eV of the energy barrier to reach its stable position, and this energy is considered relatively high, which may not be able to happen under the typical PBTi stress condition (but it may happen under higher stress condition, e.g., HCI stress). However, it is still worth

having a look at the CTL change. As shown in Fig. 6(b), 0.82 eV drops of the energy level can be observed, and the CTL of the final state is ~-0.8 eV below the CB, which locates below the middle of the Si bandgap, implying the electron trapped in defect structure has quite long trap emission time. Moreover, from the tendency of the defect reverse energy barrier, it has the similar characteristics as depicted in the second case [see Fig. 6(c)]. So for this defect, under normal PBTi measurement

FIG. 5. (a) Atomic structure of the second stretched Hf-O-Hf network. The length of the stretched Hf-O is 2.69 Å (it is stretched by ~28.1%). The moving distance is 0.676 Å ($O_a \rightarrow O_b$); (b) the MEP curve and the CTL of the corresponding structures for the second Hf-O-Hf network. The total energy barrier for the structure transition from the initial to stable state is 0.71 eV + 0.23 eV. And the change of the structure will induce ~0.83 eV drops of the CTL. The inset shows the reverse barrier from s5 to s0 at the neutral state; (c) the reverse energy barrier for the O_i at the neutral state.

FIG. 6. (a) Atomic structure of the third stretched Hf-O-Hf network. The length of the stretched Hf-O is 2.70 Å (it is stretched by $\sim 18.6\%$). The moving distance is 1.060 Å ($O_a \rightarrow O_b$); (b) the MEP curve and the CTL of the corresponding structures for the third Hf-O-Hf network. The total energy barrier for the structure transition from the initial to stable state is 0.71 eV + 0.62 eV. And the change of the structure will induce ~ 0.82 eV drops of the CTL. The inset shows the reverse barrier from s5 to s0 at the neutral state. The inset shows the reverse barrier from s5 to s0 at the neutral state; (c) the reverse energy barrier for the O_i at the neutral state.

(moderate e-field, low temperature), it acts as a shallow and switchable charge capturing center, however, if the device is stressed under a more harsh condition, e.g., high e-field, high temperature or substrate hot electron injection, it will evolve to deep level trap.

So far, we only discuss three typical stretched Hf-O-Hf networks in the amorphous HfO_2 , the initial structures of them all show the shallow electron trap characteristics under the PBTI test. Although comparing with the real situation in the amorphous HfO_2 , certain critical scenarios may not be fully included in this study, our results still give clear evidence that the disordered networks in the amorphous HfO_2 could be effective electron traps under the PBTI stress. Since disordered atomic networks are more widely existed in the amorphous structure, therefore it can be inferred that they will contribute great part of the shallow electron traps. Moreover, material deposition may induce significant stress or tension in it, which can result in higher density of disordered networks, thus more shallow electron traps may exist in those oxide. Finally, as it can be observed in the second and third cases of the stretched Hf-O-Hf that the CTL of the disorder atomic network will evolve from shallow to deep when the defect atomic structure changes. This behavior further supports the experimental observation that the defect level transfers from shallow to deep state under specific PBTI stress condition.^{6,13,53}

IV. CONCLUSION

Two components of the threshold degradation in the high- κ n-MOSFET under the PBTI stress are discussed, and experimental characterization as well as first principle simulation evidence that the V_O is the dominant shallow

electron-trapping center in the amorphous HfO_2 . However, the high V_O defect density required to accommodate the experimental measured threshold voltage degradation challenges the recognition that V_O is the only shallow electron trapping center in the amorphous HfO_2 . In view of the above dilemma, the role of the stretched Hf-O-Hf network as the electron trapping center is investigated. Our simulation results show that the stretched Hf-O-Hf networks can be effective electron capturing centers under the PBTI stress, and the fact that high density of the stretched Hf-O-Hf network in the amorphous HfO_2 helps enrich the conventional trapping model of the recoverable component in the PBTI degradation.

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APPENDIX: CALCULATION OF THE DEFECT DENSITY

As can be observed in Fig. 1 of Ref. 6, the ΔV_{th} right after one stress cycle was ~ 150 mV. The EOT of the DUT is 1.4 nm, and simply using the equation of the plate capacitor:

$$\frac{\Delta Q}{\Delta V} = C_{ox} = \frac{\epsilon \cdot \epsilon_0}{d}, \quad (A1)$$

where C_{ox} is the unit area's capacitance of the gate oxide, d is

the EOT, ΔV is the threshold voltage shift, ϵ and ϵ_0 are the relative dielectric constant of Si and vacuum dielectric constant, respectively. With Eq. (2) here, we can have the effective charge density in the order of $10^{12}/\text{cm}^2$, whose volume density is $10^{19}/\text{cm}^3$. For the HfO_2 material, the volume density of the oxygen atom is in the order of $10^{22}/\text{cm}^3$. Therefore, it shows that for every 1000 atoms, there is one vacancy.

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