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Abnormal Bias Instabilities Induced by Lateral H_2O Diffusion Into Top-Gate Insulator of a-InGaZnO Thin-Film Transistors

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ABSTRACT The environmental stability of self-aligned top-gate (SATG) a-InGaZnO thin-film transistor (TFT) was studied by performing the high-temperature high-humidity (HTHH) test. Despite the maintenance of initial electrical characteristics, the stability under positive bias stress (PBS) was considerably deteriorated, including an abnormal negative V_{th} shift (ΔV_{th}), increased off current, and degraded *SS*. Moreover, the negative ΔV_{th} was consistently enhanced with the channel length (L) decreasing. Such L dependence was clarified to originate from the lateral diffusion of H_2O in TG insulator during HTHH tests, and the PBS instabilities were caused by the ionization and migration of H_2O molecules into the a-IGZO channel, as verified by the X-ray photoelectron spectroscopy, C-V characteristics, and recovery behaviors of PBS degradation.

INDEX TERMS A-InGaZnO, self-aligned top-gate (SATG), H_2O, hydrogen, positive bias stress (PBS), environmental stability, thin-film transistors (TFTs).

I. INTRODUCTION

Recently, amorphous oxide semiconductor (AOS) thin-film transistors (TFTs), with amorphous indium-gallium-zinc oxide (a-IGZO) TFT as the representative, have been studied for next-generation displays and large-area flexible electronics, due to relatively high mobility, steep subthreshold swing (*SS*), low off current (I_{off}), and low-temperature fabrication [1], [2]. However, these superiorities were often degraded by the inherent sensitivities of AOSs to the ambience, especially H_2O vapor [3]–[11].

Among incumbent structures, H_2O-induced instabilities have been intensively investigated for bottom-gate (BG) TFTs, since their less protected channels are usually more susceptible to H_2O. Several instability models have been proposed, including the H_2O doping model [10], [11], the hydrogen bonding model [6], and the ion drift model [3]–[5]. Even with the channel in-situ protected by a top gate (TG), the moist ambience could still give rise to severe degradations [12], which cannot be fully explained by existing H_2O instability models [3]–[7], [9]–[11] proposed for BG TFTs. Considering the self-aligned top-gate (SATG) TFTs with suppressed parasitic capacitance and better scalability are preferred for advanced applications [13], it is important to clarify the humidity influences on the TG-protected AOS channel.

In this work, the effects of H_2O on SATG a-IGZO TFTs were systematically investigated. Despite the almost unchanged electrical characteristics after high-humidity tests, the significantly deteriorated bias instabilities exhibited not only abnormal degradation behaviors but also strong dependences on channel length. The underlying mechanisms were verified to be the lateral diffusion of H_2O molecules into TG insulator and their subsequent ionization/migration processes under vertical electrical field stresses.

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II. EXPERIMENTAL DETAILS

On the glass substrate, a 40-nm-thick a-IGZO film was first sputtered at room temperature with a ceramic target of In_2O_3: Ga_2O_3: ZnO = 1: 1: 2 mol%. The patterned a-IGZO active islands were treated with the nitrous oxide (N_2O) plasma at 150 °C, and subsequently covered with the gate insulator (GI) of 200-nm thick PECVD SiO_2 deposited at 300 °C. Then, a 1.5-hours anneal was specifically performed in oxygen (O_2) at 300 °C to dehydrogenate the a-IGZO [14] and passivate its defects [15]. After the sputtering of the molybdenum (Mo) film, the Mo/SiO_2 gate stack was patterned together and subjected to another anneal in O_2 at 300 °C for half an hour. Next, the self-aligned formation of n^+-IGZO source/drain (S/D) regions was realized using the argon (Ar) plasma treatment. A 200-nm-thick PECVD SiO_2 was then deposited at 150 °C as the passivation layer (PL). Finally, the Mo S/D electrodes were deposited in the contact holes of PL. A high-temperature high-humidity (HTHH) test was performed at 50 ^{o}C with relative humidity (RH) of 80%. The electrical characteristics of SATG a-IGZO TFTs were measured in a room-temperature dark environment using the Agilent B1500 semiconductor parameter analyzer and KEYSIGHT E4980A precision LCR meter.

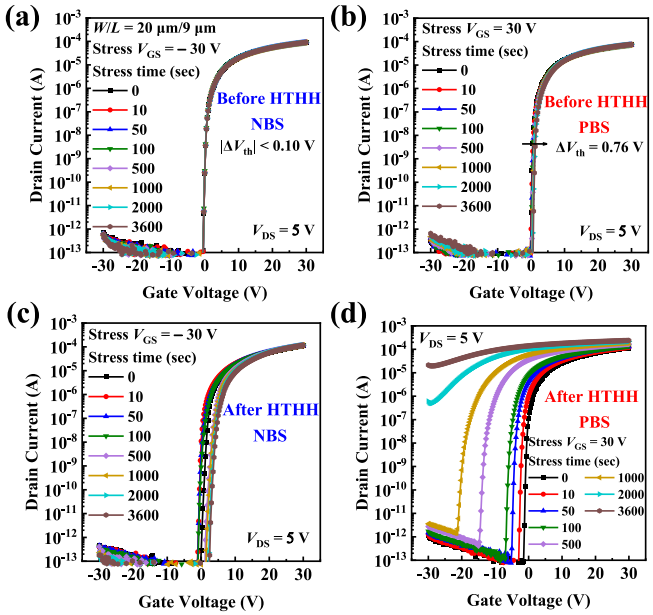

FIGURE 1. Evolutions of the transfer characteristics for SATG a-IGZO TFTs under (a, c) NBS of −30 V and (b, d) PBS of 30 V (a, b) before and (c, d) after HTHH tests.

III. RESULTS AND DISCUSSION

The initial reliability of as-fabricated SATG a-IGZO TFTs with channel width/length (W/L) of 20 μm/9 μm was first evaluated under positive/negative gate stresses (PBS/NBS) with gate voltage (V_{GS}) of ± 30 V. After 3600-sec NBS and PBS, no noticeable degradation was observed in the drain current (I_{DS}) versus V_{GS} transfer characteristics measured at a drain voltage (V_{DS}) of 5 V, as shown in Figs. 1(a) and 1(b). To quantitively evaluate instabilities, the threshold voltage (V_{th}) was extracted as the V_{GS} corresponding to the normalized $I_{DS}L/W$ of 10^{-10} A. The PBS gave rise to a slightly negative V_{GS} shift (ΔV_{th}) around 0.76 V, indicating that the channel electrons were barely trapped into GI or at GI/channel interface [16], while absolutely no ΔV_{th} could be detected when channel electrons were depleted under NBS. Together with the well-maintained *SS* during bias stresses, the high qualities of GI and interface are verified.

After the SATG a-IGZO TFTs were subjected to the 24-hours HTHH storage, neither linear- nor saturation-region characteristics exhibited observable degradations, such as more negative V_{th}, larger I_{off}, and poorer *SS*, while these are common for humidity-influenced BG AOS TFTs [3]–[7], [9]–[11]. The H_2O molecules seem to hardly reach the TG-protected a-IGZO channel during the HTHH test, plausibly consistent with the waterproof capability of metal electrodes [8].

The bias instabilities were further characterized in Figs. 1(c) and 1(d). The 3600-sec NBS led to a small ΔV_{th} around 2 V and an unchanged *SS*, while the PBS caused much more dramatic degradations. Distinct from the common PBS-induced positive ΔV_{th} [16], the transfer curves abnormally shifted towards the negative V_{GS}, together with the gradually increasing *SS*, and finally degraded into a conductor-like behavior, as shown in Fig. 1(d). Such severely deteriorated stabilities reveal the invasion of H_2O into SATG TFTs during HTHH tests, although the H_2O molecules may not directly reach the a-IGZO channel.

Among the H_2O-induced instabilities [3]–[12], such negative ΔV_{th} under PBS was often ascribed to mobile impurity ions or polar groups in GI, due to the dissociation of adsorbed H_2O molecules under electric fields [3], [4], [12]. Moreover, the degraded *SS* and I_{off} suggest the increase of interface defects and channel donors. Although the doping effects of H_2O [10], [11] and/or hydrogen [6] have been reported to bring about similar *SS* and I_{off} degradations of AOS TFTs, such mechanisms cannot explain the humidity-induced difference between NBS and PBS instabilities.

Considering both PL and GI are made of the PECVD SiO_2, their relatively permeable nature cannot thoroughly prevent vapor penetration [6], [7]. As illustrated in Fig. 2(a), the H_2O molecules are suspected to penetrate the SiO_2 PL and GI during HTHH tests, but not spontaneously diffuse through the SiO_2/a-IGZO interface, most plausibly due to the relatively low temperature and high-quality interface [17]. Such neutral H_2O in GI thus does not instantly influence the electrical characteristics. Under a sufficiently high positive V_{GS}, the O-H bonds of H_2O molecules near the GI/channel interface can be dissociated by the energetic channel electrons, and then the resulted H ions diffuse into a-IGZO to elevate channel donor concentration [6], [18], as shown in Fig. 2(b). In contrast, due to the lack of holes in AOS [19], there is no energetic carrier to trigger such H_2O ionization under NBS. Instead, a few H_2O molecules may be polarized

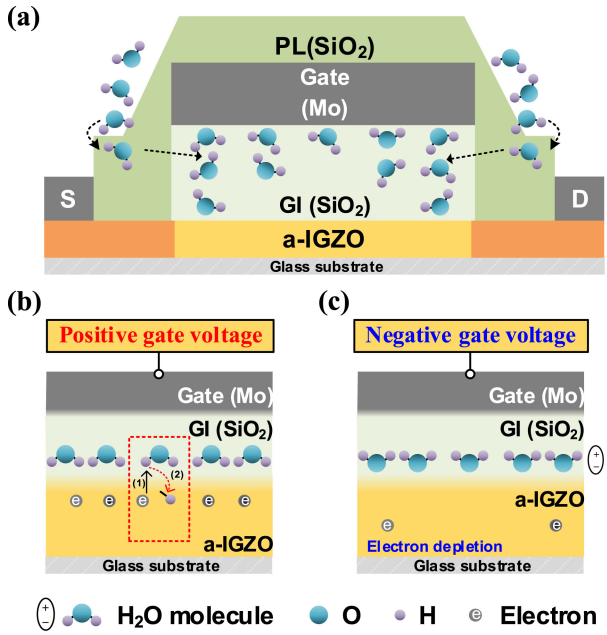

FIGURE 2. (a) Schematic diffusion process of H_2O molecules through the SiO_2 PL and GI during the HTHH test. (b) Schematic ionization and migration processes of H_2O-related species in the SATG TFTs under PBS, including (1) the O-H bond breakage and (2) the H ion migration. (c) Schematic polarization process of GI H_2O molecules under NBS.

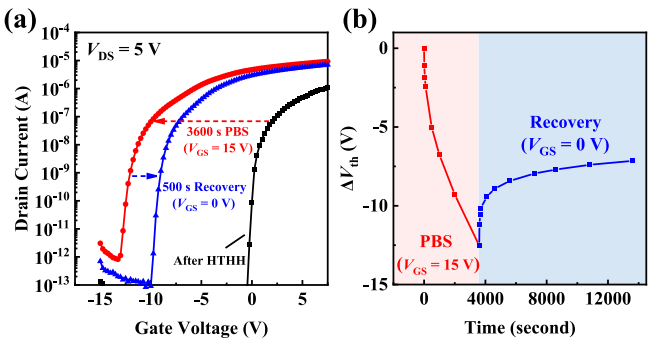

FIGURE 3. The PBS recoveries of (a) transfer characteristics and (b) ΔV_{th} for the SATG TFTs with $W/L = 20\ \mu m/84\ \mu m$ after PBS.

into electric dipoles [20], [21] and thus give rise to a positive but limited ΔV_{th}, as illustrated in Fig. 2(c).

To identify the H_2O-induced defects in the a-IGZO channel under PBS, post-PBS recovery behaviors were further analyzed. As shown in Fig. 3 (a), the 3600-sec PBS-induced negative ΔV_{th}, degraded *SS*, and elevated I_{off} were all recovered partially after only 500 seconds at a zero V_{GS}, while the main degradations could not be fully restored even after an extremely long recovery, as shown in Fig. 3(b). This suggests that the ionized H_2O mainly forms stable donors in a-IGZO, consistent with the reported irreversible doping reaction between adsorbed H_2O and AOS back channel [6]. In contrast, the recoverable short-term degradation possibly implies the transitions between subgap states.

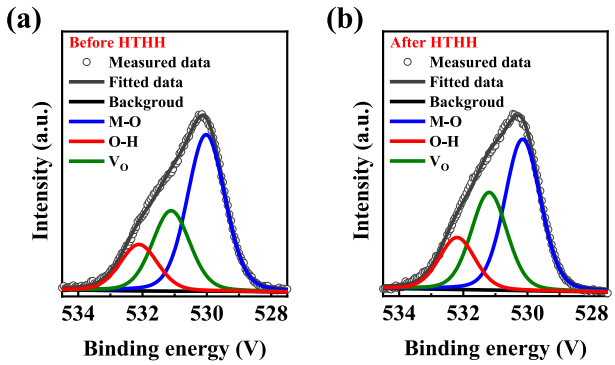

FIGURE 4. O 1s XPS results of bare a-IGZO films (a) before and (b) after HTHH tests.

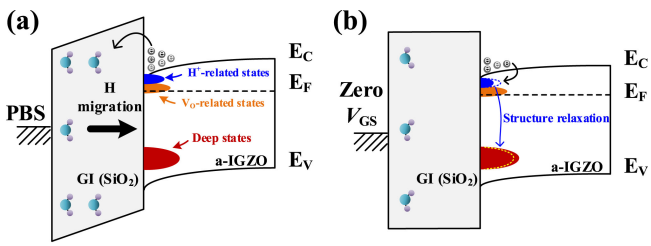

FIGURE 5. Energy band diagrams at the interface between the hydrous SiO_2 GI and a-IGZO channel under (a) positive and (b) zero V_{GS}.

The H_2O-related states in AOSs mainly include the shallow-donor hydroxyl (O^{2-}-H^+) group, relatively deeper H^- state in metal-hydrogen (M^+-H^-) bonds, and donor-like oxygen vacancy (Vo) [19], [22]–[26]. The HTHH-treated bare a-IGZO samples were thus directly analyzed using X-ray photoelectron spectroscopy (XPS). Fig. 4 shows the O 1s XPS of the a-IGZO with three deconvoluted peaks respectively corresponding to O-H bond (532.2 eV), V_O (531.2 eV), and O^{2-} ions surrounded by metal cations (529.8 eV). After the HTHH test, the area percentage of O-H subpeak only slightly increases from 16.4% to 17.2%, while that of the V_O subpeak noticeably increases from 28.4% to 32.4%. Considering the O-H bond is less stable than Vo [26], H^+ and Vo may respectively contribute to the bistable minority and relatively stable majority of the H_2O-induced channel donors during PBS.

As illustrated in Fig. 5(a), the GI H_2O molecules are dissociated by the PBS-induced energetic electrons and then enter into a-IGZO channel, generating abundant Vo donors [27] and some donor-like H^+ states [4]. Such a defective conductive channel agrees well with negative ΔV_{th} and deteriorated *SS* under PBS in Figs. 1d and 3a. As illustrated in Fig. 5(b), some H^+ states may capture the residual electrons from the conduction band under zero-V_{GS}, leading to the structural relaxation from H^+ to H^- [28], [29] and thus contributing to the short-term partial recovery in Fig. 3(b).

Distinct from the instant degradation of BG a-IGZO TFTs after HTHH tests, the H_2O cannot directly diffuse vertically into the in-situ protected channel of SATG TFT. The lateral invasion paths of H_2O may be related to the underlying

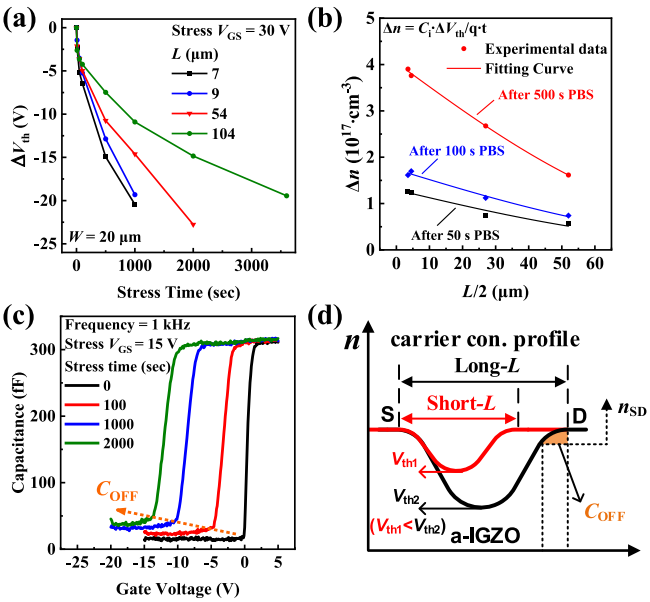

FIGURE 6. (a) Time evolutions of ΔV_{th} of the SATG TFTs with various *L*s under PBS after HTHH tests. (b) Fitting of Δn as a function of $L/2$ under various PBS times. (c) Evolutions of C-V characteristics of the SATG TFTs with W/L = 20 μm /54 μm under PBS after HTHH tests. (d) The schematic profile of carrier concentration in the channel layer.

mechanisms of unchanged I_{DS}-V_{GS} curve and abnormal PBS instabilities. Therefore, the PBS degradations were further characterized on the humidity-treated SATG TFTs with different *L*s. Figure. 6(a) compares the time evolutions of PBS-induced ΔV_{th} for these TFTs. The abnormal negative ΔV_{th} was consistently observed with L increasing from 7 μm to 104 μm, while the degradation degree was continuously relieved. This confirms the L-direction distribution of H_2O molecules within GI, originating from the diffusion process through SiO_2 during the HTHH test.

It can be reasonably inferred that the H_2O distribution is directly correlated with the change (Δn) of channel carrier concentration (n) during PBS. As shown in Fig. 6(b), the lateral distribution of Δn from source/drain (S/D) towards channel was estimated from the L dependence of ΔV_{th}. Moreover, the Δn can be well fitted as a function of $L/2$ according to Fick's second law of constant-source diffusion mode [28],

$$\Delta n|_{\text{PBS time}} = \Delta n_o \cdot \text{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

where $x = L/2$ corresponds to the lateral diffusion distance of H_2O from S/D PL into TG-GI, D is the diffusion coefficient of H_2O in SiO_2, t is the HTHH time, and Δn_o is the H_2O concentration at the edge of GI. The good fitting results for various PBS durations confirm the lateral diffusion process of H_2O molecules within SiO_2 PL and then GI during HTHH, as shown in Fig. 2(a). In addition, D extracted for different PBS times at room temperature were all around 1.2×10^{-11} cm^2 s^{-1}, close to the reported D of H_2O molecule in CVD SiO_2 [12], [29]. This consolidates that the lateral distribution of H_2O in GI is formed during the HTHH test rather than PBS.

The capacitance-voltage (C-V) measurements were also carried out to analyze the evolution of channel carrier profile during PBS. As shown in Fig. 6(c), in addition to the expected negative shift, the C-V curves significantly stretched out in *SS* and off regimes with gradually higher capacitance (C_{OFF}). As pointed out in Fig. 6(d), these imply that the PBS gradually increases the n of the central channel, while the n near channel edges is even elevated to close to S/D doping concentration (n_{SD}), respectively resulting in negative ΔV_{th} and C_{OFF} increment. Besides, due to the shorter diffusion length, the central n of the short-L channel increases to an even higher value than that of the long-L transistor, resulting in a more negative V_{th}, as illustrated in Fig. 6(d). Both I-V and C-V characteristics verify the lateral diffusion of H_2O in TG GI and the subsequent PBS-induced ionization/migration from GI into the a-IGZO channel.

IV. CONCLUSION

In conclusion, the H_2O-induced PBS instabilities in SATG TFTs were attributed to H_2O diffusion and their subsequent ionization/migration processes under vertical electrical field stresses. During the high-humidity test, the H_2O molecules could penetrate the SiO_2 PL and GI, while such neutral H_2O in GI does not instantly influence the electrical characteristics. Under PBS, the H_2O molecules in GI are dissociated by the energetic electrons and then enter into the a-IGZO channel, causing the negative ΔV_{th}, increased off current, and deteriorated *SS*. The recovery and XPS results suggest that the absorbed H_2O in a-IGZO would generate abundant Vo donors and some donor-like H^+ states in the film. Moreover, the negative ΔV_{th} was consistently enhanced with the L decreasing, resulting from the lateral diffusion of H_2O in TG insulator during HTHH tests. The clarification of the H_2O-induced instability mechanism is helpful to the design of passivation layers and active layers in SATG a-IGZO TFTs for advanced applications.

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