

Quantitative Dynamic Evolution of Unoccupied States in Hydrogen Diffused InGaZnSnO TFT under Positive Bias Temperature Stress

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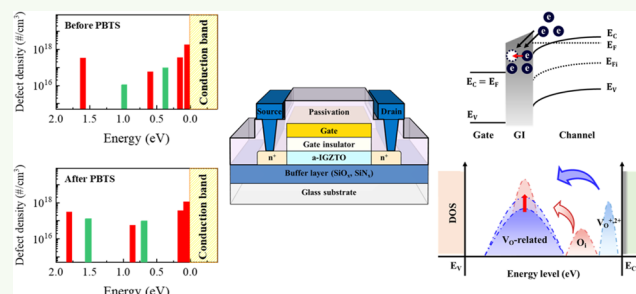
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Supporting Information

ABSTRACT: Positive bias temperature stress (PBTS)-induced defects in self-aligned top-gate coplanar amorphous indium–gallium–zinc–tin oxide (a-IGZTO) thin-film transistors (TFTs) were quantitatively extracted as a function of hydrogen concentration. As the hydrogen concentration increased, the device properties and stability improved. As the stress time increased, the two decay constants that were extracted from the recovery of PBTS increased. Under PBTS, electrons were trapped in multiple defects simultaneously. Quantitative dynamic evolution of defect measurements showed that as the stress time increased, the activation energy and density of defects changed. As electrons moved to the dielectric, the density of shallow-level defects in the channel decreased, while the activation energy and density of deep-level defects increased. With a higher hydrogen concentration in the channel, the changes in defects were smaller. These findings indicate that hydrogen improves stability by passivating electron trap sites.

KEYWORDS: quantitative analysis of defect, InGaZnO, thin-film transistor (TFT), hydrogen, positive bias temperature stress (PBTS)



1. INTRODUCTION

Amorphous indium–gallium–zinc oxide (a-IGZO) thin-film transistors (TFTs) have recently attracted attention due to their excellent electrical properties and low fabrication temperatures.^{1–3} These characteristics are particularly suitable for achieving a consistent performance over large areas. In active-matrix organic light-emitting diode (AMOLED) displays, a-IGZO TFTs have been employed as backplanes. It has been suggested that increasing indium content in a-IGZO channel material can improve electrical performance, as a 5s orbital of indium cation is able to improve the mobility of the charge carrier.⁴ However, given that indium is a scarce resource, ongoing research is exploring the substitution of indium by alternative metal cations. It is known that tin ions have a principal quantum number similar to indium ions and that spatial diffusion of s-orbitals can form a movement path of electrons.⁵ However, studies on the stability of indium–gallium–zinc–tin oxide (a-IGZTO) are still needed.

When used in the backplane of AMOLED displays, amorphous oxide semiconductor (AOS) TFTs are often exposed to positive bias temperature stress (PBTS). PBTS-induced instability can cause a decrease in the luminance and nonuniformity of AMOLED. Accordingly, it is important to understand the mechanism of PBTS-induced instability in AOS TFTs. Under positive bias temperature stress (PBTS) conditions, numerous electrons accumulate near the gate insulator, while some electrons diffuse into the gate insulator

and become trapped in defect states. Trapped electrons can partially screen the electric field from the gate. This requires a larger gate voltage to activate the TFT, which shifts the transfer curve in the positive direction. Currently, research studies that quantitatively analyze the electron trapping phenomenon caused by PBTS in AOS TFTs are very limited. Previous studies have assumed that electrons trapped in the gate insulator after PBTS are the main cause of the transfer curve shift in PBTS and that electrons are trapped in a defect state at a single energy level.^{6,7} However, it has been reported that under PBTS, the occurrence of defect states in the channel can induce a shift in the transfer curve, even without a change in the subthreshold swing (SS) value and that electrons can be simultaneously trapped in multiple defect states.^{8,9} Therefore, it is important to analyze the generation of defects and electron traps in the channel according to the PBTS.

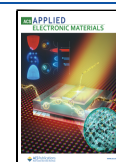
In this study, we used photoinduced current transient spectroscopy (PICTS) to quantitatively measure changes in defect characteristics as a function of time in the PBTS of a-IGZTO TFT. The quantitative defect analysis results allow an

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understanding of the relationship between defects and instability over time in PBTS.

2. EXPERIMENTAL SECTION

2.1. IGZTO TFT Fabrication and Characterization. To fabricate a self-aligned top-gate (SA-TG) structure of a-IGZTO TFTs, as shown in Figure 1, a 30 nm thick a-IGZTO active layer with an In/

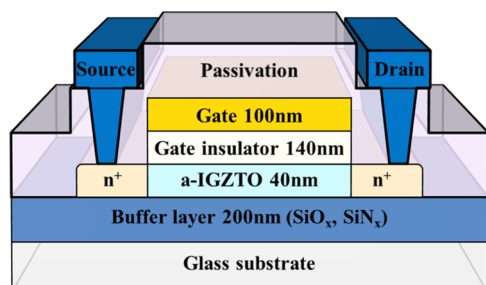


Figure 1. Cross-sectional schematic of the fabricated SA-TG a-IGZTO TFTs.

Ga/Zn/Sn composition of 28:8:8:1 at. % was deposited via radio frequency (RF) magnetron sputtering at room temperature (RT). On the active layer, a 140 nm thick SiO_x gate insulator was deposited by plasma-enhanced chemical vapor deposition (PECVD), followed by deposition of a molybdenum gate electrode. By controlling plasma power and deposition temperature in the PECVD process, the hydrogen concentration diffusing into a-IGZTO can be controlled. As the plasma power decreased, SiH₄ radical decomposition decreased, and hydrogen concentration in SiO_x increased. This could increase hydrogen diffusion into the a-IGZTO in the postprocessing steps. As the deposition temperature increased, the hydrogen concentration in the SiO_x film decreased, whereas hydrogen concentration diffusion into the a-IGZTO increased. Through this, the carrier concentration in a-IGZTO could be adjusted. Plasma power was set at (300 and 400) W. The deposition temperature was set at (280 and 300) °C. After deposition and patterning of the gate electrode and gate dielectric, SiO_x and SiN_x were deposited as an interlayer dielectric (ILD) using PECVD, and patterned to create via holes. The n⁺ a-IGZTO source (S) and drain (D) electrodes of Mo designed as via-contact types were subsequently deposited and patterned. Finally, the a-IGZTO TFT was thermally annealed at 380 °C in air to obtain a stable and uniform electrical performance. The fabricated TFTs had a channel width (*W*) and length (*L*) of 4 μm each, defined by photolithography.

Rutherford backscattering spectrometry (RBS) measurements were performed by using high-energy (2.4 MeV) He²⁺ ions (α particles) at a scattering angle of 170°. The elastic recoil detection (ERD) method involved capturing the energy spectrum of protons impacted by incident 2.4 MeV He²⁺ ions and subsequently recoiling elastically in the forward direction. By strategically employing a stopping foil of appropriate thickness on the detector, it became feasible to admit H ions for analysis while effectively excluding all scattered He ions. This exclusion encompassed the substantial He ion flux contributed by Rutherford scattering arising from other, heavier constituents within the sample. To ascertain hydrogen concentrations in the a-IGZTO films, ERD with 2.4 MeV He²⁺ ions was used.

To quantitatively analyze the defect state using PICTS, a-IGZTO TFT was irradiated with an LED ($\lambda = 405$ nm). Photocurrent was measured in the range (300 to 360) K.

The device characteristics of the a-IGZTO TFTs were measured using a semiconductor parameter analyzer. Drain current (*I_D*) was measured under a gate voltage *V_G* sweep from (−10 to 40) V while maintaining a constant drain voltage (*V_D*) of 0.1 V.

2.2. DFT Calculation Method. To investigate the formation and influence of oxygen-related defects in the a-IGZTO system, density functional theory (DFT) calculations were conducted using the

Vienna *ab initio* simulation package (VASP) with the PBEsol functional. Initially, two amorphous models were created through a melt-quench process in an *ab initio* molecular dynamics (MD) simulation.^{10,11} This simulation employed an NPT ensemble with a Langevin thermostat, γ *K*-point, and a 500 eV cutoff energy. The model compositions were set at 28 indium, 8 gallium, 8 zinc, 1 tin, and 80 oxygen atoms to match the 28:8:8:1 stoichiometry of the IGZTO. During the first phase, both models were heated to 3000 K for 12 ps using 3 fs time steps. Following this, the MD simulation cooled the models from (2000 to 300) K at a rate of 50 K/ps over 54 ps with the same time steps. Post cooling, geometric optimization was performed until the structures met the 0.01 eV/Å convergence criterion. The electronic structure and optimization processes utilized a $2 \times 2 \times 2$ *k*-points grid and a 500 eV cutoff energy.¹² The HSE06 hybrid functional was applied for more precise electronic structure prediction of the IGZTO.¹³

To examine the effects of PBTS, calculations were carried out under three different conditions: −1, neutral (+0), and +1 charged states of electrons. Separate simulations were performed for each charge state to evaluate their impact on defect formation and behavior under PBTS, providing a detailed understanding of defect dynamics and their implications for device performance under stress.

3. RESULTS AND DISCUSSION

Figure 2a shows the RBS spectra of three samples on glass substrates simulated using the Rutherford universal manipulation program (RUMP) code, which confirms the consistent elements of the three samples. The results indicated that the metal-composition ratios of the In/Ga/Zn/Sn were 28:8:8:1.

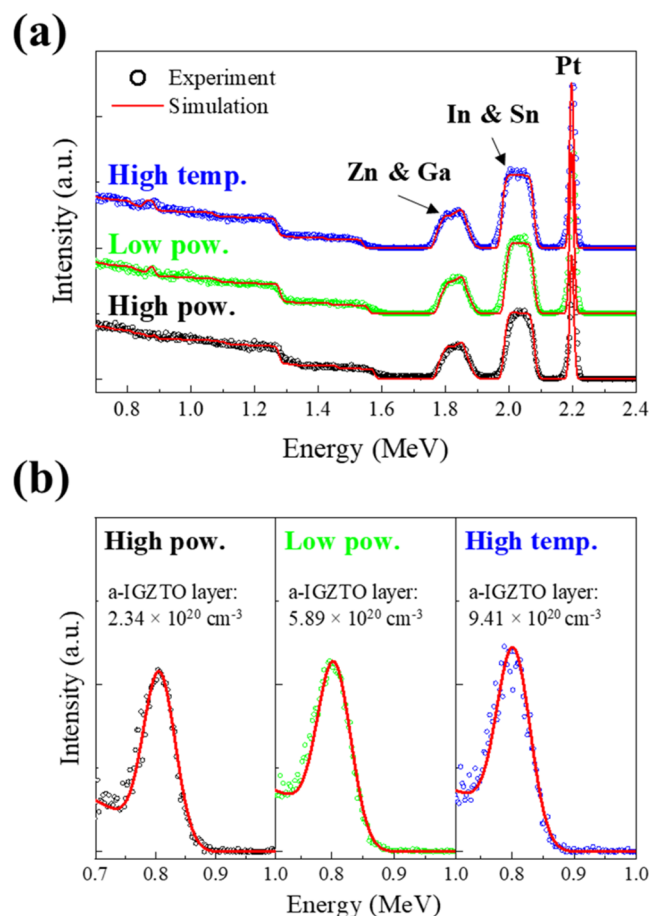


Figure 2. (a) Rutherford backscattering (RBS) spectra and (b) elastic-recoil-detection (ERD) spectra of the a-IGZTO films.

These ratios were retained for all three samples. Peak positions for each element were indexed in the RBS spectra. Here, the simulated results were almost perfectly consistent with the experimental data. Figure 2b displays the ERD spectrum for hydrogen quantities, including both simulation and experimental data. The simplest and most precise measurement that ERD can provide is the measurement of total hydrogen content (H^0 , H^+ , H^- , H_2 , O–H bonding states, etc.) within a surface layer or thin film.¹⁴ As the plasma power decreased during GI deposition, the hydrogen concentration in the a-IGZTO increased from $(2.34 \text{ to } 5.89) \times 10^{20} \text{ cm}^{-3}$. When the substrate temperature was increased to 300 °C, the hydrogen concentration increased to $9.41 \times 10^{20} \text{ cm}^{-3}$. Increasing the substrate temperature during the GI layer deposition resulted in more hydrogen diffusing into the channel layer, compared to adjusting the plasma power, which was related to an increase in the active layer conductivity.^{15,16} Hereafter, the samples are referred to as H_2 low (High power), H_2 middle (Low power), and H_2 high (High temperature), based on their hydrogen concentrations.

Figure 3a,b shows transfer curves for the fabricated SA-TG coplanar a-IGZTO TFTs under constant V_G values of (20 and -20) V, respectively, at 60 °C. As the hydrogen concentration increased from low to middle to high, the threshold voltage (V_{th}) during the initial sweep decreased from (3.41 to 2.32 to 0.12) V, respectively. Simultaneously, the field-effect mobility (μ_{FE}) increased from (22.68 to 26.15 to 35.01) $\text{cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$, respectively. The subthreshold swing (SS) decreased from (0.21 to 0.18 to 0.16) V/decade⁻¹, respectively. The electrical conductivity of AOS generally depends on oxygen deficiency or hydrogen bonding. Oxygen deficiency can increase free carriers in the AOS matrix via $V_o = V_o^{2+} + 2e^-$.¹⁷ Hydrogen in oxide semiconductors is known to act as a carrier donation center, with two types of donor states: interstitial hydrogen (H_i^+) and substitutional hydrogen (H_o^+) bonded to oxygen deficiency.¹⁸ Since the a-IGZTO was deposited under the same conditions, it was expected that there would be little difference in the oxygen deficiency between the devices. As a result, the change in electrical conductivity of a-IGZTO was more related to the hydrogen concentration. With an increased stress time, the transfer curves shifted in the positive direction under PBTS conditions. As the hydrogen concentration increased, the transfer curve shift decreased from (4.62 to 0.45 to 0.11) V under PBTS, respectively, improving device stability, while the SS value exhibited no significant changes. Previous studies on well-passivated AOS TFTs have reported that the PBTS-induced parallel shift of transfer curves can primarily be attributed to the creation of acceptor-like states below the Fermi level in the channel layer or electron injection from the channel into the gate dielectric.¹⁹ On the other hand, the transfer curves showed minimal change over time under negative bias temperature stress (NBTS), suggesting that it has little effect on the device performance. The time-dependent changes under both PBTS and NBTS conditions are summarized in Figure 3c, which shows the transfer curve shifts over time for different hydrogen concentrations.

Figure 4 shows an exponential change in ΔV_{th} over the stress/recovery time as a function of hydrogen concentration. Trapped electrons in the interfaces/bulk defects due to PBTS are released during the recovery time, leading to the recovery of ΔV_{th} . When analyzing the exponential decay of the recovery, two types of decay constants were extracted. Table 1 details

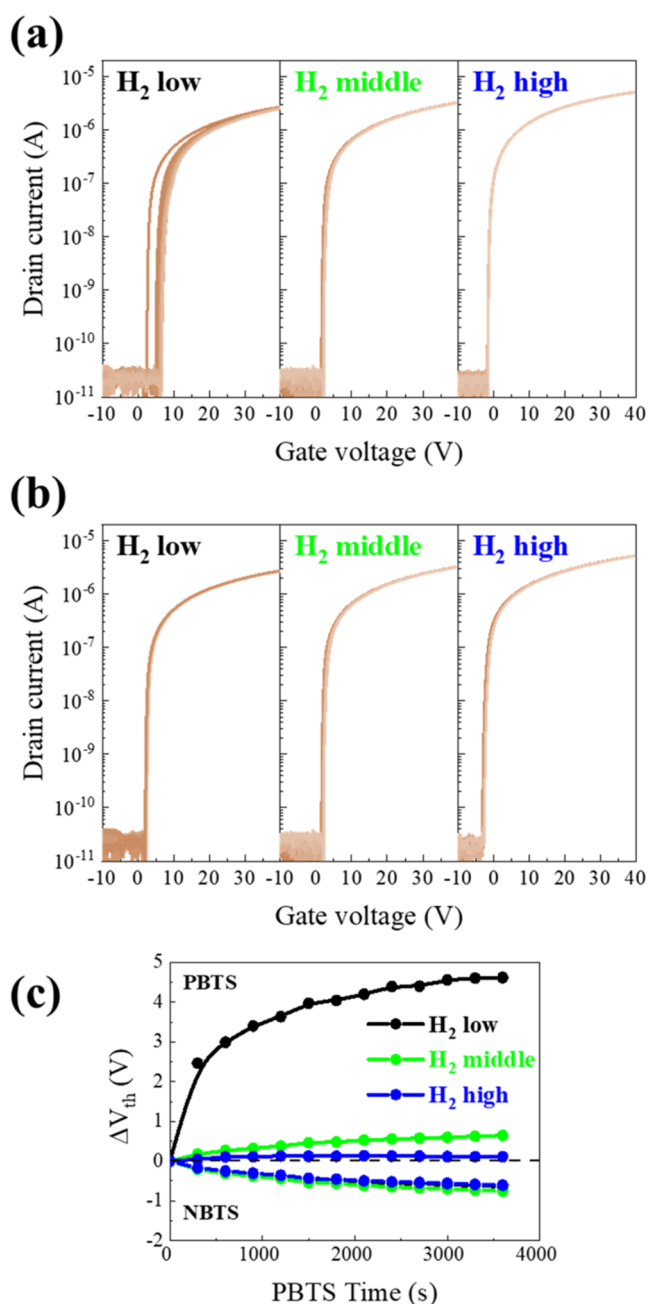


Figure 3. Transfer characteristics and threshold voltage shift of the a-IGZTO TFTs under different stress conditions. (a) Under PBTS, (b) under NBTS, and (c) threshold voltage shifts with stress time under PBTS and NBTS.

the results. The decay constant represents the time required for the trapped electrons in defects to be released²⁰

$$\tau = \tau_0 \exp(E_a/k_B T) \quad (1)$$

where E_a denotes the activation energy of defects, τ_0 is the decay constant at 0 K, and k_B is the Boltzmann constant. Consequently, PBTS can induce simultaneous trapping of electrons in two or more defects, with an increase in stress time leading to an increase in the decay constant. According to eq 1, as the PBTS application time increases, the decay constant increases while the activation energy of the defect also increases. In particular, at higher hydrogen concentrations, the decay constant increases less.

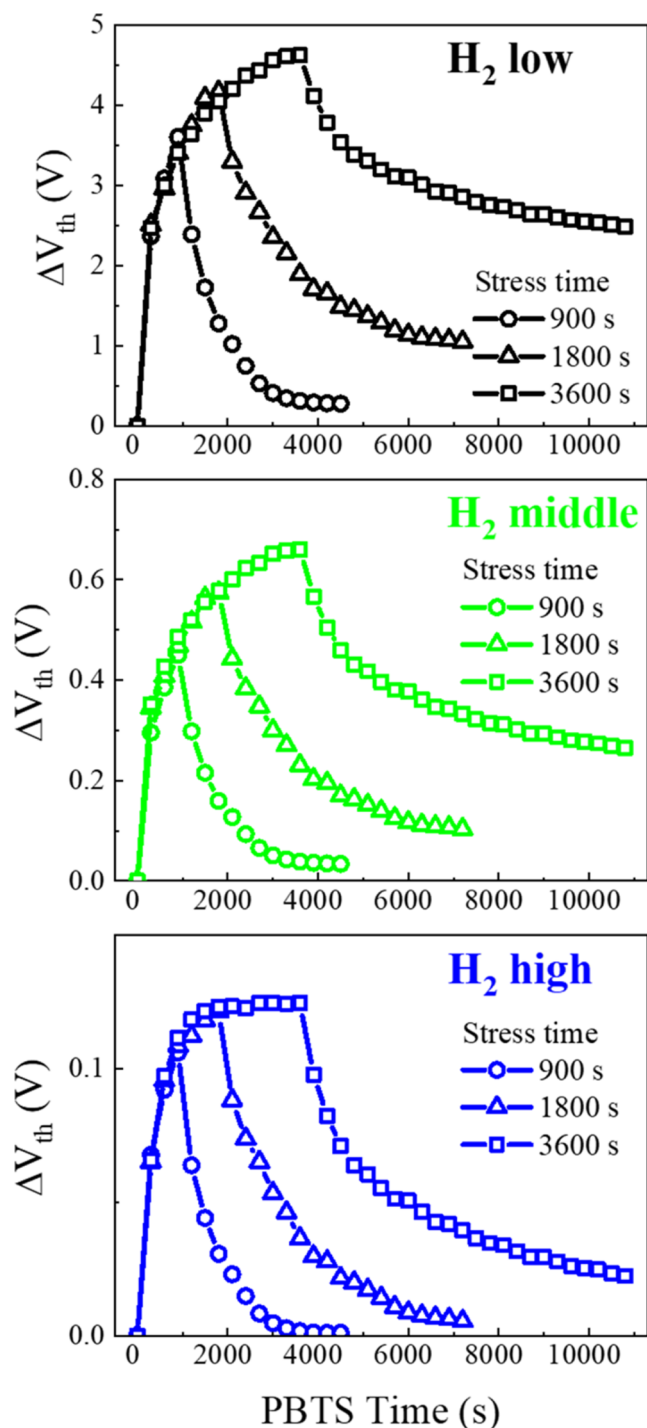


Figure 4. Time-dependent ΔV_{th} of the a-IGZTO TFTs as a function of the hydrogen concentration under various stress/recovery time pairs.

Figure 5 shows the density of states (DOS) and energy levels in the a-IGZTO under different charge states of (+1, 0,

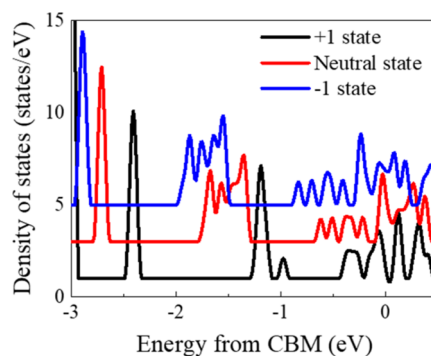


Figure 5. Density of states (DOS) of the a-IGZTO under different charge states (+1, 0, −1) calculated using DFT.

−1). Before applying PBTS, defect states primarily exist in neutral (+0) or positively charged states due to oxygen vacancies (V_O^+). Under PBTS, electrons can become trapped in these defect states, thereby transitioning them to negatively charged states. When PBTS is applied, defect states capture electrons, transitioning from neutral or positively charged states to negatively charged states. This transition leads to an increase in the energy and density of the deep-level defects. Consequently, negatively charged states exhibit higher state densities farther from the conduction band maximum (CBM). As the PBTS application time increases, the number of defects transitioning to negatively charged states increases, resulting in a further increase in both the energy and density of these deep-level defects. These results indicate that PBTS increases both the energy and density of deep-level defects, contributing to device instability. This figure demonstrates the dynamic changes in defect characteristics under different electronic conditions, emphasizing the role of electron trapping and release in the IGZTO.

Figure 6 shows the results of quantitative measurements of defects in the a-IGZTO TFTs as a function of hydrogen concentration under PBTS. After applying PBTS for (900, 1800, and 3600) s, the defects were measured using PICTS. PICTS analyzes changes in photocurrent by the trapping and detrapping of electrons in defects using light. Electrons trapped by light and those trapped by PBTS are both detrapped by thermal energy. Therefore, the decay constants of electrons trapped in the same defect are consistent in both methods. Table S1 of the Supporting Information (SI) presents the analyzed activation energy (E_a) and defect density (N_t) through PICTS. A total of six defects were identified, labeled #1 to #6. Defects were categorized into shallow-level defects and deep-level defects based on their energy levels according to the Fermi–Dirac distribution. Shallow-level defects have energies within 0.25 eV, allowing trapped electrons to be easily ionized at RT, and act as carriers through a hopping

Table 1. Decay Constants of Recovery Curves under PBTS Stress as a Function of the Hydrogen Concentration

	H ₂ low		H ₂ middle		H ₂ high	
	τ_1 (s)	τ_2 (s)	τ_1 (s)	τ_2 (s)	τ_1 (s)	τ_2 (s)
PBTS 900s	27.28	804.49	22.98	741.90	19.40	718.68
PBTS 1800s	45.96	1,024.16	29.64	944.99	27.65	878.65
PBTS 3600s	51.77	1,415.12	43.34	1,248.98	38.98	1,087.84

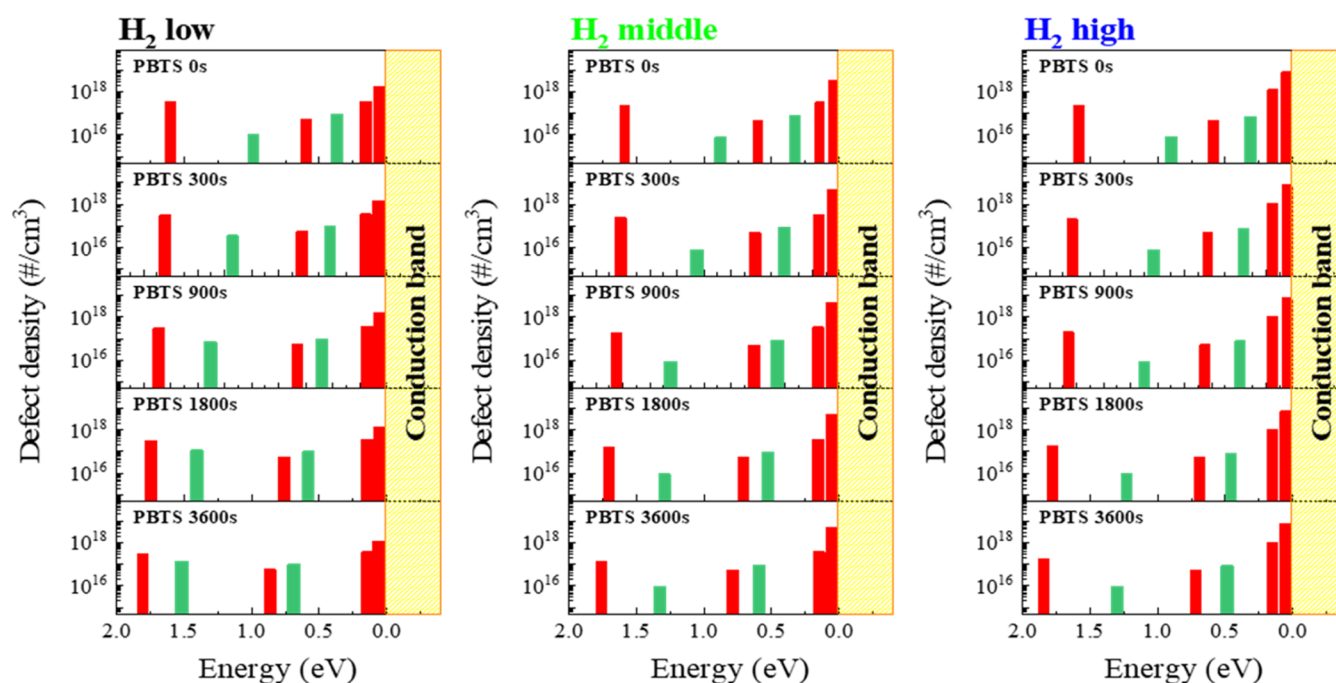


Figure 6. Time evolution of activation energy and defect density under PBTS as a function of hydrogen concentration, measured using PICTS.

process. Defects above 0.25 eV are deep-level defects, which do not naturally emit in all temperature ranges and can act as trapping sites, increasing carrier scattering.^{21,22} Importantly, the decay constant of electrons trapped by PBTS is consistent with that of electrons trapped by light, highlighting the similarity in trapping mechanisms under these conditions. For defects with the same decay constant as recovery, as the stress time increased, the E_a increased for defects #3 and #5. Among these, the N_t of defect #5 significantly increased, indicating a strong response to PBTS. In contrast, for defects #1 and #2, as the stress time increased, the E_a showed no change, whereas the N_t decreased. For defects #4 and #6, as the stress time increased, the E_a increased, while the N_t remained constant at a negligible level. These results underscore the dynamic evolution of defect states under PBTS, with specific defects exhibiting significant changes in energy and density over time.

Figure S1(a) of the SI shows a large number of electrons gathered near the gate dielectric due to energy band bending under positive gate bias. Some of these electrons were trapped in the channel trap or moved into the dielectric and became trapped in the dielectric trap. Figure S1(b) of the SI shows that electrons combine with shallow-level defects, such as oxygen vacancies (V_O) and are converted into deep-level defects ($V_O^+(V_O^{2+}) + e^- \rightarrow V_O$ (neutral)).^{23,24} Electrons also bind with oxygen interstitials (O_i) to form deep-level defects: $O_i + 2e^- \rightarrow O_i^{2-}$.^{25,26} Consequently, the density of shallow-level defects decreases, while the density of deep-level defects increases. In this process, the flow of electrons was limited, making it difficult for electrons to move and increasing the activation energy of defects. As the activation energy increased, the flow of electrons trapped in defects became more restricted, and the density of deep-level defects continued to increase. On the other hand, shallow-level defects did not significantly affect the electron movement path. Therefore, they did not significantly change the activation energy. These results show that defect #5 is highly sensitive to PBTS and that

large changes in defect density with increasing activation energy can affect the device properties.

As the hydrogen concentration increased, the changes in the E_a and N_t values under PBTS were small. Since the only difference between the three devices was hydrogen concentration, the change in defects according to stress application time was related to the hydrogen concentration in the channel. Previous studies have shown that when the Fermi energy level is close to the conduction band maximum (CBM), hydrogen can become an electron capture center in oxide semiconductors, such as $H_i^+(H_o^+) + 2e^- \rightarrow H_i^-$.²⁷ Therefore, in the a-IGZTO, H_i^+ and H_o^+ can transition to H_i^- and H_o^- by electron trapping. Hydrogen diffused from the gate insulator to the active layer can play three roles in a TFT. Initially, hydrogen can combine with oxygen to act as a shallow-level defect and generate free carriers. Under PBTS conditions, hydrogen can serve as a trap site for electrons, leading to the creation of deep-level defects. However, the passivation of electron trapping sites such as V_O and O_i can enhance stability. Therefore, hydrogen can act in different roles: (1) forming deep-level defects; and (2) reducing defect generation, the ratio of which affects the stability of the device. According to the quantitative defect measurement results, the E_a of deep-level defects increased by hydrogen was 1 eV (defect #5).

Figure 7 shows the correlation between stress time and normalized changes in N_t of defect #5 and V_{th} as a function of hydrogen concentration. The N_t for each stress time was normalized based on the N_t of defect #5 at stress 0 s. Significant alignment was observed when expressed as normalized changes in N_t and V_{th} with the stress time. Consequently, changes in V_{th} with respect to PBTS application time could be interpreted as closely linked to defect #5.

4. CONCLUSIONS

The electrical properties and defects of a-IGZTO TFTs under PBTS were investigated as a function of hydrogen concentration. Increasing the hydrogen concentration improved

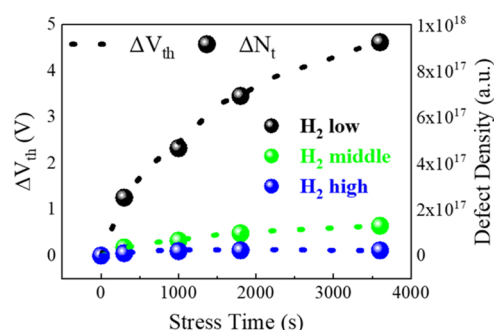


Figure 7. Correlation of ΔV_{th} and defect density in the a-IGZTO TFTs as a function of the hydrogen concentration.

device characteristics, such as field-effect mobility and subthreshold swing (SS), enhancing stability. Under PBTS, ΔV_{th} decreased with higher hydrogen concentration, showing improved stability with values of (4.62, 0.45, and 0.11) V, respectively. DFT calculations revealed that charge states influence defect densities and energy levels in the a-IGZTO (+1, 0, −1). Under PBTS, positively charged defects transition to negatively charged states, increasing the energy and density of deep-level defects. Quantitative measurements showed a decrease in shallow-level defect density and an increase in deep-level defect density. Higher hydrogen concentrations resulted in a smaller increase in the number of deep-level defects. Hydrogen modulates the stability and performance of the a-IGZTO TFTs under PBTS by passivating electron trap sites and reducing defect generation.

■ ASSOCIATED CONTENT

Data Availability Statement

The data sets that support the findings of this study are available from the corresponding author upon reasonable request.

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acsaelm.4c01430>.

Activation energy and defect density as a function of hydrogen concentration, energy band bending diagrams, and electrical response of oxygen-related defects (PDF)

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Author Contributions

H.H. and M.K. contributed equally as co-first authors. The manuscript was written through contributions of all authors. All authors have given approval to the final version of the manuscript.

Notes

The authors declare no competing financial interest.

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