The electron trap parameter extraction-based investigation of the relationship between charge trapping and activation energy in IGZO TFTs under positive bias temperature stress

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ABSTRACT

Experimental extraction of the electron trap parameters which are associated with charge trapping into gate insulators under the positive bias temperature stress (PBTS) is proposed and demonstrated for the first time in amorphous indium-gallium-zinc-oxide thin-film transistors. This was done by combining the PBTS/recovery time-evolution of the experimentally decomposed threshold voltage shift (ΔVT) and the technology computer-aided design (TCAD)-based charge trapping simulation. The extracted parameters were the trap density (NOT) = 2.6 × 10^{18} cm^{-3}, the trap energy level (ΔET) = 0.6 eV, and the capture cross section (σ0) = 3 × 10^{-19} cm^{2}.

Furthermore, based on the established TCAD framework, the relationship between the electron trap parameters and the activation energy (Ea) is comprehensively investigated. It is found that Ea increases with an increase in σ0, whereas Ea is independent of NOT. In addition, as ΔET increases, Ea decreases in the electron trapping-dominant regime (low ΔET) and increases again in the Poole–Frenkel (PF) emission/hopping-dominant regime (high ΔET). Moreover, our results suggest that the cross-over ΔET point originates from the complicated temperature-dependent competition between the capture rate and the emission rate. The PBTS bias dependence of the relationship between Ea and ΔET suggests that the electric field dependence of the PF emission-based electron hopping is stronger than that of the thermionic field emission-based electron trapping.

1. Introduction

Amorphous indium-gallium-zinc-oxide (a-IGZO) thin-film transistors (TFTs) were successfully employed in the backplane for large-screen organic light-emitting diode (OLED) displays and liquid-crystal displays (LCDs) [1,2]. These transistors were used because of their beneficial properties such as good uniformity over large areas, low processing temperatures, low-cost fabrication, compatibility with flexible substrates, and fair mobility [3,4]. Recently, the a-IGZO TFTs have been used in flexible processors, programmable units, and sensor-embedded wearable circuitry for wearable healthcare and the Internet-of-things era [5–7]. However, reliability issues, as technological challenges for more successful mass production and commercialization of IGZO TFTs, still remain.

Among the reliability issues, positive bias temperature stress (PBTS)-induced instability is very important because the PBTS corresponds to the ON condition of n-channel IGZO TFTs. Actually, current-driving TFTs in an OLED pixel and TFTs in the gate-driver circuitry are often under the influence of PBTS. Very recently, the PBTS instability of IGZO TFT was experimentally decomposed into the defect creation in the active layer and electron-charge trapping in the gate insulator (GI) [8]. Here it is worthwhile to note that the latter depends on the GI quality that varies significantly corresponding to the process or according to the GI material chosen for the fabrication, whereas the former is somewhat entangled with intrinsically IGZO material issues and thus frequently analyzed in ab initio studies [9–11]. Nevertheless, compared with the defect creation in active layers, the PBTS-induced electron trapping in IGZO TFTs has been less investigated quantitatively despite its importance for wearable circuits.

In particular, the detailed procedure of extracting the physical parameters for GI electron trap, such as spatial density, capture cross section, charge emission rate, and energy level, from the measured stress time-evolution of threshold voltage (VT) has been rarely investigated in IGZO TFTs in spite of its practical importance. Even in an
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2. Device fabrication and characterization

The a-IGZO TFTs with the inverted staggered bottom-gate top-etch stopper (ES) structure were fabricated on a glass substrate as shown in Fig. 1(a). The detailed process is as follows. A molybdenum was de-

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VT into respective instability mechanisms was proposed very recently [8].

In this paper, experimental extraction of the GI electron trap para-

eters which are only associated with charge trapping into GI under

PBTS is proposed and its detailed procedure is demonstrated for the

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parameters and the TCAD simulation reproduced the measured PBTS time-

data when the extraction of GI trap parameter is performed. However, this

approach has been rarely demonstrated because the experimental

technique for decomposing the PBTS ΔVT into respective instability

mechanisms was proposed very recently [8].

2. Device fabrication and characterization

The a-IGZO TFTs with the inverted staggered bottom-gate top-etch stopper (ES) structure were fabricated on a glass substrate as shown in Fig. 1(a). The detailed process is as follows. A molybdenum was de-

positioned on the glass substrate using an rf sputtering process, and it was patterned by dry etching. Then, the GI made up of a 100-nm-thick SiO2 layer was deposited by plasma-enhanced chemical-vapor-deposition (PECVD). The 50-nm-thick a-IGZO thin-film was DC sputter-deposited under 3 kW at room temperature in a gas mixture of Ar/O2 = 35/63 at sccm; here, the atomic ratio was In:Ga:Zn = 2:2:1. The active layer was then patterned by wet etching with diluted HF solution. Subsequently, the 100-nm-thick SiO2 was formed as the ES layer by PECVD and dry etch patterning. Molybdenum was then DC sputter-deposited and patterned by dry etching as the source/drain (S/D) electrodes. Subse-

quently, the 100-nm-thick SiO2 was PECVD-deposited as a passivation layer. Lastly, the post-annealing process was performed at 250 °C for one hour.

Geometrical parameters are as follows. The oxide thickness of GI (TGI) was 100 nm, the active layer thickness (TIGZO) was 50 nm, the channel length (L) was 50 μm, the gate-to-S/D overlap length (LOV) was 15 μm, and the channel width (W) was 25 μm.

The VT was taken from the measured I-V characteristics, which were characterized using the HP4156 semiconductor parameter analyzer. VT was measured during PBTS for 104 s and during the recovery period for additional 2 × 104 s. Here, the PBTS condition was the gate-to-source voltage (VGS) = 30 V and the drain-to-source voltage (VDG) = 0 V; the recovery condition was VGS = VDS = 0 V, when the temperature was varied from 300 to 373 K. Among the physical mechanisms of the PBTS-induced ΔVT, the contribution factor only due to the electron trapping into GI was experimentally decomposed using the method in [8]; this de-embedded ΔVT factor is shown as triangles in Fig. 2(a) and (b). Details of de-embedding ΔVT is given in [8].

3. Parameter extraction

The cross section and the energy band at a flat band voltage (VFB = VSAT) condition of the bottom-gate a-IGZO TFT are illustrated in Fig. 1(b) and (c). The physical parameters of GI electron trap can be summarized as its spatial density NOT [cm−2], capture cross section σ0 [cm2], and energy level ET [eV], respectively. As shown in Fig. 1(c), the energy level ET of electron trap is defined by ΔET [eV] which means the separation above the IGZO conduction band minimum (EC,IGZO). For simplicity, we assume that the electron trap in GI is located in a single energy level, i.e., ΔE above EC,IGZO.

In order to establish the procedure of extracting all of NOT, σ0, and ΔET from the experimentally de-embedded ΔVT, first of all, the framework of TCAD simulation was set up by using the Atlas-2D of Silvaco [15]. The Fowler-Nordheim tunneling, band-to-band tunneling, trap-assisted tunneling, and the Poole-Frenkel (PF) emission were incorporated into TCAD simulation. Here, it should be noted that all of NOT, σ0, and ΔET are TCAD-compatible parameters.

Given the stress bias (VSTR) applied to VGS and the temperature (T), the PBTS/recovery time-evolution of the de-embedded ΔVT is shown by triangles in Fig. 2(a) and (b). Here, we define the ΔVT,rec and ΔTSAT,rec as the fast recoverable ΔVT factor during recovery period and as the time when |dΔVT/dt| becomes lower than 10 μV/s, as schematically illustrated in Fig. 3(a). Then, ΔVT,rec and ΔTSAT,rec will be distinct functions of NOT, σ0, and ΔET as well as of VSTR and T. If a clear pattern exists in these functional relationships, we would be able to use those patterns in extracting parameters, such as NOT, σ0, and ΔET because ΔVT,rec and ΔTSAT,rec can be characterized experimentally under given VSTR and T conditions.

In order to find out the pattern between the trap parameters, such as

![Fig. 1. (a) Bottom-gate IGZO TFT structure. (b) Schematic cross section of bottom-gate a-IGZO TFTs. (c) Energy band structure of IGZO TFTs at the interface of active layer and gate insulator under the flat band condition.](image-url)
of the TCAD simulation was performed with varying \( T = 300, 333, \) and \( 373 \) K. From our simulation results, interestingly, three patterns were clearly observed in terms of the normalized \( t_{\text{sat,rec}}(T) \), e.g., \( t_{\text{sat,rec}}(T)/t_{\text{sat,rec}}(T = 373 \text{ K}) \); (1) the normalized \( t_{\text{sat,rec}}(T) \) is independent of \( N_{OT} \) (Fig. 4(a)), (2) it is also independent of \( \sigma_0 \) (Fig. 4(b)), and (3) it is linearly proportional to \( \Delta E_T \) and its slope increases as \( T \) increases (Fig. 4(c)). Therefore, the GI trap parameters can be extracted by comparing the experimentally characterized parameters, such as the \( t_{\text{sat,rec}}(T) \) normalized at \( 373 \text{ K}, t_{\text{sat,rec}} \) itself, and \( \Delta V_{T,\text{rec}} \), with the simulated ones at various temperatures.

Fig. 3(b) explains the procedure of parameter extraction. Details are as follows. First of all, the fundamental input parameters including the effective density-of-states (\( N_C \) and \( N_V \)), band mobility (\( \mu_{\text{band}} \)), and doping concentration (\( N_{SD} \)) are adopted with the PF emission rate factor (PF.B) which will be shown later in Eq. (3). In this step, \( N_C, N_V, \mu_{\text{band}}, \) and \( N_{SD} \) were chosen to be \( 5 \times 10^{18} \) [cm\(^{-3}\)], \( 5 \times 10^{18} \) [cm\(^{-3}\)], 10 [cm\(^2\)/V·s], and 2.3 \times 10^{17} \) [cm\(^{-3}\)], respectively. Then, the GI trap parameters are extracted in the order of \( \Delta E_T, \sigma_0, \) and \( N_{OT} \) as a unique set of parameters, whose values are adjusted by numerical iterations until all of simulated normalized \( t_{\text{sat,rec}}(T) \), \( t_{\text{sat,rec}}(T) \), and \( \Delta V_{T,\text{rec}}(t) \) agree well with the measured ones in all PBTS temperatures under the conditions of specific error factor, significant digit, and proper range. When this agreement is accomplished with the proposed parameter-extraction procedure, all parameters (\( \Delta E_T, \sigma_0, N_{OT}, \) and PF.B) can be extracted as a unique solution.

Finally extracted parameters were \( \text{PF.B} = 1 \times 10^{12} \text{ s}^{-1} \), \( N_{OT} = 2.6 \times 10^{18} \) [cm\(^{-3}\)], \( \Delta E_T = 0.6 \) eV, and \( \sigma_0 = 3 \times 10^{-19} \) cm\(^2\). The line in Fig. 2(a) and the circle in Fig. 2(b) show our TCAD simulation results where our extracted parameters are used, which suggests that this parameter-based simulation reproduces the measured PBTS time-evolution of \( \Delta V_T \) very well over a wide range of temperatures. Undoubtedly, Fig. 2(a) and (b) verify that our TCAD framework is well-calibrated and the values of extracted parameters are very reasonable.

### 4. Results and discussion

The bias-temperature-stress (BTS) time-evolution of the TFT \( \Delta V_T \) is commonly modeled by the stretched-exponential function (SEF) as

\[
\Delta V_T(T) = \Delta V_{T,\text{rec}}(T) + \Delta V_{T,\text{sat}}(T) + \Delta V_{T,\text{dep}}(T)
\]
follows \([16,17]\):

\[
\Delta V_T = \Delta V_{\text{iso}} \times \left[ 1 - \exp \left( -\frac{t}{\tau} \right)^\beta \right]
\]  

(1)

where \(\Delta V_{\text{iso}}\) is the \(\Delta V_T\) at infinite time, \(\tau\) is the characteristic time constant, and \(\beta\) is the stretching exponent with a value smaller than 1. The SEF for BTS/recovery has its own set of parameters, such as \(\Delta V_{\text{iso}}\), \(\tau\), and \(\beta\), whose values are dependent on the BTS temperature \(T\).

Consistently, in our case, the line in Fig. 2(b) shows that the PBTS time-evolution of \(\Delta V_T\) is well fitted with SEF model (except the recovery time) for both the experimentally de-embedded \(\Delta V_T\) (triangle) and the simulated one (circle). Our PBTS temperature-dependent SEF parameters are shown in Fig. 2(c), where the stress time can be much longer than the experimental test because the data are taken from TCAD simulation.

The activation energy \(E_a\) for BTS instability can be commonly acquired from the temperature dependence of the SEF parameter \(\tau\) using the formula of 
\[
\tau = \tau_0 \times \exp \left( \frac{E_a}{kT} \right)
\]

where \(\tau_0\) is the pre-exponential factor, \(E_a\) is the activation energy, \(k\) is Boltzmann's constant, and \(T\) is the temperature. Due to the variability of physical parameters, the activation energy \(E_a\) for BTS instability is usually applied to a range of materials and devices. In our case, we use the simple form above to calculate the activation energy for BTS instability, which is different from the traditional form of activation energy.

Finally, the PBTS voltage \(V_{\text{STR}}\) dependence is shown in Fig. 7(a). The \(V_{\text{STR}}\) then decreases slightly because the decreased \(c_n\) causes a reduction in the temperature dependence of electron trapping.

In contrast, in the PF emission/hopping dominant regime, the \(e_n\) increases very abruptly with an increase in \(\Delta E_T\) because the energy distance between the \(E_T\) and the \(E_{\text{CIGZO}}\) increases as shown in Fig. 6(b), and the electron trapping becomes more difficult \([18]\). The \(E_a\) then decreases slightly because the decreased \(c_n\) causes a reduction in the temperature dependence of electron trapping.

In our well-calibrated TCAD simulation framework, the relationship between the GI electron trap parameters and the \(E_a\) of electron trapping in IGZO TFTs under PBTS was investigated more in detail, which is practically very important use of our parameter-extraction technique. As shown in Fig. 5(a) and (b), \(E_a\) increases with an increase of \(\sigma_0\), whereas \(E_a\) is independent of \(N_{\text{OT}}\). The \(N_{\text{OT}}\) increases only the absolute amount of electron trapping \([12]\), but does not affect \(\tau\), so there is no \(N_{\text{OT}}\) dependence of \(E_a\). The \(\sigma_0\)-dependent \(E_a\) increase occurs because when electron trapping is activated by \(\sigma_0\), the temperature dependence of \(\tau\) becomes more prominent \([18–20]\). However, the \(\Delta E_T\) dependence of \(E_a\) suggests that there are two regimes different from each other; this is shown in Fig. 5(c). The former regime is the thermal field emission-based electron trapping dominant regime, whereas the latter is the PF emission/hopping dominant regime. The two mechanisms are explained associated with the capture rate \(c_n\) \([18–21]\) and emission rate \(e_n\) \([22,23]\) as shown in Fig. 6. We express the \(c_n\) considering tunneling probability \((f_T) [24,25]\) and \(e_n\) as:

\[
c_n = \nu_0 \nu_f N_{\text{OT}} (1 - f_T) N_N \tau \times W L L_{\text{lin}}
\]

(2)

\[
e_n = PF \times \exp \left( \frac{(3.75 - \Delta E_T) - q \sqrt{\Phi / \nu_f}}{kT} \right)
\]

\[
e_n \approx PF \times \exp \left( \frac{(3.75 - \Delta E_T) - q \sqrt{V_{\text{STR}} / \nu_f}}{kT} \right)
\]

(3)

where \(\nu_0\) is the thermal velocity of electrons (units: \(\text{cm/s}\)), \(f_T\) is Fermi-Dirac distribution function in the GI trap, \(N_N\) is channel electron density considering PBTS condition (units: \(\text{cm}^{-3}\)), \(\tau\) is channel thickness, \(q\) is the elementary charge of an electron, \(F\) is electric field in GI, and \(v\) is the
the temperature dependence of $c_n$ increases (see Fig. 7(b)). In addition, the critical $\Delta E_T$ decreases with the increase of $V_{STR}$ (see Fig. 7(c)) because the balance between $c_n$ and $e_n$ is obtained at a deeper $E_T$ level from $E_{CT}$ as the $V_{STR}$ increases. This provides a very important quantitative insight that the electric field dependence of the PF emission-based electron hopping is stronger than that of the thermionic field emission-based electron trapping.

5. Conclusion

Experimental extraction of the GI electron trap parameters which are only associated with charge trapping into GI under PBTS is proposed and its detailed procedure is demonstrated for the first time in a-IGZO TFTs. Our extraction technique is established by combining the

PBTS/recovery time-evolution of the experimentally decomposed threshold voltage shift ($\Delta V_T$) and the technology computer-aided design (TCAD)-based charge trapping simulation. Our parameters and TCAD simulation reproduced the measured PBTS time-evolution of $\Delta V_T$ very well over a wide range of temperatures. Furthermore, we found that $E_a$ increases when $\sigma_0$ increases, whereas $E_a$ is independent of $N_{CT}$ by comprehensively investigating the relationship between the GI trap parameters and the $E_a$ value. It was also found that the cross-over $\Delta E_T$ point originates from the complicated T-dependent competition between $c_n$ and $e_n$. The $V_{STR}$ dependence of the relationship between $E_a$ and $\Delta E_T$ proved that the electric field dependence of the PF emission-based electron hopping is stronger than that of the thermionic field emission-based electron trapping.

Our results are potentially useful for the quantitative analysis and
joint-optimization of the GI and the IGZO film for the TFT process integration in wearable healthcare monitoring systems and in display backplanes.

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