Simulation and modeling of off-leakage current in InGaZnO thin-film transistors

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Abstract. We investigate the mechanism of off-leakage current in InGaZnO (IGZO) thin-film transistors with the help of a two-dimensional device simulator. The deep donorlike states probably originating from the oxygen vacancies are introduced in the IGZO channel, and it is shown that these trap states significantly affect the characteristics in the off-state region through the pinning of the channel potential. A simple analytical model to explain the simulation results is proposed, which suggests that the off-leak characteristics is controlled by the amount and the depth of the deep donorlike states as well as the thicknesses of IGZO and SiO2 layers in TFT.

Keywords: InGaZnO, thin film transistor, device simulation, leakage current

1. Introduction

In recent years, InGaZnO (IGZO) has attracted much attention as a promising channel material for thin film transistors (TFTs) [1] used in, e.g., mobile device applications [2] and new memories [3]. One of the prominent characteristics of IGZO TFTs is ultra-low off-state leakage current owing to its wide band gap nature (\(E_G = 3.05\) eV [4]), and it has been reported that measured leakage currents are actually very low (< \(10^{-20}\) A/\(\mu m\)) [3, 5, 6, 7]. However, their conduction mechanisms have not been fully understood yet. Shi et al. [8] performed the device simulation to investigate the effect of the deep donorlike states originated from oxygen vacancies on the \(a\)-IGZO performance. Moreover, Jeong et al. [9] also simulated the off-leakage characteristics and suggested that it sensitively depends on the active layer thickness due to Fermi-level pinning caused by the deep donorlike states. Although these previous studies have pointed out the significant influence of the deep donorlike states on the off-leakage current, its effect on the off-state \(I_d - V_g\) characteristics were not intensively investigated. In this study, we present an in-depth simulations to understand the behavior of off-state current as a function of the gate voltage [10], and discuss the essential mechanisms with the help of a two-dimensional device simulator.
2. Simulation Method

Figure 1 shows the cross-sectional view of the TFT structure simulated in this study. The structure consists of an a-IGZO active layer with a thickness of \( t_{\text{IGZO}} = 50 \) nm and an SiO\(_2\) gate insulator layer with a thickness of \( t_{\text{ox}} = 300 \) nm. The channel length \( L \) and width \( W \) are 10 \( \mu \)m and 8 \( \mu \)m, respectively. This structure mimics the device used in [3], in which more detailed information about the structure and the fabrication process is described. A two-dimensional device simulator ATLAS [11] was used to simulate the electrical characteristics of this device, and the material parameters for a-IGZO were taken from [4]. Contacts between source/drain electrodes and the a-IGZO layer were described by the Schottky model with a metal work function of \( \Phi_{m,\text{sd}} = 4.33 \) eV and the electron affinity of 4.16 eV for a-IGZO [4]. In order to fit the \( I_d - V_g \) characteristics for \( V_g > 0 \) V to the measured data [6], we have adjusted the metal gate work function (\( \Phi_{m,g} = 4.73 \) eV) as well as the density-of-states (DOS) of the acceptorlike band tail states in the a-IGZO layer:

\[
g_{\text{ta}}(E) = N_{\text{ta}} \exp \left( \frac{E - E_G}{W_{\text{ta}}} \right), \tag{1}
\]

where \( E \) is the electron energy measured from the valence band top \( E_V \), \( W_{\text{ta}} \) the characteristic slope, and \( N_{\text{ta}} \) the DOS at the bottom of the conduction band. Furthermore, we have also taken into account the Gaussian-distributed donorlike states to model the deep traps originated from, e.g., oxygen vacancies [8]:

\[
g_{\text{gd}}(E) = N_{\text{gd}} \exp \left[ - \left( \frac{E - E_{\text{gd}}}{W_{\text{gd}}} \right)^2 \right], \tag{2}
\]
where $N_{gd}$, $E_{gd}$, and $W_{gd}$ are the peak density, the mean energy (measured from $E_V$), and the standard deviation of the states, respectively. It has been pointed out that the deep donorlike states affect the off-state leakage current in TFTs [8, 9], which is the main interest of this work.

In order to investigate the off-state leakage current, the generation-recombination mechanisms associated with band-to-band (BBT) and trap assisted tunneling (TAT) processes were taken into account. In this study, the generation rate due to BBT was expressed as a function of the local electric field $F$ assuming Kane’s model [12] as

$$ G_{bbt}(F) = q^2 F^2 m_r^2 \frac{\exp \left( - \frac{m_r^2}{2 \hbar^2 E_G} \right)}{18 \pi \hbar^2 E_G^2}, $$

where $m_r$ is the tunnel mass assumed to be the same value as the conduction band effective mass ($0.34m_0$ [13]), $m_0$ is the free electron mass, $q$ the elementary charge, $\hbar$ the Planck constant. To consider the effect of defect states, Shockley-Read-Hall recombination/generation was taken into account, where the carrier capture cross-sections for the defect states were assumed to be $10^{-15}$ cm$^2$ regardless of the trap types. In addition, TAT mechanism based on [14] was also incorporated into the recombination/generation rate, although its effect was not significant.

Regarding the numerical techniques, we assumed that the trap DOS was distributed continuously in the band gap, and the integral equations for the charge and recombination were evaluated using a numerical integral scheme. Furthermore, all the computations were done in extended precision mode of 256 bit [11], which is essential to accurately evaluate the ultra-low leakage current in wide bandgap materials.

3. Results and Discussion

3.1. Effect of donorlike states

Figure 2 shows the simulated transfer characteristics for $V_d = 5$ V at 300 K. The experimental data are also plotted for comparison, showing that good agreement was obtained in the positive $V_g$ region. On the other hand, in the off-state conditions, the simulation results are many orders of magnitude less than the measured currents. Without BBT mechanism, the current conduction is considered to be carried by the thermal electrons surmounting the barrier energy comparable to $E_G$, and their population is indeed very low, estimated from the Boltzmann factor at room temperature; $\exp(-E_G/k_BT) \sim 10^{-51}$. Even if the effects of BBT and the acceptorlike tail states ($N_{ta} = 10^{18}$ cm$^{-3}$, $W_{ta} = 80$ meV) were incorporated, the magnitude of the simulated current was still much lower than the measured data. Here, it should be noted that the experimental data [6] does not necessarily indicate the intrinsic leakage currents through the a-IGZO active layer, but the parasitic components would be involved. On the other hand, the others have subtracted the parasitic component by comparing the data for different channel widths [7], and reported the off-leakage current of 380 yA/μm at 85°C in the c-axis aligned crystal-IGZO transistor [5]. Although they expected off-state
Figure 2: $I_d - V_g$ characteristics of a-IGZO TFT at $V_d = 5$ V per unit channel width. The simulation results (lines) are compared with the experimental data (dots) [6].

current at room temperature is $\sim 1$ yA/µm, it is still much higher than our simulation results shown in Fig. 2.

One of the possible origin to enhance the off leakage current is the Fermi level pinning due to the deep donorlike states [8, 9]. When the negative gate voltage is applied, the donorlike states become positively charged by emitting an electron. Then, the rise of the channel potential would be suppressed due to electric field termination by the positive charges. This mechanism could explain why the observed drain leakage current is many orders of magnitude larger than the expected level as shown in Fig. 2, considering that the subthreshold leakage current is exponentially dependent on the channel potential [15]. In this study, we intensively investigated this scenario with the aid of the device simulator.

Figure 3 shows the simulation results calculated with DOS of donorlike states as well as the acceptorlike states included in Fig. 2. To investigate the effect of the trap depth, a narrow distribution with $W_{gd} = 0.1$ eV was assumed, and $E_{gd}$ was varied from 1 eV to 2.2 eV. The simulation results indicate that the off-state $I_d - V_g$ characteristics are significantly affected by the deep donorlike states. For example, looking at the case of $E_{gd} = 2.1$ eV, the current once exhibits plateau behavior with decreasing $V_g$, and then abruptly drops at $V_g \sim -13$ V, followed by the regrowth at $V_g \sim -23$ V. The behavior after the plateau is similar to that for $N_{gd} = 0$, except for the voltage shift of $\Delta V \sim 12$ V. In Fig. 3, the experimental data are also plotted, and it can be confirmed that the measured leakage level is reproduced with $E_{gd}$ around 2.1 – 2.2 eV, although, as mentioned above, we consider it indicates an upper limit of the current.

We have also investigated the effect of $N_{gd}$ as shown in Fig. 4. Note that the width of the plateau region, i.e., $\Delta V$, is dependent on $N_{gd}$. Figure 5 shows $\Delta V$ extracted from the shift of
Figure 3: Effect of donorlike states with various $E_{gd}$ on the off-leakage current. (a) DOS of defect states assumed in the simulation. (b) Simulated $I_d - V_g$ characteristics at $V_d = 5$ V plotted together with the experimental data (open circles).

Figure 4: Effect of donorlike states with various $N_{gd}$ on the off-leakage current. (a) DOS of defect states assumed in the simulation. (b) Simulated $I_d - V_g$ characteristics at $V_d = 5$ V plotted together with the experimental data (open circles). An arrow indicates $\Delta V$ for $N_{gd} = 0.5 \times 10^{18}$ cm$^{-3}$. 

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$V_g$ at the same $I_d (= 10^{-26} \text{ A/}\mu\text{m})$ indicating the linear dependence of $\Delta V$ on $N_{gd}$.

![Figure 5: $N_{gd}$ dependence of $\Delta V$ extracted from Fig. 4. The solid line represents the calculation result with the analytical form (shown later in Sec. 3.2.)](image)

**3.2. Discussion**

Finally, let us discuss the mechanisms responsible for the simulation results shown in Sec. 3.1. Figure 6 shows the conduction band edge ($E_C$) profiles in the active layer of the TFT simulated with various gate voltages. At $V_g = 0$ V, the potential distribution was almost flat in the channel region consistent with the the MOSFET behavior operating in subthreshold region [15]. However, when decreasing $V_g$ from $-2$ V to $-14$ V, a different behavior was observed due to the charging of the deep traps; when the donorlike state levels are raised above the quasi Fermi level, they are positively charged and significantly affect the potential distribution. Unlike the free carriers, these charges are immobile, and thus the potential gradient was induced along the channel direction. Moreover, as they terminate the electric field from the gate, the potential profile becomes insensitive to the change of $V_g$, which is also the case for the energy barrier against the source electrons. Consequently, the plateau behavior of the $I_D - V_g$ characteristics was caused as shown in Figs. 3 and 4. With further decreasing $V_g$, after all the donorlike states had been depleted (i.e., positively charged), then the channel potential was controlled by $V_g$ again. Finally, when large enough negative $V_g (< -16$ V) was applied, the $E_C$ was also pinned this time due to the accumulation of holes generated though the SRH and BBT mechanisms.

The width of the plateau is thus related to the total areal density of the deep-donor states. As shown in Fig. 6 (b), the potential variation along the vertical direction was less significant in the simulated structure. In this case, we can derive a simple analytical form to interpret the simulation results by approximately ignoring the the thickness of the $a$-IGZO layer. Considering the Gauss' law relating the gate oxide field and the positive charges of
Figure 6: Conduction band edge profiles in the a-IGZO active layer along (a) the horizontal direction (see, line A in Fig. 1) and (b) the vertical direction (line B in Fig. 1). Simulations were done with various $V_g$ varied from 0 V down to −18 V.

the unoccupied donor-like states, we obtain:

$$\Delta V = \frac{\sqrt{\pi} q W_{gd} N_{gd} t_{IGZO}}{C_{ox}},$$

where $C_{ox}(\equiv \epsilon_{ox}/t_{ox})$ is the gate oxide capacitance per unit area, and $\epsilon_{ox}$ is the dielectric constant of SiO$_2$. As shown in Fig. 5, the simulated results were well explained by the model. Eq. (4) also suggests that $\Delta V$ depends on the thicknesses of the IGZO and SiO$_2$ layers, which was confirmed in Fig. 7.

Based on the above consideration, the donor-like states are expected to be located in the band gap of a-IGZO at (or below) ~ 2.1 eV from the valence-band maximum with a concentration of > $5 \times 10^{18}$ cm$^{-3}$. At present, the origin of such states remains unclear, but let us speculate it finally. To date, there have been many experimental studies of the trap states in IGZO [16], but, to the best of our knowledge, the detection of such donor-like states has not been reported so much; e.g., the transient photoconductivity measurement, which is a special case of deep-level transient spectroscopy (DLTS), has suggested the existence of the activation states with an activation energies around ~ 1.1 eV [17]. On the other hand, theoretical studies base on the density functional theory (DFT) have pointed out that the oxygen vacancy $V_O$ in crystalline InGaO$_3$(ZnO)$_m$($m = 1$) exhibits a negative-$U$ behavior with a charge transition level $\epsilon(2+/0)$ located at ~ 1 eV below the conduction band minimum (i.e., ~ 2 eV above the valence band maximum) [18, 19]. As the Fermi level moves upward and crosses this level, the charge state transition occurs from the +2 to the neutral charge state. It is considered that the transition levels can be observed in experiments where the final charge state can fully relax to its equilibrium configuration after the transition, such as in DLTS, and these thermodynamic transition levels correspond to thermal ionization en-
ergies [20, 21]. We think that such properties of V$_O$ could be an origin of the donorlike states assumed in this study. However, one of the ambiguous point is that in amorphous there would be no definite state levels; DFT calculation has revealed that the V$_O$ transition levels are widely distributed depending on the local atomic configuration [22]. Further investigations, both experimental and theoretical, are thus necessarily to further understand the mechanism controlling the leakage current in IGZO TFTs.

4. Conclusions

The mechanism of the off-leakage current in a-IGZO TFTs has been investigated with the use of the device simulator. It has been demonstrated that in the off-state region the deep donorlike states significantly affect the leakage current; the positively charged donorlike states induce the pinning of the channel potential and create the plateau region in $I_d$ - $V_g$ characteristics. A simple analytical model to explain the simulated behavior has been proposed, which suggests that the control of the amount and depth of the deep donorlike states as well as the thicknesses of IGZO and SiO$_2$ layers in the device structure.

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