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## Localized Tail States and Electron Mobility in Amorphous ZnON Thin Film Transistors

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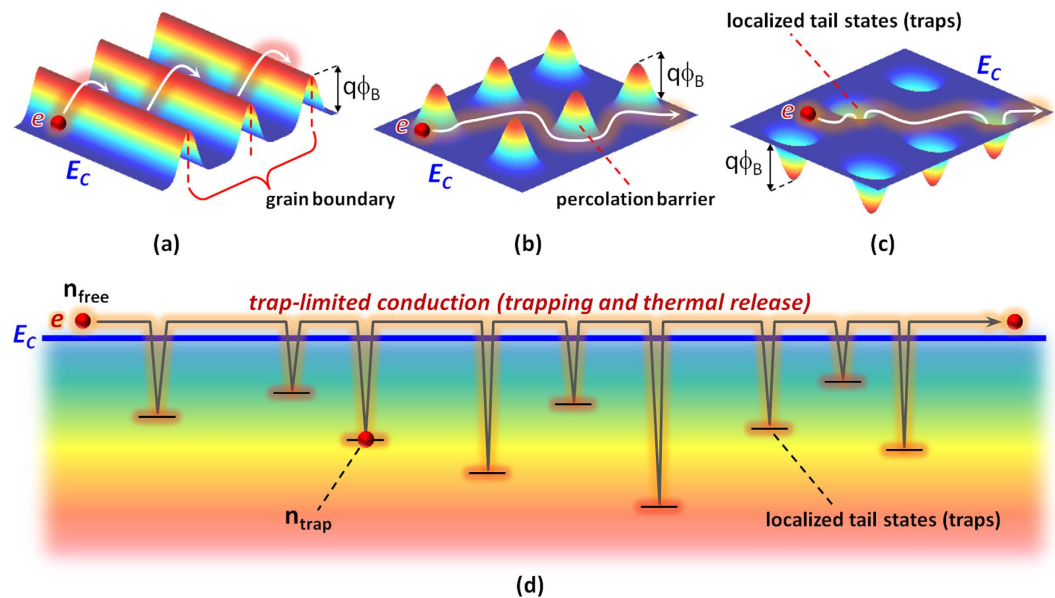
The density of localized tail states in amorphous ZnON (a-ZnON) thin film transistors (TFTs) is deduced from the measured current-voltage characteristics. The extracted values of tail state density at the conduction band minima ( $N_{tc}$ ) and its characteristic energy ( $kT_t$ ) are about  $2 \times 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$  and 29 meV, respectively, suggesting trap-limited conduction prevails at room temperature. Based on trap-limited conduction theory where these tail state parameters are considered, electron mobility is accurately retrieved using a self-consistent extraction method along with the scaling factor ' $1/(\alpha + 1)$ ' associated with trapping events at the localized tail states. Additionally, it is found that defects, e.g. oxygen and/or nitrogen vacancies, can be ionized under illumination with  $h\nu \gg E_g$ , leading to very mild persistent photoconductivity (PPC) in a-ZnON TFTs.

Oxide semiconductors shows great promise as a high mobility channel layer in thin film transistors (TFT) fabricated at low or even room temperatures<sup>1,2</sup>. A classical oxide material is ZnO, which has mostly a poly-crystalline (pc) structure, i.e. pc-ZnO, suggesting the presence of potential barriers at the grain boundaries, which lowers the mobility (see Fig. 1a)<sup>3,4</sup>. To suppress these potential barriers, metal cations, such as Ga and In, were incorporated into the binary system, thereby stabilizing the amorphous phase over the crystalline phase. But the addition of Ga and In introduces compositional disorder, and these cation states create potential fluctuations in the conduction band minima ( $E_c$ )<sup>5,6</sup>. Although this tends to reduce the overall electron mobility as shown in Fig. 1b, the approach has been successful due to the low temperature processability and high mobility in the amorphous phase<sup>1,7</sup>.

As another approach for high mobility and optical stability in oxide semiconductors, anions, instead of cations, can be added<sup>8</sup>. For example, fluorine (F) can be used for n-type doping of  $\text{SnO}_2$ . However, F does not affect electron mobility as it is an anion, which puts disorder into the valence band not the conduction band<sup>9</sup>. As another example, when nitrogen (N) is incorporated into ZnO, this does not cause p-type doping but it forms an amorphous alloy, where the anion site disorder stabilizes the amorphous phase, making amorphous ZnON (a-ZnON). Again, this does not lower the electron mobility because the disorder is in valence band states, and not the conduction band states. Another important effect is that the N 2p orbital lies higher than the O 2p orbital, so that the new N 2p states raise the valence band maxima (VBM) above its energy in ZnO<sup>9</sup>. It is known that the photo-induced instabilities of ZnO and IGZO are related to states due to O vacancies and interstitials that lie in the lower band gap region. These states are now covered up by the higher VBM states, so they can no longer give rise to such instabilities and persistent photoconductivity (PPC)<sup>10,11</sup>, which is a strong benefit for the N containing materials.

According to the recent literature<sup>11</sup>, the electron effective mass of a-ZnON ( $\sim 0.19 m_0$ ) can be larger than that of crystalline ZnN (i.e. c-ZnN) and smaller compared to ZnO films. This may be explained with a disorder of a-ZnON, especially in amorphous phase. Indeed, the conduction band minima (CBM) of a-ZnON is also composed of both Zn 4s and N 2p, similar to c-ZnN<sup>12,13</sup>. Here, N 2p is sensitive to bonding angle tilt in amorphous phase, thus high disorder in a-ZnON, although Zn 4s is spherical and

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**Figure 1.** Schematic profiles of the conduction band minima ( $E_C$ ) in (a) poly-crystalline ZnO, (b) amorphous InGaZnO, and (c) amorphous ZnON, respectively. Here, 'e' denotes a free electron, released into conduction band. In (a),  $\phi_B$  is the potential barrier height at the grain boundary in poly-crystalline ZnO. In (b),  $\phi_B$  is the potential barrier height due to compositional disorder in amorphous InGaZnO. (d) Schematic diagram to describe trap-limited conduction associated with the localized tail states. Here,  $n_{free}$  and  $n_{trap}$  denote free and trapped carrier densities at band tail states, respectively.

less sensitive to bonding angle disorder. This can yield a high density of localized tail states near the CBM in a-ZnON (see Fig. 1c). For a TFT with a-ZnON channel, the field-effect mobility is strongly affected by the presence of the localized tail states. This can be explained with trap-limited conduction theory (i.e. multiple trapping and thermal release events) (see Fig. 1c,d)<sup>5,14</sup>. One of the ways to reduce the localized tail state density is by thermal annealing, resulting in higher mobility (up to 110 cm<sup>2</sup>/V-s) reported in Ref. 8.

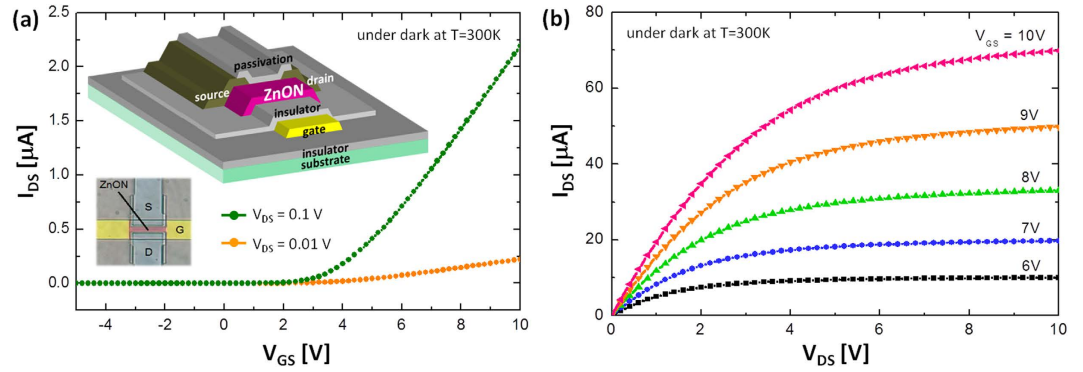
In this paper, we extract the density of localized tail states in a-ZnON TFTs, using current-voltage characteristics of the device. The extracted values of tail state density at the CBM ( $N_{tc}$ ) and characteristic energy ( $kT_t$ ) are about  $2 \times 10^{20}$  cm<sup>-3</sup>eV<sup>-1</sup> and 29 meV, respectively, thus  $kT_t > kT$  (i.e. thermal energy) at  $T = 300$ K. This implies that trap-limited conduction is dominant at room temperature. In addition, it is found that the extracted field-effect mobility and its gate voltage-dependence are strongly dependent on the pre-factor  $1/(\alpha + 1)$ , where  $\alpha = 2(kT_t/kT - 1)$  for  $kT_t > kT$ . Here, we derived a more accurate field-effect mobility expression, using the proposed self-consistent extraction method. Also, a weak persistent photoconductivity in a-ZnON TFTs with Mo electrode is observed under visible light illumination, suggesting ionization of defects, such as oxygen and/or nitrogen vacancies, located near the VBM. To check the effect of electrode on leakage current and PPC, we replaced the Mo with Cr for electrodes. It is found that the leakage current slightly increases, but the effect of illumination is maintained, suggesting the PPC is arising from a change in the intrinsic property of the channel layer.

## Results and Discussion

**Localized Tail States.** Since the current-voltage ( $I$ - $V$ ) characteristics of the TFT are largely determined by the density of localized states, e.g. tail states in the channel layer, the density of localized states can be retrieved from the measured terminal characteristics<sup>15-17</sup>. As a first step, the free carrier density ( $n_{free}$ ) is extracted from the measured  $I$ - $V$  characteristics. Note that linear characteristics of the drain current vs. gate voltage ( $I_{DS}$ - $V_{GS}$ ) are required rather than saturation regime characteristics<sup>16,17</sup>,

$$n_{free} = \frac{1}{\epsilon_s kT} \left( \frac{L \cdot I_{DS}}{\mu_{band} \cdot W \cdot V_{DS}} \right)^2. \quad (1)$$

Here,  $\mu_{band}$  is the band mobility of the ZnON layer (note that this is a constant and the main unknown),  $\epsilon_s$  the permittivity of a-ZnON (which is about  $11\epsilon_0$ , where  $\epsilon_0$  is vacuum permittivity),  $kT$  the thermal energy,  $W$  the channel width,  $L$  the channel length, and  $V_{DS}$  the drain voltage. Also, the carrier density



**Figure 2.** (a) Linear  $I_{DS}$ - $V_{GS}$  characteristics measured at a small  $V_{DS}$  (0.01 V and 0.1 V). Inset: Schematic 3-D view of the fabricated a-ZnON TFTs along with this micro-photo. Here, the gate insulator is  $Si_3N_4$ , stacked layer of  $SiO_2$  and  $Si_3N_4$  is used as Passivation, and Mo and Cr are used for source, drain, and gate terminals in two different devices, respectively. (b) Measured output characteristics, i.e.  $I_{DS}$ - $V_{DS}$ , of the examined TFTs for different  $V_{GS}$ .

of the free carriers ( $n_{free}$ ) and trapped carriers ( $n_{trap}$ ) at tail states can be derived with Poisson's Equation along with Gauss's law as follows,

$$\frac{d^2\varphi}{dx^2} = \frac{q}{\epsilon_S} (n_{free} + n_{trap}), \quad (2)$$

$$E = -\frac{d\varphi}{dx}, \quad (3)$$

where  $x$  is the distance from the front channel interface along the channel depth, and  $\varphi$  the channel potential along  $x$ . Based on Equations (2) & (3), the carrier densities can be connected to gate voltage using a charge balance Equation:  $E(x=0) = C_{ox}(V_{GS} - V_{Te})$ . Here,  $C_{ox}$  is the gate-insulator capacitance and  $V_{Te}$  is an effective threshold voltage which can be represented as  $[1/V_{GS} + 1/V_T]^{-1}$  for  $V_{GS} > 0$  and  $V_T > 0$ , where  $V_T$  is a threshold voltage to be extracted with a linear extrapolation at a linear regime. This yields the following,

$$E(x=0) = \sqrt{\frac{2q}{\epsilon_S} \int_0^{\varphi_s} (n_{free} + n_{trap}) d\varphi} \approx \frac{C_{ox}(V_{GS} - V_{Te})}{\epsilon_S}. \quad (4)$$

Squaring Equation (4) and taking its first derivative with respect to the surface potential  $\varphi(x=0) = \varphi_s$ ,  $n_{trap}$  can be obtained as,

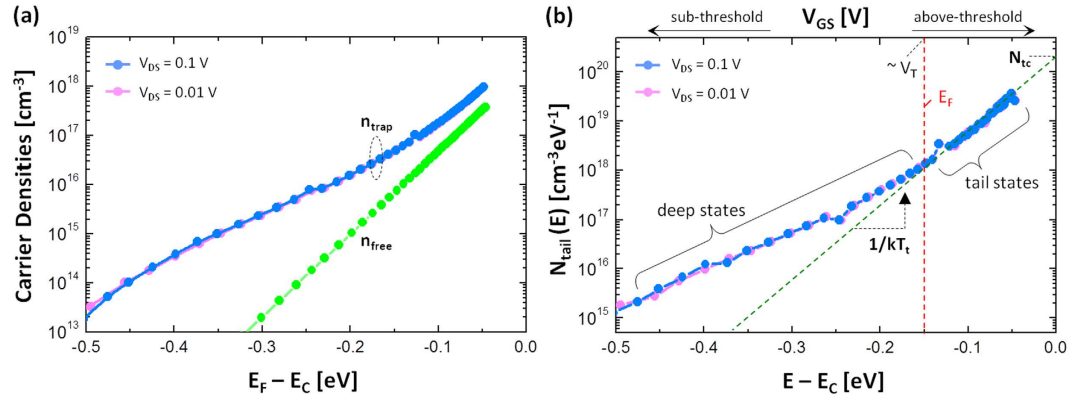
$$n_{trap} = \frac{\epsilon_S}{2q} \frac{dE^2(x=0)}{d\varphi_s} - n_{free}. \quad (5)$$

Based on Equations (1), (4), and (5), the density of tail states ( $N_{tail}(E)$ ) can be given as the first derivative of Equation (5),

$$N_{tail} = \left. \frac{dn_{trap}}{d\varphi_s} \right|_{E_F \rightarrow E}. \quad (6)$$

Here,  $q\varphi_s = E_F - E_{F0}$  where  $E_{F0}$  is the Fermi level at flat band (see the Supplementary Information for more detailed derivation procedure).

Based on the above extraction method, the density of localized tail states was retrieved using a-ZnON TFTs with  $W = 50 \mu m$  and  $L = 10 \mu m$ . Here, the linear  $I_{DS} - V_{GS}$  characteristics were measured at a small  $V_{DS}$  (e.g. 0.01 V and 0.1 V), as seen in Fig. 2(a,b) shows output characteristics for different  $V_{GS}$  (see also Figure S2 in the Supplementary Information). The basic parameter to be extracted from each I-V curve is  $V_T$ . The  $V_T$  values of these two cases ( $V_{DS} = 0.01 V$  and  $0.1 V$ ) are 4.4 V and 4.3 V, respectively. The other unknown parameters,  $\mu_{band}$  and  $C_{ox}$  are  $110 cm^2/V\cdot s$  and  $19 nF/cm^2$ , respectively<sup>8</sup>. Here,  $\mu_{band}$  can be the maximum achievable mobility and the  $C_{ox}$  value was calculated using a thickness of 300 nm and measured permittivity of  $\sim 6.5\epsilon_0$  for the gate insulator  $Si_3N_4$ . Using these parameters and Equations (1–6), the carrier densities ( $n_{free}$  and  $n_{trap}$ ) and density of tail states ( $N_{tail}(E)$ ) were extracted as seen in Fig. 3a,b,



**Figure 3.** (a) Extracted carrier densities ( $n_{\text{free}}$  and  $n_{\text{trap}}$ ) and (b) density of tail states denoted as  $N_{\text{tail}}(E)$ . The extracted  $N_{\text{tail}}(E)$  for different  $V_{\text{DS}}$  is similar to each other, suggesting that the extraction method is almost independent on  $V_{\text{DS}}$  when  $V_{\text{DS}}$  is small enough. This also implies that contact resistance effects are negligible at small  $V_{\text{DS}}$ , e.g. 0.1 V and 0.01 V.

respectively. As indicated in Fig. 3b, the tail states (i.e. gap states near the  $E_C$ ) can be approximated as an exponential distribution<sup>14–16</sup>,

$$N_{\text{tail}}(E) = N_{\text{tc}} \exp\left(\frac{E - E_C}{kT_t}\right). \quad (7)$$

Here,  $N_{\text{tc}}$  is the tail state density at  $E = E_C$  (i.e. conduction band minima), and  $kT_t$  is the characteristic energy of the tail state. Applying Equation (7) into the plot shown in Fig. 3b,  $N_{\text{tc}}$  and  $kT_t$  values were extracted as  $2 \times 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$  and 29 meV, respectively.

**Electron Mobility.** To incorporate the effect of tail states into the field effect mobility ( $\mu_{\text{FE}}$ ), the trap-limited conduction theory is employed,

$$\mu_{\text{FE}} \equiv \mu_{\text{band}} \left( \frac{n_{\text{free}}}{n_{\text{free}} + n_{\text{trap}}} \right). \quad (8)$$

Here,  $n_{\text{free}}$  (with Boltzmann's approximation for  $|E_F - E_C| > kT$ ) and  $n_{\text{trap}}$  (for  $kT_t > kT$ ) are represented analytically as a function of Fermi level ( $E_F$ )<sup>16,17</sup>, respectively, as follows,

$$n_{\text{free}} = N_C \exp\left(\frac{E_F - E_C}{kT}\right), \quad (9)$$

$$n_{\text{trap}} = N_{\text{tc}} kT_t \exp\left(\frac{E_F - E_C}{kT_t}\right), \quad (10)$$

where  $N_C$  is an effective free carrier density [ $\text{cm}^{-3}$ ]. Note that the  $N_C$  value of ZnON is about  $2 \times 10^{18} \text{ cm}^{-3}$ , which is calculated with an electron effective mass  $\sim 0.2 m_0$ <sup>10,11</sup>, where  $m_0$  is the electronic rest mass. With Equations (9) & (10), Equation (8) can be rewritten as a function of  $E_F$ , assuming  $n_{\text{free}} < n_{\text{trap}}$

$$\mu_{\text{FE}} \approx \mu_{\text{band}} \left( \frac{N_C}{N_{\text{tc}} kT_t} \right) \exp\left( (E_F - E_C) \left( \frac{1}{kT} - \frac{1}{kT_t} \right) \right). \quad (11)$$

Here,  $E_F - E_C (= E_{F0} + q\varphi_S - E_C)$  can be given as a solution of Equation (4), replacing  $V_{\text{Te}}$  by  $V_T$  just for the above-threshold regime,

$$E_F - E_C = kT_t \ln\left( \frac{C_{\text{ox}}^2 (V_{\text{GS}} - V_T)^2}{2\varepsilon_S N_{\text{tc}} (kT_t)^2} \right). \quad (12)$$

Using Equations (11) & (12), Equation (11) can be represented as a function of  $V_{\text{GS}}$ , following a power law,

Parameters	$V_{DS}$	
	0.01 V	0.1 V
$N_{tc}$ [ $\text{cm}^{-3}\text{eV}^{-1}$ ]	$2.15 \times 10^{20}$	$2.17 \times 10^{20}$
$kT_t$ [meV]	29.1	29.2
$1/(\alpha + 1)$	0.79	0.78
$\psi$	0.21	0.22
$\mu_{gm}$ [ $\text{cm}^2/\text{V}\cdot\text{s}$ ] (peak)	38.4	38.6
$\mu_{FE}$ [ $\text{cm}^2/\text{V}\cdot\text{s}$ ] (peak)	30.2	30.1

**Table 1. Summary of Extracted Parameters for a different  $V_{DS}$ .**

$$\mu_{FE} = \xi (V_{GS} - V_T)^\alpha, \quad (13)$$

$$\xi \equiv \mu_{band} \left( \frac{N_C}{N_{tc} kT_t} \right) \left( \frac{C_{ox}^2}{2\varepsilon_S N_{tc} (kT_t)^2} \right)^{\alpha/2}, \quad (14)$$

where  $\alpha = 2(kT_t/kT - 1)$ . Note that  $\xi$  is a prefactor independent on  $V_{GS}$ . As seen in Equation (13), the field-effect mobility ( $\mu_{FE}$ ) is a function of  $V_{GS}$ , and linked with localized tail states in terms of the exponent ( $\alpha$ ) and constant ( $\xi$ ) in the power law. Along with Equation (13), the current-voltage relation can be derived based on a drift transport equation, and approximated with the condition,  $V_{GS} - V_T \gg V_{DS}$  (i.e. linear approximation), as follows,

$$I_{DS} \approx \mu_{FE} C_{ox} \left( \frac{W}{L} \right) (V_{GS} - V_T) V_{DS}. \quad (15)$$

Due to the presence of the exponent ( $\alpha$ ) and gate-voltage dependence in the  $\mu_{FE}$  expression seen in Equation (13), the first derivative of Equation (15) with respect to  $V_{GS}$  (i.e. transconductance ( $g_m$ )) is given as follows,

$$\frac{\partial I_{DS}}{\partial V_{GS}} = \frac{\partial \mu_{FE}}{\partial V_{GS}} C_{ox} \left( \frac{W}{L} \right) V_{DS} (V_{GS} - V_T) + \mu_{FE} C_{ox} \left( \frac{W}{L} \right) V_{DS}. \quad (16)$$

Note that the first term of Equation (16) cannot be zero since  $\mu_{FE}$  is a function of  $V_{GS}$ . So, the conventional way to get  $\mu_{FE}$  seems to be insufficient and inconsistent. In Equation (16), the first derivative of  $\mu_{FE}$  is shown and can be expanded with Equation (13), as follows,

$$\frac{\partial \mu_{FE}}{\partial V_{GS}} = \alpha \mu_{FE} (V_{GS} - V_T)^{-1}, \quad (17)$$

With Equation (17), Equation (16) can be rewritten as follows,

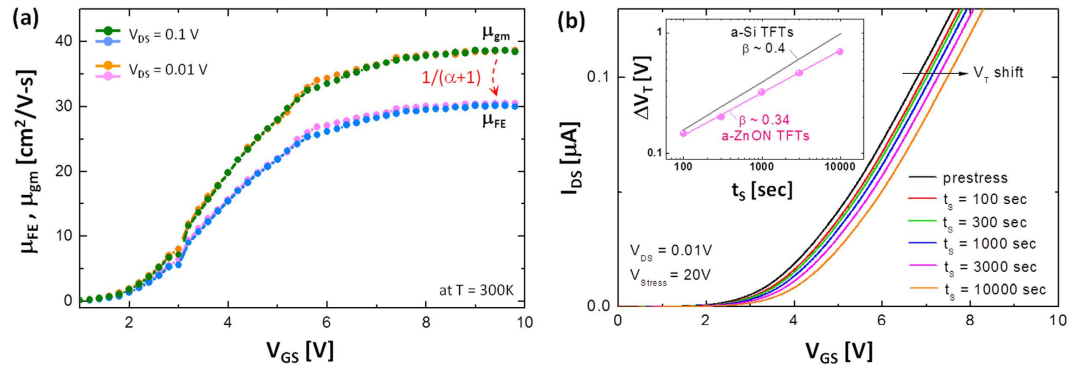
$$\frac{\partial I_{DS}}{\partial V_{GS}} = \alpha \mu_{FE} C_{ox} \left( \frac{W}{L} \right) V_{DS} + \mu_{FE} C_{ox} \left( \frac{W}{L} \right) V_{DS}. \quad (18)$$

From Equation (18),  $\mu_{FE}$  is now given as follows,

$$\mu_{FE} = \frac{1}{\alpha + 1} \left( \frac{\partial I_{DS}}{\partial V_{GS}} \right) \frac{1}{C_{ox} (W/L) V_{DS}} \equiv \frac{1}{\alpha + 1} \mu_{gm}. \quad (19)$$

As can be seen in Equation (19), due to the presence of  $\alpha$  associated with localized tail states, the mobility can be reduced by the ratio of  $1/(\alpha + 1)$ . Here, we defined the parameter ' $1/(\alpha + 1)$ ' as the mobility scaling factor due to trapping events in the localized tail states. So, the conventional way yields an over-estimated value and hence an inconsistency. So, we believe that Equation (19) provides a more accurate  $\mu_{FE}(V_{GS})$  while capturing the effects of localized tail states with the parameter  $\alpha$ . Using Equation (19),  $\mu_{FE}(V_{GS})$  was extracted using the retrieved value of  $kT_t$  seen in Table 1. In addition, the following equation can also be defined to explain the portion of trapping ( $\psi$ ) as,

$$\psi = \frac{\alpha}{1 + \alpha}. \quad (20)$$



**Figure 4.** (a) Field effect mobility (i.e. gate voltage dependent mobility) as a function of  $V_{GS}$  for different  $V_{DS}$ : 0.1 V, 0.01 V. Here,  $\mu_{FE}$  is shown from using Equation (19) in comparison with  $\mu_{gm}$  calculated by the conventional way with transconductance ( $g_m$ ). (b)  $I_{DS}$ - $V_{GS}$  characteristics measured after applying 20 V stress for each stress period ( $t_s$ ). Here, the gate voltage applied ( $V_{Stress}$ ) is 20 V (Inset: retrieved  $\Delta V_T$  vs.  $t_s$ ).

This can be used as a measure of how trapping significantly affects the electron mobility. As shown in Fig. 4(a),  $\mu_{FE}$  (at  $V_{GS} = 9$  V) is about  $30.2 \text{ cm}^2/\text{V}\cdot\text{s}$  for  $V_{DS} = 0.01$  V which is reduced by 21% (i.e.  $\psi = 0.21$ ) compared to the conventional extraction route where  $\mu_{FE}$  is considered as a constant ( $38.4 \text{ cm}^2/\text{V}\cdot\text{s}$  without considering  $\alpha$ ), i.e.  $\mu_{gm}$ . Note that we also tested the proposed mobility extraction method for  $V_{DS} = 0.1$  V. It is found that there is a discrepancy less than 1% compared to the case of  $V_{DS} = 0.01$  V, as summarized in Table 1. Here, we believe that the case of  $V_{DS} = 0.01$  V provides higher accuracy compared to  $V_{DS} = 0.1$  V since a smaller  $V_{DS}$  is always better to satisfy the assumption that  $V_{GS} - V_T \gg V_{DS}$ , relating to Equation (15).

The band tail states not only affect the electron mobility but also affect bias instability. Indeed, it is known that the density of band tail states determines the rate of instability creation, e.g. threshold voltage shift ( $\Delta V_T$ ). The  $\Delta V_T$  as a function of time ( $t$ ) is defined by the following relation<sup>18</sup>,

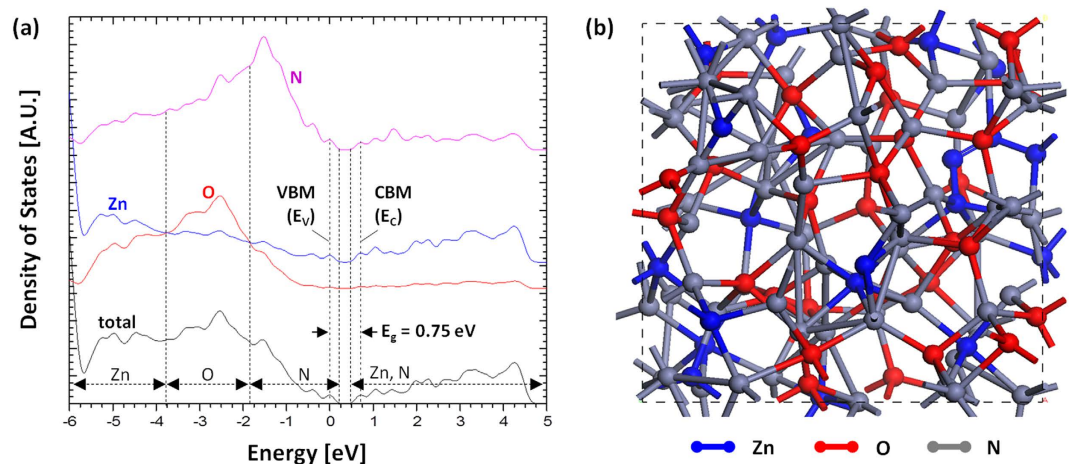
$$\Delta V_T = (V_{Stress} - V_{T0})(t/t_0)^\beta. \quad (21)$$

Here,  $V_{Stress}$  is the bias stress,  $V_{T0}$  the pre-stress threshold voltage ( $\sim 4.3$  V), and  $t_0$  the characteristic time constant. In particular,  $\beta$  is a power-law exponent, which is proportional to the tail state density ( $N_{tc}$ ,  $\text{cm}^{-3}\text{eV}^{-1}$ ). So the following relation can be deduced,

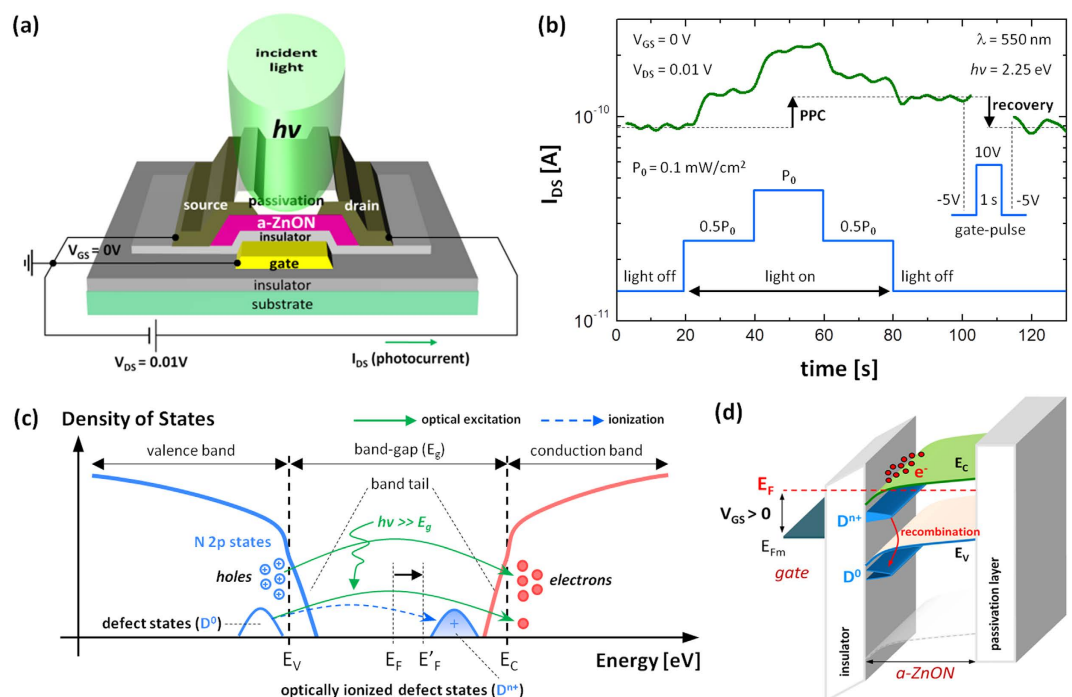
$$\beta = \zeta N_{tc}, \quad (22)$$

where  $\zeta$  is a constant in the dimension of  $\text{cm}^3\text{eV}$ . To extract the values of  $\beta$  and  $t_0$ , the I-V characteristics were measured after applying 20 V bias stress for each stress period, as seen in Fig. 4b. Based on this, the  $\Delta V_T$  as a function of time is retrieved, as seen in the inset of Fig. 4b, yielding  $\beta \sim 0.34$  and  $t_0 \sim 10^8$  sec. Here, it is found that the value of  $\beta$  is smaller compared to a-Si TFTs  $\sim 0.4$ <sup>18</sup>. As can be seen in Equation (22), this can be explained with a smaller  $N_{tc}$  of a-ZnON TFTs  $\sim 2 \times 10^{20} \text{ cm}^{-3}/\text{eV}$  compared to a-Si TFTs  $\sim 10^{22} \text{ cm}^{-3}/\text{eV}$ <sup>19</sup>.

**Persistent Photoconductivity.** Additionally, we performed computations of the density of states (DOS) in a-ZnON. Figure 5 shows the computed total DOS and projected DOS (PDOS) onto Zn, O, and N atoms for a-ZnON. Note that the fabricated a-ZnON film composition has been measured with the Rutherford backscattering spectrometry (RBS) (see the Supplementary Information). As shown in Fig. 5a, it is clear that the N forms the VBM, and is located from  $-1.8$  eV to  $0$  eV. This implies that oxygen defects (e.g. vacancies and interstitials), viewed as the origin of the PPC, are filled with N. Also, the band-gap is about  $0.75$  eV, as indicated in Fig. 5, suggesting that photon energies in the range from  $0.75$  eV  $\sim 2.55$  eV may not give rise to the PPC in a-ZnON. To check this, we measured the drain current as a function of time (i.e.  $I_{DS}$ -time plot) when  $V_{GS} = 0$  V and  $V_{DS} = 0.01$  V under illumination with  $550$  nm wavelength light (equivalent to  $2.25$  eV photon energy,  $h\nu$ ), as seen in Fig. 6a. Here, the maximum optical power  $P_0$  is  $\sim 0.1$  mW/cm<sup>2</sup>. As shown in Fig. 6b, the drain current ( $\sim 2.3 \times 10^{-10}$  A) under  $P_0$  is increased by 2 times more than that ( $\sim 1.2 \times 10^{-10}$  A) under  $0.5P_0$ . This suggests that the drain current under illumination is associated with excess carrier generation, which is linearly proportional to incident optical power, rather than electron trapping into gate insulator. After removal of illumination (after  $t = 80$  s), the drain current is almost recovered, thus the examined a-ZnON is optically very stable. However, we find a small difference (i.e.  $I_{PPC} \sim 3.4 \times 10^{-11}$  A) between the initial ( $I_{DS} \sim 9.1 \times 10^{-11}$  A) and final ( $I_{DS} \sim 1.25 \times 10^{-10}$  A) stages. Thus, persistent photoconductivity (PPC) still exists, albeit mild as seen in Fig. 6b, implying that some of the excess electrons are generated from optically irreversible states.

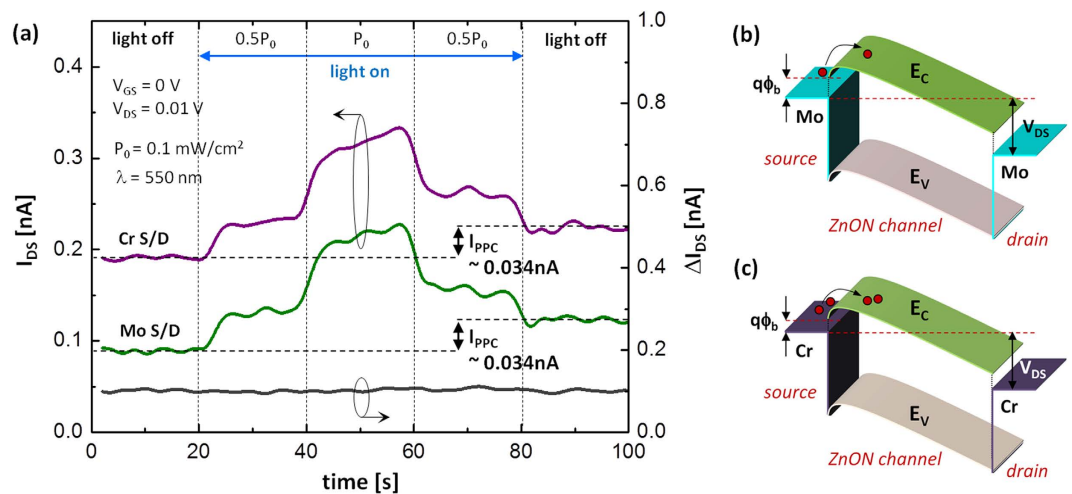


**Figure 5.** (a) Computed total electronic density of states (DOS) and projected DOS (PDOS) for the Zn, O, and N atoms in a-ZnON. The VBM energy level is set to 0 eV, and retrieved band-gap energy ( $E_g$ ) is about 0.75 eV as indicated. (b) The model unit cell of a-ZnON obtained from the melt-quench simulations.



**Figure 6.** (a) Schematic 3-D view of the transistor examined with the light illumination and DC bias on  $V_{DS}$ . (b) Measured drain current ( $I_{DS}$ ) of the examined device with Mo electrode as a function of time. Here, light pulse is applied as described in the inset. (c) Possible density of states picture with respect to optical carrier generation mechanisms and PPC. Here, the generated electrons are denoted as 'e',  $E_F$  and  $E'_F$  denote Fermi levels before and after illumination, respectively, and  $E_V$  is the valence band maxima. (d) Schematic 3-D band diagram along the channel depth. Here, we show the effect of the positive gate bias on the recombination of ionized deficiency defects with induced electrons.

So, the PPC may be associated with some of the unfilled oxygen defects ( $O_D$ ). Besides oxygen-related defects, we also consider nitrogen-related defects ( $N_D$ ), such as nitrogen vacancies ( $N_V$ ), which exist especially at the vicinity of the valence band maxima<sup>20–22</sup>. Under illumination, they can also be ionized as  $N_V^0 \rightarrow N_V^{n+} + ne^-$ , where  $n$  is an integer, e.g.  $1 \sim 3$ <sup>20,22</sup>. Since these constitute negative U-defects, the ionization process is irreversible even after removal of light, thus giving rise to the mild PPC<sup>22</sup>. These defects, collectively denoted as  $D^0$ , can be ionized under illumination ( $D^0 \rightarrow D^{n+} + ne^-$ ), relocating to the vicinity of the  $E_C$ <sup>10,11,20–25</sup>. This maintains the increased Fermi level ( $E_F$ ) even after illumination, as



**Figure 7.** (a) Measured IDS vs. time for two devices with different metal electrodes, e.g. Mo and Cr, respectively. Also, the current difference is shown on y-axis on the right hand side. Horizontal band diagrams for the cases of (b) Mo and (c) Cr electrodes, respectively.

described in Fig. 6c. Since we have a very mild PPC (see Fig. 6b), we should assume that the density of defects, including oxygen and nitrogen vacancies, is small, implying that the photocurrent under illumination mostly consists of electrons generated from the N 2p states in the valence band. In order to estimate the number of the ionized deficiency defects ( $N_{idd}$ ,  $\text{cm}^{-2}$ ), we may use the following relation,

$$I_{PPC} \approx \mu_{FE} \frac{W}{L} q N_{idd} V_{DS}. \quad (23)$$

Using the values of the parameters extracted in the previous sections (e.g.  $I_{PPC} = 3.4 \times 10^{-11}$  A,  $\mu_{FE} = 30.2 \text{ cm}^2/\text{V}\cdot\text{s}$ ,  $W/L = 5$ ,  $V_{DS} = 0.01$  V), the  $N_{idd}$  is retrieved as  $1.43 \times 10^8 \text{ cm}^{-2}$ . To electrically remove these ionized defects, we employed a positive gate-pulse scheme<sup>25</sup>, as seen in Fig. 6b. This yields a fully recovered current level ( $I_{DS} \sim 9.2 \times 10^{-11}$  A) which is similar to the current level before illumination. Hence, it is suggested that these ionized defects ( $D^{n+}$ ) were eliminated with the forced recombination with the electrons ( $ne^-$ ) induced during the positive gate-pulse width (+10 V), i.e.  $D^{n+} + ne^- \rightarrow D^0$ , as described in Fig. 6d. Here, the number of induced electrons (i.e.  $N_e \approx C_{ox} \times (10 - V_{+})/q \approx 6.7 \times 10^{11} \text{ cm}^{-2}$ ) are much more than the  $N_{idd} \sim 1.43 \times 10^8 \text{ cm}^{-2}$ , thus it is enough for a full recombination.

In addition, we replaced Mo with Cr for electrodes to check effects of metal on leakage current and PPC. Figure 7a shows the measured  $I_{DS}$  vs. time for two devices with different metal electrodes, e.g. Mo and Cr, respectively. It is found that there is a small current difference before and after illumination for each case. And the difference (i.e.  $I_{PPC}$ ) is almost the same as 0.034 nA. This implies that the choice of electrode metal doesn't affect the PPC. And the current difference between the Mo and Cr cases ( $\Delta I_{DS}$ ) is shown on the right-hand-side y-axis. It is found that this current difference is always approximately 0.1 nA, suggesting that the leakage current is changed globally regardless of illumination and PPC. This can be explained with the reduced barrier height at source side ( $q\phi_b$ ) due to a smaller work-function of Cr ( $\sim 4.5$  eV) compared to Mo ( $\sim 4.6$  eV), as shown in Fig. 7b,c. These results indicate that the choice of metal for electrodes does not affect the PPC.

## Conclusions

In conclusion, the density of localized tail states in ZnON thin film transistors (TFTs) has been extracted using current-voltage characteristics of the TFTs. The extracted values of  $N_{tc}$  and  $kT_t$  are about  $2 \times 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$  and 29 meV, respectively. Considering trap-limited conduction theory, the field-effect mobility expression has been derived and shown to be represented in terms of tail state parameters. In particular, the exponent ( $\alpha$ ) has been strongly connected to the mobility through  $kT_t$  which is a key measure of the degree of the disorder of the channel layer. This suggests that a reduction of  $kT_t$  is needed to achieve higher mobility. Additionally, it has been revealed that the examined ZnON is optically very stable showing only weak PPC which is thought to be arising from ionization of defects, such as oxygen and/or nitrogen vacancies, located in vicinity of the valence band maxima. This happens equivalently in both ZnON TFTs with Mo and Cu electrodes, suggesting the PPC is associated with a change of the intrinsic property of the channel.



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## Author Contributions

S.L. and A.N. designed the experiments and also did analysis with the proposed theories and method. S.L. carried out the experiments. Y.Y. fabricated and characterized the samples. Y.G. and J.R. performed the computations for PDOS. All the authors contributed to discuss on the paper. S.L., A.N. and J.R. wrote the paper.

## Additional Information

**Supplementary information** accompanies this paper at <http://www.nature.com/srep>

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