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Device performance and bias instability of Ta doped InZnO thin film transistor as a function of process pressure

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The device performance and bias instability of radio frequency (RF) sputtered Ta doped InZnO thin film transistors (TFTs) were investigated as a function of deposition process pressure. Under low process pressure, the electrical characteristics of TaInZnO TFTs were enhanced with amorphous physical structure and the decrease of oxygen deficient bonding states. These changes were correlated with the evolution of electronic structure, such as band alignment and band edge states below the conduction band. As the process pressure decreased, the energy difference between conduction band minimum and Fermi level and the band edge states was decreased. In particular, the relative energy level of band edge states was moved into the deep level within bandgap, with the increase of process pressure. © 2013 American Institute of Physics. [http://dx.doi.org/10.1063/1.4794941]

Transparent amorphous oxide semiconductors (AOSs) have been paid wide attention as an attractive active channel layer with high switching speed, for various electronic device applications, including liquid crystal displays (LCDs) and active-matrix organic light emitting diodes (AMOLEDs).1–3 Compared with conventional amorphous/poly-silicon thin film transistors (TFTs), oxide TFTs have significant advantages, such as high electron mobility, transparency, low temperature, and low cost process, with the preservation of amorphous structure.4 Various semiconductors based on indium and zinc oxide compounds have been intensively studied, since the 2004 report on amorphous indium-gallium-zinc oxide TFTs with high device performance.5

However, for practical mass production, higher device performance and better device instability still remain as some of the most important and critical issues. Recently, many efforts have been made to seek alternative oxide semiconductors with good stability under bias and illumination stress, using combinatorial material design.5,6 Various metals doped InZnO based oxide semiconductors have been considered as a device channel to enhance the device characteristics by controlling the carrier concentration and mobility.7,8 Also, several research groups have studied modifying the device structure, materials, and process parameters, in order to understand and improve the degradation of device performance and instability.9–11 Even if previous results have suggested that the device operation and the stress induced device instabilities are caused by the charge trapping mechanism related to oxygen defects, their origins and interpretations of device instability have not yet become apparent.12,13 Moreover, detailed and systematic approaches are necessary, in terms of the electronic structure of oxide semiconductor, because it is strongly correlated to the charge transport and trapping behaviors, which are subject to the device characteristics.

In the present work, device performance and bias instability of TaInZnO (TIZO) oxide thin film transistors are studied as a function of RF-sputtered process pressure, with respect to the electronic structure of band alignment and band edge states below the conduction band, which are correlated to the chemical bonding states. TIZO active layer deposited in lower process pressure shows better device characteristics, with smaller oxygen deficient chemical bonding states and band edge states.

Heavily doped p-type Si wafer with thermally grown SiO2 (100 nm) wafer was used as substrates onto which TIZO films were deposited, without substrate heating, by a radio frequency sputtering system. The RF power and process pressure were set to 75 W and changed from 1 mTorr to 5 mTorr, respectively. The active area was defined using a shadow mask during TIZO film deposition. After that the indium-tin-oxide (ITO) source/drain (S/D) electrode was deposited and patterned again using shadow masks. The fabricated TFTs had a bottom gate structure, and a channel width (W) and length (L) of 1000 μm and 150 μm, respectively. Finally, TIZO TFTs were annealed at 300 °C for 1 h, by using a furnace system. In order to analyze the physical and electronic properties of TIZO films, separated TIZO films were prepared on identical substrates and underwent the same heat treatments as for the TFT devices. The composition was ~5% Ta doping into InZnO, and the ratio of In was slightly changed within ~2%, as a function of process pressure and annealing temperature, when investigated by Rutherford backscattering (RBS). The physical structure, measured by x-ray diffraction (XRD), is preserved as an amorphous structure, regardless of process pressure. Hall measurements were employed to investigate the electrical properties of films, such as carrier concentration and mobility, using a van der Pauw configuration, with a permanent magnet of 0.55 T at room temperature. Chemical bonding states were also examined by x-ray photoelectron spectroscopy (XPS), using a monochromatic AlKα source, with a pass energy of 20 eV. The electronic structures, related to changes in band alignment and band edge states below the conduction band, were investigated by XPS and spectroscopic ellipsometry (SE). The SE measurements were performed by a rotating analyzer system with an auto retarder, in the energy...
range of 0.75 eV to 6.4 eV, with incident angles of 65°, 70°, and 75°.

Figure 1(a) shows the representative transfer characteristics of the TFTs with the TIZO active layer deposited in the different process pressures of 1 mTorr, 3 mTorr, and 5 mTorr, respectively. The field effect mobility (μ_{FE}) and threshold voltage (V_{th}) in the saturation region (V_{DS} = 10.1 V) were calculated by fitting a straight line to the plot of the square root of I_{DS} versus V_{GS}, according to the expression for a field-effect transistor. The subthreshold gate swing (S.S) value was extracted from the linear part of the log(I_{DS}) vs. V_{GS} plot. A significant improvement of the device performance was observed for the TFTs with the TIZO active layer deposited in a process pressure of 1 mTorr, and the detailed device parameters are summarized in Table I. As process pressure decreased from 5 mTorr to 1 mTorr, the μ_{FE} and S.S values in TIZO TFTs significantly improved, from 1.12 cm²/Vs and 0.62 V/decade to 6.99 cm²/Vs and 0.27 V/decade, respectively. These imply that the process pressure is a critical factor in changing the charge-trapped defects in the TIZO semiconductor and/or interface (TIZO/SiO₂), because of improving mobility and S.S values.

The bias instability of the TFTs with TIZO active layers was also investigated as a function of process pressure under negative bias stress (NBS) condition, with a gate bias of −20 V after 10, 100, 1000, and 3600 s, as shown in Figure 1(b). As the stress time passes, transfer characteristics of TIZO TFTs systematically shift in the negative direction, without any significant changes of mobility and S.S values. TFT with lower process pressure shows a smaller shift in the negative direction of the transfer curves. The V_{th} of the TFT in 5 mTorr shifts by −1.4 V, while that in 1 mTorr exhibited only a −0.3 V shift in V_{th}. This suggests that the charge trapping mechanism may be dominant in the bias instability of oxide TFTs. Under our investigations, the origin for the negative V_{th} shift of TIZO TFTs under various deposition process pressures can be strongly related to the change trap densities, such as oxygen related traps in the channel bulk and at the gate insulator/channel interface. The S.S value of a given TFT device is generally correlated to the total trap density, including the bulk (N_{SS}) and semiconductor–insulator interfacial traps (D_{it})

$$SS = \frac{qk_BT(N_{SS}t_{ch} + D_{it})}{C_i \log(e)},$$

where q is the electron charge, k_B is Boltzmann’s constant, T is the absolute temperature, and t_{ch} is the channel layer thickness. N_{SS} and D_{it} in the TIZO TFTs were calculated by setting one of the parameters to zero and are summarized in Table I, as well. The N_{SS} and D_{it} values for the TFT in 1 mTorr were 2.38 × 10^{17}/eVcm³ and 9.53 × 10^{13}/eVcm², respectively. However, these values were considerably increased to 5.47 × 10^{17}/eVcm³ and 2.19 × 10^{13}/eVcm² for the TFT in 5 mTorr. Thus, the decrease of trap density was consistent with improvement of the NBS instability, as the process pressure decreased from 5 mTorr to 1 mTorr. Figure 1(c) shows the electrical properties, including the carrier concentration and Hall mobility of a-TIZO films as a function of process pressure. TIZO film deposited at a process pressure of 5 mTorr has the carrier concentration and Hall mobility of 2.4 × 10^{14} cm⁻³ and 1.0 × 10⁻¹ cm²V⁻¹s⁻¹, respectively. When the process pressure decreased to 1 mTorr, the carrier concentration and Hall mobility monotonically increased to 7.1 × 10^{13} cm⁻³ and 22.35 cm²V⁻¹s⁻¹, respectively. Similar to TFT characteristics as a function of process pressure, the electrical properties of TIZO films were significantly enhanced with the decrease of process pressure from 5 mTorr to 1 mTorr. The dependence of electrical properties on the process pressure could be related to the negative V_{th} shift of TIZO TFTs under various deposition process pressures.

### Table I. TFTs parameters including μ_{FE}, I_{on/off} ratio, V_{th}, S.S., and N_{created} with width/length = 1000/150 μm as a function of process pressure. The mobility was extracted from maximum transconductance, and V_{th} was defined by the gate voltage, which induces a drain current of 10 nA at V_{DS} of 5.1 V. The subthreshold gate swing (S.S) value was extracted from the linear part of the log(I_{DS}) vs. V_{GS} plot.

<table>
<thead>
<tr>
<th>Process Pressure (mTorr)</th>
<th>μ_{FE} (cm²/Vs)</th>
<th>I_{on/off} ratio</th>
<th>V_{th} (V)</th>
<th>S.S. (V/decade)</th>
<th>N_{SS} (10^{17}/eV cm³)</th>
<th>D_{it} (10^{13}/eV cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.99</td>
<td>~107</td>
<td>0</td>
<td>0.27</td>
<td>2.38</td>
<td>9.53</td>
</tr>
<tr>
<td>3</td>
<td>1.56</td>
<td>~108</td>
<td>2</td>
<td>0.39</td>
<td>3.44</td>
<td>13.77</td>
</tr>
<tr>
<td>5</td>
<td>1.12</td>
<td>~107</td>
<td>3.5</td>
<td>0.62</td>
<td>5.47</td>
<td>21.88</td>
</tr>
</tbody>
</table>

FIG. 1. (a) Transfer characteristics, (b) shift of threshold voltage under negative bias stress (−20 V) of TIZO TFTs with L = 150 μm and W = 1000 μm, and (c) carrier concentration and Hall mobility of TIZO films as a function of process pressure.
the defect concentration in the deposited films, which is subject to the device performance and instability. In order to interpret the detailed origin of device performance and instability in TIZO TFTs, more discussion is provided below and considers the chemical bonding states and electronic structure, including the band alignment and band edge states below the conduction band.

The chemical bonding states were observed by XPS, and changes in O 1s spectra are shown in Figure 2(a). XPS spectra were measured after eliminating the surface contamination by adsorbed OH, C, H2O, etc., and minimizing the preferred sputtering of light elements, using Ne ions at 500 eV. In order to differentiate the detailed oxygen states, the O 1s spectra were carefully deconvoluted into 3 peaks (O1, O2, O3), using Gaussian fitting with the subtraction of a Shirley type background and by considering a previous report.18 The low binding energy peak (O1) at 529.9 eV is related to the O2− ions on metal oxides, indicating Ta-In-Zn-O bonds.19 The higher binding energy peak (O3) around 532.7 eV is usually attributed to chemisorbed or dissociated oxygen or OH species on the surface of the TIZO films, such as CO3− adsorbed H2O, or adsorbed O2. The peak at the medium binding energy (O2) of the O 1s spectrum is associated with OH bonding species and with O2− ions that are in the oxygen-deficient Ta-In-Zn-O bonding matrix.20 The density of oxygen deficient bonding states (O2) increases upon the increase of process pressure, as shown in the relative ratio of the O2 peak (O2/Ototal) of Figure 2(b). This means that the TIZO films deposited in higher process pressure have larger oxygen related defects by oxygen deficient bonding states, which induce the degradation of device performance and instability.16,21

Figures 3(a)–3(c) show the valence band spectra and bandgap measured by XPS and SE using the extrapolation method and the schematic energy diagram for TIZO films as a function of process pressure. The corresponding values of the bandgap (Eg), and the relative energy difference between the Fermi level (EF) and valence band maximum (ΔEVb), and between EF and conduction band minimum (ΔECb), are indicated below the diagram. The extracted bandgap is increased from 3.32 eV to 3.49 eV with the increase of process pressure, and the valence band offset (ΔEVb) has a similar value, regardless of process pressure, which is related to the slight decrease of the In ratio in TIZO film. As a result, the relative position of the Fermi level (ΔECb) shifts far from the conduction band minimum, from 0.18 eV (1 mTorr) to 0.31 eV (5 mTorr). This result is strongly correlated to the decrease of carrier concentration shown in Figure 1(c) and could be the plausible origin of degraded device operation and electrical properties.
In order to investigate the electronic structure of the TIZO films, including the band edge states below the conduction band, SE data were analyzed as a function of process pressure in Figure 4. Figure 4(a) shows the imaginary dielectric function \( (\varepsilon_2) \) spectra from SE measurements for TIZO film deposited in 1 mTorr with the deconvoluted Gaussian band edge states (D1, D2), by a simple four-phase model comprised of a Si substrate, SiO\(_2\) overlayer, TIZO overlayer, and ambient layer. As the process pressure increased, the evolution of band edge states represents that the shallow band edge state (D1) is drastically increased, and the deep band edge state (D2) is slightly increased, which is totally related to the increase of oxygen deficient chemical bonding states, such as oxygen vacancies.\(^{22}\) In previous study, we have tried to interpret the two distinct band edge states of ZnO film annealed in various annealing ambient atmosphere using analysis of SE data, which are correlated to the electrical properties of ZnO film, such as carrier concentration and mobility, depending on the relative position within bandgap.\(^{23}\) Based on the previous interpretation for ZnO film,\(^{21}\) TIZO film deposited in higher process pressure (5mTorr) is considered to provide larger carrier concentration and a little slower mobility, because of the increase of shallow (D1) and deep (D2) band edge states, respectively. However, herein conflict results, for the drastic decrease of carrier concentration and mobility, could be caused by the relative energy position from conduction band minimum, as shown in Figure 4(c). The relative energy positions of D1 and D2 shift to the deep level energy position from the conduction band minimum with the increase of process pressure: D1: 0.34 eV → 0.68 eV, D2: 1.01 eV → 1.24 eV. This shift to deep level of D1 and D2 (especially D1) within the bandgap may contribute to larger degradation of mobility, by the increase in charge scattering during carrier transport due to energy level far from the conduction band, not to the increase of carrier concentration, similar to the previous results. In addition, the decrease of mobility by the increase of band edge states, and their shift to deep energy level, could lead to the degradation of device performance and instability with the relative position of the Fermi level and oxygen deficient bonding states.

In summary, the device performance and bias instability of TaInZnO oxide TFTs were evaluated as a function of RF-sputtered process pressure. TFTs properties under lower process pressure are dramatically improved with a good field effect mobility of \((\sim 6.99 \text{ cm}^2/\text{V s})\) and small threshold voltage within 0.5 V. TIZO film deposited in the lower process pressure has the smaller conduction band offset \((\Delta E_{\text{CB}} = E_g - \Delta E_{\text{VB}})\) and smaller band edge states below the conduction band, related to oxygen deficient bonding states. In addition, the band edge states are moved into deep energy level from the conduction band minimum, with the increase of process pressure. These evolutions of electronic structure, such as the band alignment and band edge states of TIZO film, are strongly correlated to the device characteristics of TIZO TFTs, depending on the process pressure.

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