A comprehensive density-of-states model for oxide semiconductor thin film transistors

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Received: 16 June 2021 / Accepted: 9 September 2021 / Published online: 1 November 2021
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Abstract
In this paper, a novel and comprehensive density-of-states model is presented to understand the origin of conductivity and the performance of p-type and n-type oxide semiconductor thin film transistors (TFTs). To validate the model, the simulated $I–V$ characteristics are compared with measured results of p-type Cu$_2$O and SnO and n-type SnO$_2$ TFTs. It was observed that cation vacancies are responsible for hole conduction in p-type TFTs, while anion vacancies and/or metal interstitials are responsible for electron conduction in n-type TFTs. This was observed by assigning the cation vacancies to acceptor-like Gaussian states and anion vacancies and/or metal interstitials to donor-like Gaussian states. The characteristic slopes in conduction/valence band-tail states are due to disorders present in the oxide semiconductors. The model successfully delivers the physical insight and pathway to circuit simulation of large-scale integration of pixel circuits in active matrix liquid crystal display/active matrix organic light-emitting diodes.

Keywords Density of states (DOS) · Thin film transistors (TFT) · Cuprous oxide (Cu$_2$O) · Tin oxide (SnO$_2$)

1 Introduction

Oxide semiconductor (OS) thin film transistors (TFTs) have emerged as an important technology in transparent electronics and opto-electronic display devices when comparing poly-Si and amorphous silicon TFTs [1]. OSs show remarkably high field-effect mobility, a wide bandgap and high uniformity over larger areas [2]. These properties help in the development of many high-performance display technologies, such as active matrix liquid crystal display (AMLCD) and active matrix organic light-emitting diodes (AMOLED) [3]. In the past few years, the display industry has been transformed into a multi-billion-dollar business market, expected to reach $87.2 billion by the year 2025 [1]. Recently, display companies, such as Samsung, LG and Sharp, have already touted 70-inch ultra-definition (UD) 3D-TVs with high scanning frequency of 240 Hz [1]. Due to the room-temperature fabrication capability of OSs [4], flexible electronics are becoming the applications of the future which are thinner, lighter and easier to carry [5]. Apart from displays, oxide semiconductors are still used in other applications, including solar cells, electrochromic windows, invisible security circuits, gas sensors and memory devices. [6, 7].

Back panels for AMLCD/AMOLEDs often use n-type TFTs with indium tin oxide [8] and amorphous indium gallium zinc oxide (a-IGZO) [9], due to their high field effect mobility of $> 10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and high ON/OFF current ratio of $> 10^7$ [1]. However, complementary metal oxide semiconductor (CMOS) transistors result in improved switching characteristics, with architectural simplicity, which offers a logic voltage swing with $> 85\%$ of high output voltage [10]. Therefore, they demand an efficient p-type OS for future high-speed and high-density displays. A few metal oxides are native p-type OSs, such as Cu$_2$O and SnO; however, they show limited effective mobility due to restrictions in localized O 2p orbitals of the valence band [11].

Computer-aided design (CAD)-based numerical simulation tools, such as technology-CAD (TCAD) and electronic design automation (EDA) tools, are often used to design and analyze semiconductor devices and circuits. They use physical models to describe the carrier transport, reaction to external electrical signals and optical nature of semiconductor devices. Although oxide semiconductors have been known for over five decades [12], major debate persists regarding the source of conductivity. This makes them one
of today’s least well known semiconductor groups, largely due to a lack of understanding of the microscopic nature of the amorphous oxides. In particular, the development of defects in the generation of carriers and carrier localization behavior are far from fully known. Therefore, carrier transport properties such as mobility and scattering phenomena also need detailed study.

This paper presents a comprehensive physical model of density of states (DOS) in oxide semiconductors. The model is proposed to incorporate device modeling into TCAD tools. The validity of the model is addressed with measured results of early reports. The model helps to investigate the influence of various defects on carrier transport mechanisms and device performance. In the following sections, we present the development of a comprehensive DOS model of OSs. Based on the model, in Sect. 3, we simulate Cu$_2$O, SnO and SnO$_2$ TFTs to study the current–voltage ($I–V$) characteristics. The physics and origin of the device performance using the DOS model are discussed in detail. This physical model of the OS helps device engineers and industries to design and optimize high-performance transparent electronic circuits.

2 Density of states for oxide semiconductors

Defects control the optical and electronic properties of OSs and play a crucial role in the reaction of the material to external stimuli. In general, any divergence from the ideal crystalline lattice is a defect. It could be a point defect like an interstitial or vacancy, an impurity or an extended defect such as stacking fault or dislocation. In OS material, these defects and disorders are intrinsically available, leading to spreading of the electronic state $g(E)$ into the forbidden states, often referred to as tail states, shown in Fig. 1.

Theoretical interpretation of tail states in OSs has been explained by various researchers. Cohen et al., in 1969 [13], explained the properties of amorphous semiconductor alloys through a simple band model. The model presumes the presence of sharp mobility edges $E_C$ and $E_V$ that separate the extended and localized states in both conduction bands (CB) and valence bands (VB), respectively. In this model, the density of conduction and valence band tail states are extended into the bandgap and overlap each other as shown in Fig. 1. It is worth noting that the mobility in the extended states (delocalized states) is considerably larger in comparison with localized states. Later, the Cohen model was compared with the measured DOS at ($E=E_F$) for chalcogenide glass [14]. It was found that $g(E)$ was on the order of $10^{19}$ cm$^{-3}$ eV$^{-1}$. However, the model could not explain the well-defined localization states of elemental and compound amorphous semiconductors.

Later, the model was improved by Davis et al. [15], who separated the energy range for localized tail states for the CB and VB by introducing $\Delta E_C (E_C - E_A)$ and $\Delta E_V (E_B - E_V)$, respectively, as shown in Fig. 2. In addition to this, they assumed a band of localized state in the middle of the forbidden band. Regardless of the amorphous nature of OSs, they exhibit good electrical properties, particularly a high electron mobility of > 50 cm$^2$V$^{-1}$ s$^{-1}$ [16]. The conduction band minimum (CBM) holds the electron transport path which consists of overlapped $s$ orbitals of spherically shaped metal cations. This creates a conducting path for free electrons, provided by oxygen vacancies, with small effective mass [4, 17]. This in turn increases the electron mobility. However, achieving such a high mobility for holes is difficult. This is due to their transport path in the valence-band maximum (VBM), which comprises localized oxygen $2p$ orbitals. This
makes holes heavier and results in low mobility. Also, the creation of holes is hindered by the high formation energy of the cation vacancies, which are native acceptors.

Based on the observations from disorders and defects in OSs, a comprehensive DOS model was proposed which summarizes all effects, as shown in Fig. 3. The model has exponentially declining states called band tail states and deep-level sub-band mid-gap states also called Gaussian states. These states are presented as a schematic in Fig. 3. It is necessary to identify the origins of these states that contribute to the DOS model.

The spherical s orbitals in the CB are immune to structural disorders. For this reason, the n-type OSs show smaller tails in the CB. On the other hand, the O 2p orbitals near the VBM are highly affected by direction-dependent disorders. This results in larger tails in the VB [4, 18]. Considering these facts, the tail states of the CB and VB are described as [15, 19]:

\[ G_{TA}(E) = g_{TA}(E)e^{-\frac{(E-E_{c})}{U_{TA}}} \]  

(1)

\[ G_{TD}(E) = g_{TD}(E)e^{-\frac{(E-V_{b})}{U_{TD}}} \]  

(2)

where \( E \) is the trap energy. \( G_{TA}(E) \) (acceptor-like states) and \( G_{TD}(E) \) (donor-like states) are exponential decaying tail states with respect to the CB edge densities \( g_{TA}(E) \) (cm\(^{-3}\) eV\(^{-1}\)) at \( E = E_{C} \) and VB edge densities \( g_{TD}(E) \) (cm\(^{-3}\) eV\(^{-1}\)) at \( E = E_{V} \). \( U_{TA} \) and \( U_{TD} \) are characteristic slopes of \( g_{TA} \) and \( g_{TD} \), respectively. These slopes signify the disorder present in the material.

Deep states or Gaussian states are induced in the OS due to a large divergence in the coordination number as compared with a crystalline one, such as vacancies. At the lower half of the bandgap, below the \( E_{F} \) [20], the Gaussian state is present due to the variation in the coordination number of oxygen atoms. Similarly, mis-coordinated cations were suggested to be the source of deep states in the upper half of the forbidden band [21], shall be described as [15, 19]:

\[ G_{GA}(E) = g_{GA}(E)e^{-\frac{(E-E_{U})}{U_{GA}}} \]  

(3)

\[ G_{GD}(E) = g_{GD}(E)e^{-\frac{(E-E_{G})}{U_{GD}}} \]  

(4)

Here, \( G_{GA}(E) \) and \( G_{GD}(E) \) are acceptor-like and donor-like mid-gap states with their respective Gaussian distribution densities \( g_{GA} \) and \( g_{GD} \) with peak energies \( E_{U} \) and \( E_{G} \). \( U_{GA} \) and \( U_{GD} \) are characteristic slopes of \( g_{GA} \) and \( g_{GD} \), respectively.

The total DOS, \( G(E) \), can be written as [15, 19]:

\[ G(E) = G_{TA}(E) + G_{TD}(E) + G_{GA}(E) + G_{GD}(E) \]  

(5)

The DOS model was essentially first developed for amorphous hydrogenated silicon (a-Si:H) material-based TFTs, as demonstrated by Davis et al. [15]. Later, the model was extended for amorphous indium gallium zinc oxide (a-IGZO)-based TFTs by Fung et al. [22] which gives a very high performance compared to a-Si:H TFTs.

### 3 Numerical simulations of OS TFTs

CAD-based numerical simulations are often used since they provide detailed physical insight into the device operation. For the simulation of the TFT device, the TCAD Silvaco (Atlas) tool was employed [23]. It solves the coupled equations, consisting of Poisson, continuity and charge transport equations, for the given device boundary. It also allows the physics of defect states in the active layer using the DOS model. The simulation was performed on staggered bottom-gate TFTs. From the accuracy point of view, high-density meshing has been employed near the active layer/dielectric interface along the Y-axis. Necessary models like field-dependent mobility, defect model, Fermi–Dirac model and interface trap model were applied to the active layer. Along with that, boundary conditions were set for the active layer to regulate the carrier movement within the source and drain electrodes. Moreover, for electrodes, tunneling and thermionic models, along with ohmic contact models, were also used. A discrete DOS model consisting of acceptor-like (ACC) and donor-like (DON) states with 128 trap states each was employed for the simulation. Using this simulation setup, we have simulated the cuprous oxide (Cu₂O)-, tin monoxide (SnO)- and tin oxide (SnO₂)-based TFTs with the comprehensive DOS model.

Fig. 3 Comprehensive DOS model for oxide semiconductors
### 3.1 p-Type Cu$_2$O and SnO TFTs

In general, p-type OSs are rare due to dominant O 2p orbitals which strongly localize the hole and restrict p-type conduction. To overcome this problem, Kawazoe et al. proposed an alternative way to reduce the localization of 2p orbitals, known as chemical modulation of the valence band [24]. In this approach, the 2p orbital undergoes hybridization with metal d or s orbitals of equivalent energy levels. This results in the formation of an extended valence band in the form of bonding and anti-bonding levels. This shifts the valence band edge to an anti-bonding level from the O 2p level due to the closed-shell electronic configuration of both cations and anions. The modification of the band diagram in the VB greatly helps to reduce the localization of holes, and hence improves the hole mobility within the material. This phenomenon is shown in Fig. 4. Based on this, several closed-shell d$_{10}s^0$ and d$_{10}s^2$ metals were identified as a possible choice for the development of p-type OSs [25, 26].

Cuprous oxide, Cu$_2$O (CuI), was recognized as a potential candidate, since it has a closed d$_{10}$ shell whose energy is comparable with oxygen 2p orbital energy [26]. Because it is cation-deficient, it acts as p-type (hole conduction). It has a simple cubic structure with a lattice constant of 4.27 Å. Generally, a copper oxide system at a fixed metal-oxide ratio (stoichiometry) has two stable phases (Cu$_2$O and CuO) and one meta-stable phase paramelaconite (Cu$_4$O$_3$). However, during a synthesis process like sputtering, the copper oxide system becomes non-stoichiometric due to copper vacancies. This makes it possible to tune the electronic properties of semiconducting Cu$_2$O by varying the oxygen partial pressure of the deposition scheme.

To analyze further, first-principles density functional theory (DFT) simulations were performed, which offer valuable insight into defects with various functionality [27]. This helps to compute the formation energy and the transition phase of defects, which influences the electronic structures and hence affects the electrical and optical properties of the system. From the simulation, it was found that the cation deficiency is due to copper vacancies ($V_{Cu}$). These defects have lowest formation energies under both Cu-rich and Cu-poor conditions [26]. The VBM, which mostly consists of Cu$_{d_{10}}$(d$_{10}$) orbitals, is an anti-bonding state. Its acceptor ionization energy or transition level ε(0/−1) is located at $E_V +0.28$ eV, which is relatively shallow. The covalence property allows band broadening that leads to small effective mass and ultimately good carrier mobility [24]. Based on several studies, Cu$_2$O has shown remarkable Hall mobility of > 100 cm$^2$V$^{-1}$s$^{-1}$ [28]. Although there are several computational and experimental works on defects in Cu$_2$O systems, there are no reports on the modeling of p-type conduction using the DOS model. This can be addressed by adopting the proposed DOS model in numerical simulation to fit the measured I–V characteristics of fabricated Cu$_2$O TFTs.

Nam et al. reported the fabrication and characterization of a p-type Cu$_2$O TFT using radio-frequency (RF) magnetron sputtering [29]. On a heavily doped p-type Si substrate, acting as a gate electrode, a 100-nm SiO$_2$ dielectric was thermally grown. Thereafter, a 45-nm thin film of Cu$_2$O was deposited using RF magnetron sputtering followed by annealing at 500 °C for 7 min. Subsequently, using an evaporation technique, Ni contacts were deposited and patterned as source and drain with channel width and length of 1000 μm and 100 μm, respectively. A realistic simulation of a Cu$_2$O TFT was performed with the device structure shown in the inset in Fig. 5b. For the fitting of transfer characteristics, initially noted physical parameters including the effective mass of electrons and holes ($m_e = 0.98 m_0$ and $m_h = 0.66 m_0$) [30] and band hole mobility (47.5 cm$^2$V$^{-1}$s$^{-1}$) [29] are considered. The details of the input parameters are listed in Table 1.

![Fig. 4 Chemical modulation of the valence band between a closed or pseudo-closed metal configuration and an oxide ion [24]](image-url)
For the simulation of the TFT, there are a few key DOS parameters which significantly influence the I–V characteristics. These parameters are $g_{GA}$, $g_{GD}$, $U_{TA}$ and $U_{TD}$. Based on the first-principles study by Raebiger et al. [26], it was found that Cu$_2$O exhibits p-type conduction due to the presence of copper vacancies ($V_{Cu}$). These are acceptor-like vacancies which are present near the VBM. In simulation, we have imitated $V_{Cu}$ with the $g_{GA}$ parameter. Figure 5a shows the effect of $g_{GA}$ on the simulated I–V characteristics. As the $g_{GA}$ value increases, the OFF current of Cu$_2$O TFT increases. This is due to the presence of more acceptor-like vacancies ($V_{Cu}$), which allow more hole current to flow across the channel. With regard to Raebiger et al., the concentration of $g_{GA}$ is quite comparable to the $V_{Cu}$, which is above $10^{20} \text{cm}^{-3} \text{eV}^{-1}$. However, the change in the ON current due to $g_{GA}$ is small. Similarly, the $U_{TD}$ parameter was varied from 60 to 70 meV, and it was found that there are substantial changes in the drain current (inset Fig. 5a). To understand this phenomenon, a probe was placed near the active/dielectric interface layer, and the computed $(E_F - E_v)$ as a function of $V_{GS}$ was plotted for different $U_{TD}$, as shown in Fig. 5b. We can see that as $U_{TD}$ decreases, the Fermi energy $E_F$ approaches $E_v$, which indicates the band-bending phenomenon. Moreover, $U_{TD}$ also signifies the disorders present in the material. These disorders are due to variations in the bond angle, bond lengths and coordination numbers present in the active layer. This causes a rise in the tail states with exponential distribution ($U_{TD}$), also referred to as Urbach energy [31].

Like hole producers ($V_{Cu}$), there are potential hole neutralizers in Cu$_2$O in the form of oxygen vacancies ($V_O$) and copper interstitials (Cui) [26]. However, the formation energy $\Delta H$ is very high in the case of Cui, so we have not considered the effect of Cui in the simulation [26]. Like $V_{Cu}$, $V_O$ also has low formation energy, which can affect the hole.

Fig. 5  a Comparison of simulated transfer characteristics of Cu$_2$O TFTs for various $g_{GA}$ with measured results (RMS error = 3.8%) (inset: variation in $U_{TD}$), b effect of $V_{GS}$ on $(E_F - E_v)$ at the probe (inset: structure of Cu$_2$O TFT), c comparison of simulated transfer characteristics of Cu$_2$O TFTs for various $g_{GD}$ with measured results, d extracted DOS of Cu$_2$O TFT (measured data: [29])
carrier concentration. Since oxygen vacancies contribute to giving away the electrons, they are donor-like states. In our simulation, we relate \( V_0 \) with \( g_{GD} \). Figure 5c shows the simulated transfer characteristics for different \( g_{GD} \). We can observe that higher values of \( g_{GD} \) significantly affect the hole current. The concentration of \( g_{GD} \) is lower than \( g_{GA} \) by an order of magnitude of \(-3\) based on the literature [26]. However, the DOS parameter \( U_{TA} \) does not affect the hole current in any manner. Figure 5a, d shows the fitted \( I-V \) characteristics with experimental data [29] and the DOS profile extracted for the same, respectively.

An alternative approach to the hybridization of O 2p orbitals is to use an electronic structure having a pseudo-closed-shell configuration as shown in Fig. 4 [25], for instance, tin monoxide (SnO), beryllium oxide (Be2O3) and lead oxide (PbO). Amongst these, SnO shows promising results in terms of p-type conductivity [32]. SnO exhibits a tetragonal layer crystal structure, and the formation of the Sn–O–Sn layer is in the <011> direction. At the VB, there is a significant overlap between Sn 5s and O 2p orbitals, which leads to a reduction in the localization of holes [33]. Several research articles have reported on SnO-based p-type TFTs showing field-effect mobility > 3 cm² V⁻¹ s⁻¹, ON/OFF ratio > 10⁵ and subthreshold swing ~ 100 mV/dec [34]. This is largely due to the presence of Sn vacancies (\( V_{Sn} \)) having low defect-formation energy which act as native acceptor-like defects. Its acceptor ionization energy or transition level \( \varepsilon \) (0/−1) is located at \( E_V +0.1 \) eV. For the simulation of the SnO TFT, we have considered the measured results of our earlier works [34, 35]. A bottom-gate staggered TFT configuration was used, where a heavily doped n-type silicon gate was taken as a substrate. On top of it, a hafnium oxide (HfO₂) dielectric of 50 nm thickness was deposited by employing an e-beam evaporation method and later annealed for dielectric activation. After that, a very thin layer of 8-nm thickness of SnO, acting as an active layer, was coated on the dielectric. Thereafter, nickel-based source/drain electrodes were deposited with the help of e-beam evaporation and patterned for channel length and width of 60 and 560 \( \mu \)m, respectively.

Figure 6a, b shows the effect of \( g_{GA} \) and \( U_{TD} \) on the simulated \( I-V \) characteristics of SnO, respectively. As the \( g_{GA} \) value increases, the OFF current of SnO TFT increases. This is due to the presence of more acceptor-like vacancies (\( V_{Sn} \)), which allow more hole current to flow across the channel [36]. Similarly, changes in the \( U_{TD} \) significantly affect the drain current. However, the effect of \( g_{GD} \) is minimal. This is due to the \( V_0 \) defect concentration which is not sufficient to neutralize the \( V_{Sn} \) [36]. Table 1 shows the simulation parameters for SnO TFTs.

### 3.2 n-Type SnO2 TFTs

To validate the compatibility of the DOS model for an n-type OS, we have considered an n-type tin oxide (SnO₂)-based TFT. SnO₂ is possibly the simplest material among OSs. It exhibits a rutile structure where each tin atom is enclosed by six oxygen atoms [37]. Again, each of these oxygen atoms is surrounded by three other tin atoms. It has a direct bandgap of 3.6 eV and oxidation state of 4 (Sn⁴⁺) [37]. The n-type nature of SnO₂ is due to its conduction band minimum (CBM), which consists of Sn 5s orbitals overlapping each other. This allows the free movement of electrons, leading to the low electron effective mass which is between 0.23 and 0.3\( m_0 \) where \( m_0 \) is the mass of the electron (9.1 × 10⁻³¹ kg s). However, its VBM is nearly flat, and thus it has a large hole effective mass. This is due to the presence of oxygen 2p states which are highly localized, hence restricting hole conduction. Although there are various reports on the successful implementation of the DOS model of n-type a-IGZO TFTs [22, 38] and boron indium oxide TFTs [39]; however, SnO₂-based TFTs are rarely modeled [40]. Saji et al. successfully demonstrated the fabrication of a SnO₂ TFT using RF sputtering [41], as follows: from a Sn metal target, a 25-nm thin film of SnO₂ was deposited on the bottom Si substrate (gate electrode) using RF sputtering under different oxygen flow rates. On the top, 100-nm SiO₂ was thermally grown followed by a patterned Ni/Au source and drain deposition using an e-beam evaporation technique with channel width and length of 500 and 500 \( \mu \)m, respectively [41].

Similar to the Cu₂O TFT, the same approach was tested on a SnO₂ TFT for various \( g_{GD}-g_{GA}, U_{TD} \) and \( U_{TA} \). Godinho et al. reported the first-principles study of SnO₂, and it was found that n-type conductivity was due to the presence of

| Symbols | Units | \( Cu_2O \) | SnO | SnO₂ |
|---------|-------|---------|-----|-----|
| \( N_C \) | cm⁻³ | \( 2.47 \times 10^{19} \) | \( 2.41 \times 10^{18} \) | \( 3.51 \times 10^{18} \) |
| \( N_V \) | cm⁻³ | \( 1.11 \times 10^{19} \) | \( 9.13 \times 10^{19} \) | \( 1.13 \times 10^{19} \) |
| \( g_{TA} \) | cm⁻³ eV⁻¹ | \( 2.47 \times 10^{21} \) | \( 2.43 \times 10^{20} \) | \( 1 \times 10^{20} \) |
| \( g_{TD} \) | cm⁻³ eV⁻¹ | \( 1 \times 10^{21} \) | \( 5 \times 10^{20} \) | \( 1.13 \times 10^{21} \) |
| \( U_{TA} \) | meV | 30 | 30 | 20 |
| \( U_{TD} \) | meV | 65 | 70 | 40 |
| \( E_g \) | eV | 2.7 [29] | 0.9 [25] | 3.6 [37] |
| \( \chi_e \) | eV | 3 [29] | 3.7 [43] | 4 [37] |
| \( E_{GA} \) | eV | 0.32 | 0.1 | 0.1 |
| \( E_{GA} \) | eV | 1.5 | 0.52 | 0.8 |
| \( E_{GD} \) | eV | 2.5 | 0.9 | 3.3 |
| \( U_{GD} \) | eV | 0.2 | 0.2 | 0.25 |
| \( g_{GD} \) | cm⁻³ eV⁻¹ | \( 4 \times 10^{17} \) | \( 1 \times 10^{17} \) | \( 1.3 \times 10^{18} \) |
| \( g_{GA} \) | cm⁻³ eV⁻¹ | \( 6.5 \times 10^{20} \) | \( 2 \times 10^{19} \) | \( 2 \times 10^{18} \) |
| \( \mu_p \) | cm²V⁻¹ s⁻¹ | \( 47.5 \times 29 \) | \( 4.8 \times 44 \) | \( 18.6 \times 41 \) |
| \( \xi_t \) | cm²V⁻¹ s⁻¹ | \( 7.6 \times 45 \) | \( 15 \times 43 \) | \( 9 \times 37 \) |

Table 1: Key simulation parameters in the DOS model for \( Cu_2O \), SnO and SnO₂ TFTs

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doubly ionized positively charged oxygen vacancies ($V_{\text{O}}^{2+}$) [42]. According to Kröger–Vink notation, the charge balance can be written as:

$$O_{\text{X}}^X \rightarrow V_{\text{O}}^{2+} + 2e' + \frac{1}{2}O_2(g)$$  \hspace{1cm} (6)

where $O_{\text{X}}^X$ represents oxygen at the oxygen site with a neutral charge. Oxygen anions, according to this equation, escape from the oxygen site and form $V_{\text{O}}^{2+}$ with free electrons. These electrons will go to the conduction band and hence improve the current conduction. Similarly, Zunger et al. reported that low formation energies for both oxygen vacancies and tin interstitial (Sn$_i$) contributed to n-type conduction [37]. Based on these observations, we have varied the $g_{\text{GD}}$ to imitate $V_{\text{O}}^{2+}$ and/or Sn$_i$ to fit the measured results. When $g_{\text{GD}}$ concentration increases from low to high, more electrons are induced into the CB, which results in more drain current, as shown in Fig. 7a. No substantial changes were observed due to the change in the $U_{\text{TD}}$. This could be because the CB of SnO$_2$ is derived from Sn 5s states, as they are spherically symmetrical and immune to directionally dependent disorders. The same is not possible for Cu$_2$O and SnO, since their VB is derived from hybridized Cu–3d–O 2p and Sn 5s–O 2p, respectively. This leads to a large value of VB Urbach energy ($U_{\text{TD}}$) [18]. In this perspective, achieving $U_{\text{TD}}$ less than 30 meV is highly unrealistic based on the available fabrication methods for OS development. Similarly, we have also varied the $g_{\text{GA}}$ which relates to the $V_{\text{Sn}}$. However, the formation energy of $V_{\text{Sn}}$ is larger than the $V_{\text{O}}^{2+}$, so it is highly unlikely to affect the drain current in a realistic scenario [33]. In addition, no changes were observed for different $U_{\text{TD}}$ values on the drain current. Figure 7b–d shows the fitted transfer and output characteristics with the measured data and DOS of SnO$_2$, respectively [41].

Table 2 lists the overall performance of TFTs based on different channel layer materials. It was observed that the performance of n-type TFTs are much better than p-type TFTs, especially the a-IGZO TFT reported by Fung et al.
However, many researchers are still actively developing high-performance p-type TFTs. Caraveo et al. demonstrated a high-performance SnO TFT by carefully controlling the SnO phase [32]. This yielded high field-effect mobility of 6.75 cm² V⁻¹ s⁻¹, which is the highest overall among p-type-based TFTs. However, it still has high SS and low ON/OFF current ratio. This is due to the presence of traps/defects at/near the channel/interface of the TFT. To suppress these defects, techniques such as plasma fluorine treatment of SnO have been employed [34]. Rajshekar et al. studied...
this technique through TCAD simulation and found that these defects are tin and oxygen vacancies [35].

Figure 8 summarizes the physical modeling of OS-based TFTs. It shows the probability of various defects in the material system based on their formation energy. It was found that cation vacancies were responsible for hole conduction in p-type TFTs, while anion vacancies and/or metal interstitials were responsible for electron conduction in n-type TFTs. This was observed by assigning the cation vacancies to $g_{GA}$ and anion vacancies and/or metal interstitials to $g_{GD}$.

4 Conclusion

This paper presents a comprehensive physical model for the TCAD-based simulation of n- and p-type TFTs with OSs. The model is developed from the earlier understanding of the density of states in conduction/valence bands and a forbidden bandgap. The model gives insight into the physics of carrier transport and device operation in TFTs. It was observed that the tail states due to disorders and deep states due to bulk defects of OSs are responsible for the p- and n-type conductivity. Validation of the proposed model was performed by comparing the simulated $I$–$V$ characteristics with measured results of p-type and n-type TFTs. With an RMS error of <4%, an excellent fitting was observed, and the density of tail and defect states was computed successfully. These understandings and specifications of OSs may help engineers and industries in developing high-performance circuits for high-definition displays, solar cells and flexible electronics.

Acknowledgements The authors thank the Council of Scientific and Industrial Research (CSIR), Government of India, for the financial support (File No. 09/844(046)/2018-EMR-I). The authors thank Dr. C. H. Cheng of National Taiwan Normal University, Taiwan, Dr. Uma Mahendra Kumar, Vellore Institute of Technology, Vellore, and Dr. S. Parthiban of PSG Institute of Advanced Studies, Coimbatore, India. The authors also thank the Editor and the anonymous reviewers for their useful comments and suggestions.

Author contributions Kadiyam Rajshekar contributed to the development of a comprehensive density-of-states model for oxide semiconductors and applied the model on thin film transistors of various oxide
semiconductors through numerical simulations. D. Kannadan has supervised and supported the research works with Kadiyan Rajsherek.

Funding No funding source information is available.

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

References

1. Fortunato, E., Barquinha, P., Martins, R.: Oxide semiconductor thin-film transistors: a review of recent advances. Adv. Mater. 24(22), 2945–2986 (2012). https://doi.org/10.1002/adma.201103228

2. Hosono, H., Yasukawa, M., Kawazoe, H.: Novel oxide amorphous semiconductors: transparent conducting amorphous oxides. J. Non Cryst. Solids 203, 334–344 (1996). https://doi.org/10.1016/0022-3093(96)00367-5

3. The Magic of Transparent Technology/Pro Display. https://prodisplay.com/the-magic-of-transparent-technology/. Accessed 17 Feb 2021

4. Nomura, K., Ohta, H., Takagi, A., et al.: Room-temperature fabrication of transparent flexible thin-film transistors using amorphous oxide semiconductors. Nature 432, 488–492 (2004). https://doi.org/10.1038/nature03090

5. Lim, W., Jang, J.H., Kim, S.H., et al.: High performance indium gallium zinc oxide thin film transistors fabricated on polyethylene terephthalate substrates. Appl. Phys. Lett. 93, 082102 (2008). https://doi.org/10.1063/1.2975959

6. Chopra, K.L., Major, S., Pandya, D.K.: Transparent conductors—a status review. Thin Solid Films 102, 1–46 (1983)

7. Lewis, B.G., Paine, D.C.: Applications and processing of transparent conducting oxides, MRS Bull. 25, 22–27 (2000). https://doi.org/10.1557/mrs2000.147

8. Le, Y., Shao, Y., Xiao, X., et al.: Indium-tin-oxide thin-film transistors with in situ anodized Ta2O5 passivation layer. IEEE Electron Device Lett. 37, 603–606 (2016). https://doi.org/10.1109/LED.2016.2548785

9. Cho, M.H., Seol, H., Yang, H., et al.: High-performance indium gallium zinc oxide thin-film transistors fabricated by atomic layer deposition. IEEE Electron Device Lett. 39, 688–691 (2018). https://doi.org/10.1109/LED.2018.2812870

10. Martins, R., Nathan, A., Barros, R., et al.: Complementary metal oxide semiconductor technology with and on paper. Adv. Mater. 23, 4491–4496 (2011). https://doi.org/10.1002/adma.201102232

11. Nandy, S., Banerjee, A., Fortunato, E., Martins, R.: A review on Cu2O and Cu-based p-type semiconducting transparent oxide materials: promising candidates for new generation oxide based electronics. Rev. Adv. Sci. Eng. 2, 273–304 (2013). https://doi.org/10.11066/rase.2013.1045

12. Hogarth, C.A.: Hall constant of cadmium oxide [3]. Nature 167, 521–522 (1951). https://doi.org/10.1038/167521a0

13. Cohen, M.H., Fritzschke, H., Ovshinsky, S.R.: Simple band model for amorphous semiconductor alloys. Phys. Rev. Lett. 22, 1065–1068 (1969). https://doi.org/10.1103/PhysRevLett.22.1065

14. Nwachuku, A., Kuhn, M.: Tunneling into amorphous germanium films. Appl. Phys. Lett. 12, 163–165 (1968). https://doi.org/10.1063/1.1651936

15. Davis, E.A., Mott, N.F.: Conduction in non-crystalline systems. V. Conductivity, optical absorption and photocconductivity in amorphous semiconductors. Philos. Mag. 22, 903–922 (1970). https://doi.org/10.1080/14786437008221061

16. Leeneheer, A.J., Perkins, J.D., Van Hest, M.F.A.M., et al.: General mobility and carrier concentration relationship in transparent amorphous indium zinc oxide films. Phys. Rev. B—Condens. Matter Mater. Phys. 77, 1–5 (2008). https://doi.org/10.1103/PhysRevB.77.115215

17. Hosono, H., Kikuchi, N., Ueda, N., Kawazoe, H.: Working hypothesis to explore novel wide band gap electrically conducting amorphous oxides and examples. J. Non Cryst. Solids 198–200, 165–169 (1996). https://doi.org/10.1016/0022-3093(96)80019-6

18. Robertson, J.: Disorder and instability processes in amorphous conducting oxides. Phys. Status Solidi Basic Res. 245, 1026–1032 (2008). https://doi.org/10.1002/pssb.200743458

19. Kemp, M., Meunier, M., Tannous, C.G.: Simulation of the amorphous silicon static induction transistor. Solid State Electron 32, 149–157 (1989). https://doi.org/10.1016/0038-1101(89)90182-2

20. Sallis, S., Butler, K.T., Quackenbush, N.F., et al.: Origin of deep subgap states in amorphous indium gallium zinc oxide: chemically disordered coordination of oxygen. Appl. Phys. Lett. (2014). https://doi.org/10.1063/1.4883257

21. Körner, W., Urban, D.F., Eilsässer, C.: Origin of subgap states in amorphous In–Ga–Zn–O. J. Appl. Phys. (2013). https://doi.org/10.1063/1.4826895

22. Fung, T.C., Chuang, C.S., Chen, C., et al.: Two-dimensional numerical simulation of radio frequency sputter amorphous In–Ga–Zn–O thin-film transistors. J. Appl. Phys. 106, 1–10 (2009). https://doi.org/10.1063/1.3234400

23. Silvaco: Technology computer aided design (TCAD) software (2013). https://doi.org/10.1201/b14860

24. Kawazoe, H., Yasukawa, M., Hyodo, H., et al.: P-type electrical conduction in transparent thin films of CuAlO2. Nature 389, 939–942 (1997)

25. Ogo, Y., Hiramatsu, H., Nomura, K., et al.: Tin monoxide as an s-orbital-based p-type oxide semiconductor: electronic structures and TFT application. Phys. Status Solidi 206, 2187–2191 (2009). https://doi.org/10.1002/pssa.200881792

26. Kohn, W., Sham, L.J.: Self-consistent equations including exchange and correlation effects. Phys. Rev. 140, A1133 (1965). https://doi.org/10.1103/PhysRev.140.A1133

27. Matsuzaki, K., Nomura, K., Yanagi, H., et al.: Epitaxial growth of high mobility Cu2O thin films and application to p-channel thin film transistor. Appl. Phys. Lett. 93, 3–6 (2008). https://doi.org/10.1063/1.3026539

28. Nam, D.-W., Cho, I.-T., Lee, J.-H., et al.: Active layer thickness effects on the structural and electrical properties of p-type Cu2O thin-film transistors. J. Vac. Sci. Technol. B Nanotechnol. Microelectron. (2012). https://doi.org/10.1116/1.4764110

29. Goltzene, A., Schwab, C., Wolf, H.C.: Carrier resonance in Cu2O. Solid State Commun. 18, 1565–1567 (1976). https://doi.org/10.1016/0038-1098(76)90394-X

30. Urbach, F.: The long-wavelength edge of photographic sensitivity and of the electronic Absorption of Solids [8]. Phys. Rev. 92, 1324 (1953). https://doi.org/10.1103/PhysRev.92.1324

31. Caraveo-Frescas, J.A., Nayak, P.K., Al-Jawhari, H.A., et al.: Record mobility in transparent p-type thin monoxide films and devices by phase engineering. ACS Nano 7, 5160–5167 (2013). https://doi.org/10.1021/nn400852r
33. Ogo, Y., Hiramatsu, H., Nomura, K., et al.: p-channel thin-film transistor using p-type oxide semiconductor. SnO 032113, 1–4 (2012). https://doi.org/10.1063/1.2964197
34. Chen, P.C., Chiu, Y.C., Zheng, Z.W., et al.: Influence of plasma fluorination on p-type channel tin-oxide thin film transistors. J. Alloys Compd. 707, 162–166 (2017). https://doi.org/10.1016/j.jallcom.2016.11.294
35. Rajshekar, K., Hsu, H.H., Kumar, K.U.M., et al.: Effect of plasma fluorination in p-type SnO TFTs: experiments, modeling, and simulation. IEEE Trans. Electron Devices 66, 1314–1321 (2019). https://doi.org/10.1109/TED.2019.2895042
36. Togo, A., Oba, F., Tanaka, I., Tatsumi, K.: First-principles calculations of native defects in tin monoxide. Phys. Rev. B 74, 195128 (2006). https://doi.org/10.1103/PhysRevB.74.195128
37. Çetin, K., Zunger, A.: Origins of coexistence of conductivity and transparency in SnO. Phys. Rev. Lett. 2, 7–10 (2002). https://doi.org/10.1103/PhysRevLett.88.095501
38. Stewart, K.A., Gouliouk, V., Mcglone, J.M., et al.: Side-by-side comparison of single- and dual-active layer oxide TFTs: experiment and TCAD simulation. IEEE Trans. Electron Devices 64(10), 1–6 (2017)
39. Stewart, K.A., Gouliouk, V., Keszler, D.A., Wager, J.F.: Sputtered boron indium oxide thin-film transistors. Solid-State Electron. 137, 80–84 (2017)
40. Shang, Z.W., Ma, J., Liu, W.D., et al.: Performance investigation of an n-type tin-oxide thin film transistor by channel plasma processing. IEEE J. Electron Devices Soc. 8, 485–489 (2020). https://doi.org/10.1109/JEDS.2020.2986172
41. Saji, K.I., Mary, A.P.R.: Tin oxide based p and n-type thin film transistors developed by RF sputtering. ECS J. Solid State Sci. Technol. 4, Q101–Q104 (2015). https://doi.org/10.1149/2.0091509jss
42. Godinho, K.G., Walsh, A., Watson, G.W.: Energetic and electronic structure analysis of intrinsic defects in SnO2. J. Phys. Chem. C 113, 439–448 (2009). https://doi.org/10.1021/jp807753t
43. Quackenbush, N.F., Allen, J.P., Scanlon, D.O., et al.: Origin of the bipolar doping behavior of SnO from X-ray spectroscopy and density functional theory. Chem. Mater. 25(15), 3114–3123 (2013). https://doi.org/10.1021/cm401343a
44. Fortunato, E., Barros, R., Barquinha, P., et al.: Transparent P-type SnOx thin film transistors produced by reactive RF magnetron sputtering followed by low temperature annealing. Appl. Phys. Lett. 97, 52105 (2010). https://doi.org/10.1063/1.3469939
45. Madelung, O., Rossler, U., Schulz, M., et al.: Cuprous oxide (Cu2O) dielectric constant. In: Non-Tetrahedrally Bonded Elements and Binary Compounds I, pp. 1–2 (2005). https://doi.org/10.1007/10681727_58
46. Rajshekar, K., Hsu, H.H., Kumar, K.U.M., et al.: physical modeling of p-type fluorinated Al-doped tin-oxide thin film transistors. IEEE J. Electron Devices Soc. 8, 1–1 (2020). https://doi.org/10.1109/jeds.2020.3018463
47. Singh, S., Chakrabarti, P.: Simulation fabrication and characterization of ZnO based thin film transistors grown by radio frequency magnetron sputtering. J. Nanosci. Nanotechnol. (2012). https://doi.org/10.1166/jnn.2012.5194

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