



Modeling of the Density of States in Field-Effect Zinc Oxide Semiconductor Devices Fabricated by Ultrasonic Spray Pyrolysis on Plastic Substrates ⁺

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Abstract: In this work, using a physically based simulator, the modeling of the density of states (DOS) through the fitting of the electrical characteristics in field-effect devices is presented. The transfer characteristic of zinc oxide (ZnO) thin-film transistors is simulated, along with the capacitance–voltage curves in metal-insulator-semiconductor capacitors using ZnO as an active layer. The ZnO semiconductor devices were fabricated by high-frequency ultrasonic spray pyrolysis on poly-ethylene terephthalate plastic substrates. Different aspects were considered and discussed to model the device interfaces.

Keywords: density of states; ZnO; spray pyrolysis; TFTs; MIS capacitor

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1. Introduction

Metal-oxide semiconductors have received considerable attention due to their relevance in thin-film transistor (TFTs) technologies [1,2]. In addition, their low-temperature process (≤ 200 °C), transparency, high stability, structural uniformity and compatibility with large-area substrates make them very attractive for commercial applications [3]. The main bottleneck for the commercialization of these devices is the understanding of the density of states (DOS) within the bandgap, which is the key to develop analytical models enabling the design of new circuits.

The simulation of these systems before their achievement is useful to calculate the electrical characteristics through numerically solving semiconductor equations [4], where the device structure, material properties and physical models are used to describe the carrier transport properties and the electronic states [5]. Notably, the electronic properties of these oxide semiconductors are still not completely understood, and the role of tail and deep states within the bandgap in transport properties of oxide TFTs is still under investigation [6]. This motivates the modeling of the DOS and makes this research crucial to reproduce the electrical characteristics of oxide TFTs [7].

In this study, the modeling of the DOS through the fitting of the transfer characteristics of zinc oxide (ZnO) TFTs and the capacitance–voltage curves in metal-insulator-semiconductor (MIS) capacitors using ZnO as an active layer is presented. The ZnO semiconductor devices were fabricated by high-frequency ultrasonic spray pyrolysis on polyethylene terephthalate plastic substrates [8]. We propose an accurate estimation of the DOS through calculations performed in similar field-effect devices of the same dielectric–semiconductor interface, since this interface plays an important role to induce conductive channels in TFTs, as well as in the accumulation and depletion regions of MIS capacitors. The results show the agreement existing between the experimental data and the simulated electrical characteristics of ZnO field-effect devices. In this work, different aspects were considered and discussed to model the DOS.

2. Experimental

Figure 1 shows the schematic structures of the fabricated devices. The plastic substrates used were made of commercial ITO-coated PET, purchased from Sigma-Aldrich and used as is. The transparent dielectric consists of a thin film of spin-on glass (SOG). The SOG precursor solution was prepared by 33% of LSF47 solution in 66% of LSFD1 diluent, provided by Filmtronics Inc. PA, USA. The SOG solution was deposited onto the ITO/PET substrates by spin-coating at 3000 rpm for 30 s and cured for 10 min at 100 °C and 2 h at 200 °C, resulting in 85 nm-thick SOG film. For TFTs, 100 nm-thick aluminum ebeam evaporated was patterned as source and drain electrodes, followed by the ultrasonic deposition of 90 nm-thick ZnO. The ZnO precursor solution was prepared from 0.2 M of zinc acetate (Sigma-Aldrich) diluted in methanol. For MIS capacitors, the same substrate, dielectric film and ZnO films were used. The top contacts were made of ITO films ultrasonically deposited, using an ITO precursor solution prepared from indium chloride (Sigma-Aldrich) at a molar concentration of 0.3 M, and tin chloride (Sigma-Aldrich) diluted in methanol at a molar concentration of 5 wt%.



Figure 1. (a) Schematic cross-sectional view of the bottom-gate coplanar TFT, (b) schematic crosssectional view of the MIS capacitor, (c) photograph of ZnO TFTs fabricated onto PET substrates and (d) photograph of MIS capacitor fabricated on PET substrates.

3. Simulation

The electrical properties of amorphous materials are strongly related to the DOS [9]. In our approach, it is assumed that the total density of states is composed by acceptor-like states (near the conduction band) and donor-like states (near the valence band), both are composed by the sum of tails' states and deep states. Therefore, a numerical approximation of the DOS distribution, g(E), is given by [10–12]:

$$g(E) = N_{TA} \exp\left(\frac{E - E_C}{W_{TA}}\right) + N_{TD} \exp\left(\frac{E_v - E}{W_{TD}}\right) + N_{GA} \exp\left(\frac{E_{GA} - E}{W_{GA}}\right) + N_{GD} \exp\left(\frac{E - E_{GD}}{W_{GD}}\right), \tag{1}$$

where N_{TA} and N_{GA} are the density of tail-acceptor and deep-acceptor states' distribution respectively, W_{TA} and W_{GA} are the characteristic decay energies of tail-acceptor and deep-acceptor states, N_{TD} and N_{GD} are the density of tail-donor and deep-donor states, W_{TD} and W_{GD} are the characteristic decay energy for donor states and E_{GA} and E_{GD} are the peak energy distribution for both acceptor and donor states. The results presented are representative of devices with channel lengths, L, from 10 to 65 μ m and a channel width, W, of 120 μ m. Discrete trap energy levels were considered in the calculations.

4. Results and Discussion

Figure 2 shows the experimental and simulated electron transfer characteristics of the ZnO TFTs we have achieved on plastic substrates. The parameters used for the DOS calculation are summarized in Table 1. These values are in the range of the ones reported in the literature for other ZnO TFTs [12–18]. Although it is usually hard to reproduce the subthreshold region of TFTs, since this region is more affected by the DOS, our simulated curve is found to be consistent with the electrical characteristics exhibited below and above the threshold region [19].



Figure 2. Experimental and simulated transfer characteristics of the ZnO TFTs at V_{ds} = 25 V.

On the other hand, since the DOS was modeled in MIS capacitors of the same dielectric–semiconductor interface and g(E) affects the surface potential (ϕ_s), the capacitance– voltage curves should depend on g(E) [20,21]. The electrons trapped in the localized states are exited and transferred towards the conduction band, which affects the capacitance.

Figure 3 shows the C-V characteristics simulated and measured in MIS capacitors. The experimental data match with the calculations obtained using the DOS parameters presented in Table 1. In this process, the DOS was modeled by fitting the electrical characteristics for both the TFTs and the MIS capacitors. The DOS parameters were adjusted to fit the experimental data. The simulations also accounted for the contact resistance effects, which are known to have an important effect in the electrical characteristics of field-effect devices. In Ref. [12], a higher density of acceptor-like states was necessary to compensate the contact resistance contribution. In order to compensate parasitic contributions, the contact resistance was set to 0.1 ohm-cm² for each contact.



Figure 3. Simulated and experimental C-V characteristics of ZnO MIS capacitors.

Table 1. Main parameters used in the simulations.

Parameters	ZnO	Description
Eg (eV)	3.05	Energy gap
Nта (ст ⁻³ eV ⁻¹)	3.5×10^{20}	Density of tail-acceptor states
Ntd (cm ⁻³ eV ⁻¹)	4.0×10^{20}	Density of tail-donor states
WTD (eV)	0.05	Decay energy of tail-donor states
Wta (eV)	0.025	Decay energy of tail-acceptor states
N_{GA} (cm ⁻³ eV ⁻¹)	1.0×10^{17}	Density of deep-acceptor states
N_{GD} (cm ⁻³ eV ⁻¹)	1.5×10^{19}	Density of deep-donor states
Wgd (eV)	0.1	Decay energy of deep-donor states
Wga (eV)	0.05	Decay energy of deep-acceptor states
$E_{GD}(eV)$	0.1	Peak energy of deep-donor states
Ega (eV)	0.35	Peak energy of deep-acceptor states
μ_n (cm ² /Vs)	15	Electron band mobility
$\mu_p (\mathrm{cm}^2/\mathrm{Vs})$	0.1	Hole band mobility

5. Conclusions

In summary, the DOS was modeled to successfully reproduce the experimental electrical characteristics of ZnO TFTs and MIS capacitors. An accurate estimation of the DOS was also obtained by fitting the electrical characteristics in both TFTs and MIS capacitors. The advantage of using physically based simulations is that the DOS of oxide semiconductor films in field-effect devices can be modeled by separating the contribution of each device interface.

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Data Availability Statement: Data is contained within the article.

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