An Effective-Medium TCAD Model of Amorphous In-Ga-Zn-O (a-IGZO) Suitable For Large-Area Devices

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***Abstract*—a-IGZO is a disordered material whose transport is typified by percolative flow through a rolling landscape of a spatially-varying conduction-band-edge. Our previous Microscopic TCAD model of a-IGZO replicated percolative flow via directly simulating this spatial variation. However, this is difficult for large-area devices as it requires fine spatial resolution. Here we introduce a new Effective-Medium TCAD model that is shown to be accurate (relative to both the Microscopic model and experiment) in the coarse-gridding and large-device regime.**

Keywords—IGZO, TCAD, amorphous oxide semiconductors

I. Introduction

Amorphous indium gallium zinc oxide (a-IGZO) is a material with ever-growing interest for a variety of applications owing to its wide band-gap, intrinsic n-type doping, amorphous nature and unusually high mobility (relative to other amorphous materials). The importance of being amorphous relates to the fact that it can be applied conformally both in thin-films and to geometries with extreme aspect ratios. Since a-IGZO has such a wide band-gap this conformal film will also be transparent, which is what motivated its first applications as a thin-film transistor channel material for optical displays that may be applied to a flexible substrate [1].

Furthermore, beyond that, since an amorphous material (unlike a crystalline material) will have no unsatisfied dangling chemical bonds at a material surface, a-IGZO films exhibit extremely low interface trap densities and thus extremely good subthreshold swings. This behavior, coupled with the possibility for high-quality conformal deposition and high mobility, has also made a-IGZO an attractive channel material in vertical NAND applications [2]. In these devices, an extremely deep hole is etched and must be contoured conformally with a thin channel material. Conventionally, silicon has been used for this purpose but the need for conformal deposition in such extreme aspect ratios has meant that the resulting channel was of a very poor quality and heavily polycrystalline.

A final key feature of a-IGZO is its low OFF-current. This property is again partially owed to its wide band-gap and intrinsic n-doping. In addition, the chemical bonding environment of oxygen within a-IGZO, which is highly directional and anisotropic and thus impedes the flow of holes in the valence band when in the amorphous state, plays an important role. This low OFF-current has also prompted investigation into a-IGZO's potential as a selector transistor in DRAM [3] which serves to prevent the escape of accumulated charge from the memory capacitor (and thus should be highly resistive to carrier flow when the selector is in the OFF state).

However, a generic feature of disordered materials, like a-IGZO, is that their conduction band edge (the valence band can be neglected due to intrinsic n-type doping and wide-band

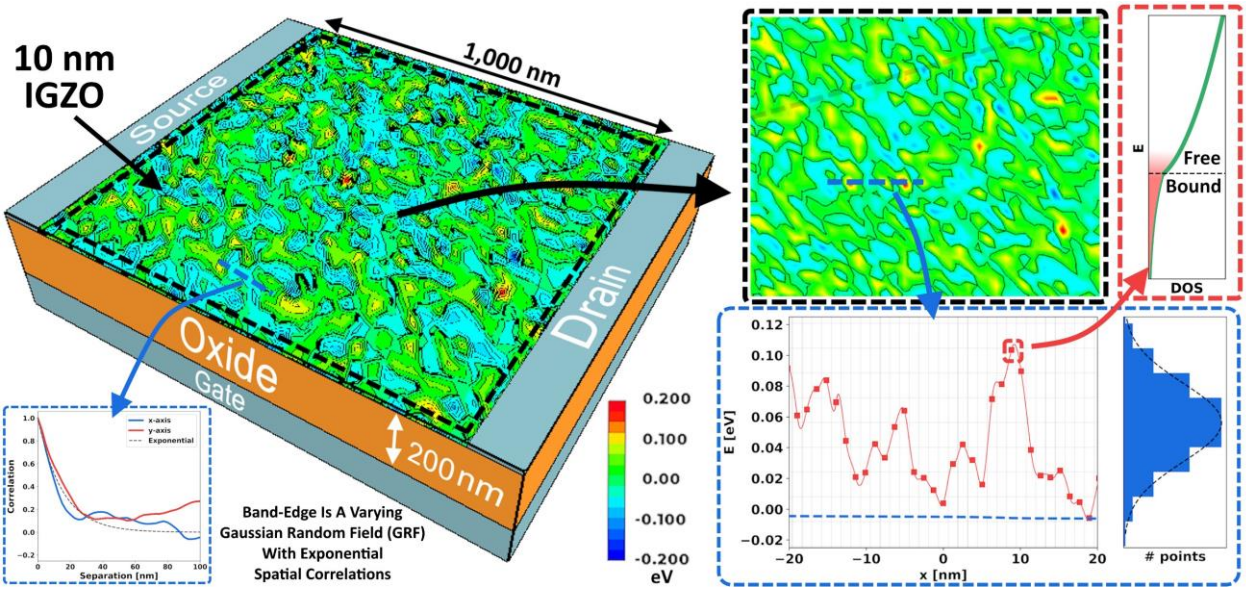

Figure 1: Conceptual breakdown of Microscopic model where a spatially correlated Gaussian Random Field is generated resulting in a rolling landscape band-edge. Band tails are also included.

gap) becomes blurred in both space and energy [4,5]. This can be conceptualized (see Figure 1) as the conduction band becoming a rolling landscape of "hills" and "valleys" where each point on that landscape has an energy spectrum that includes both a range of energies higher than the band-edge energy representing bulk-like free carriers and an exponentially decaying band-tail for energies below the band-edge, in the band-gap, that represents bound carriers.

Transport through this disordered landscape is then highly percolative in nature and any mobility model must take this into account. Previously in [6], we developed a "Microscopic Variability Model" of IGZO that generated a spatially-correlated Gaussian Random Field (GRF) to act as the band-edge whose tunable correlation length would act as the characteristic size of "hills" and "valleys". This model captured percolative transport in a straightforward and natural way as carriers flow through the landscape. In order to ensure numerical stability despite the wide band-gap of a-IGZO, a solver was used based on quasi-Fermi-level-transport (QFT) [7], a reworking of the drift-diffusion (DD) formalism to handle ultra-low carrier concentrations. This Microscopic model was not only a mobility model but also a variability model with each unique instance of the landscape affecting the results. We also showed that this model can very accurately reproduce experimental data from [8] on a 10 nm thick back-gated IGZO TFT (see Figure 3).

However, a fundamental shortcoming of this model is that the gridding in a device must be much smaller than the correlation length in order for the "hills" and "valley" to be sufficiently resolved and accurate percolation to be captured. This is an issue given that, as was mentioned, one of the key application areas of a-IGZO is TFTs [1], which are often microns large. Thus there is a need for an "Effective-Medium" (or just "Effective") model of a-IGZO suitable for TCAD simulation on large devices. Here we construct such a model.

II. Methods and Discussion

Our TCAD model is based on the compact model of Nenashev et al [9] which envisions the same sort of rolling landscape as the Microscopic model, where the conduction band edge, $E_c(r)$, varies in space throughout the film. This landscape is concretely defined by a Gaussian distribution

$$\mathrm{G(E_c)} = exp\left(-\frac{1}{2}\left(\frac{E_c - E_{c0}}{\delta_c}\right)^2\right)/\sqrt{2\pi\delta_c^2}$$

with a standard deviation of δ_c that represents the fraction of the system volume that has a conduction band-edge between E_c and $E_c + dE_c$.

In the Nenashev model the equation for the total effective carrier concentration in the amorphous system (n_{am}) is then:

$$\mathrm{n_{am}} = \int_0^\infty G(E_c) n_r(E_c, E_F) dE_c$$

where n_r represents the expected bulk carrier concentration if the system had a uniform non-varying conduction band-edge of E_c. Thus, the interpretation is that the effective concentration results from an integral over the carrier concentration of each region with a given E_c weighted by the relative volume fraction of the system with that E_c.

This equation for the carrier concentration contains no aspect of percolative behavior as all carriers, regardless of their location in the landscape, contribute their charge to the system and thus are relevant to the electrostatics.

However, percolation physics are injected into this model by how the conductivity is then defined:

$$\mathrm{\sigma_{am}} = \int_{\theta_c}^\infty G(E_c)\sigma_r(E_c, E_F) dE_c$$

which is written in terms of the functions σ_r, which represent the regular bulk conductivity of a carrier given a band-edge of E_c.

Note that the fundamental difference between the definition of the effective carrier concentration, n_{am}, and the effective conductivity, σ_{am}, in the Nenashev model is that the integral in σ_{am} is bounded from below by a certain percolation threshold, θ_c. The effect of this is to enforce the conceptual idea that in this rolling landscape only carriers above a certain "altitude" or critical E_c have a clear percolative path from one end of the system to the other without being trapped in any valley or blocked by any ridge.

Here we extend this compact model to a TCAD model by applying it on a per-mesh-point basis. First the electrostatic Poisson system is solved to determine the necessary charge or electron density at a given point as normal. However, when a quasi-Fermi-level is derived from that density we instead use the Gaussian weighted expression n_{am} instead of the regular bulk $n(E_{c0}, E_F)$ and thus determine at each point an "amorphous" Fermi level, $(E_F)_{am}$, that is different from that for a conventional system. Since the expression for n_{am} is not analytical, calculation is aided by building a dynamically growing look-up table for $n_{am} \rightarrow (E_F)_{am}$ as the simulation runs. This amorphous Fermi-level is then used to calculate the conductivity and thus mobility according to σ_{am}. The workings of this Effective-Medium TCAD model are described in Figure 2.

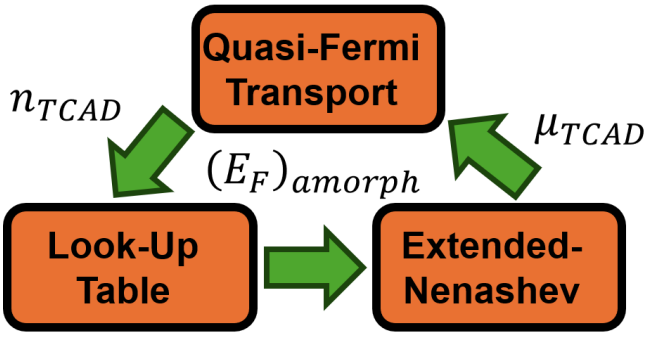

Figure 2: Flow of Effective-Medium TCAD model. Regular drift-diffusion is solved to determine, at each point, charge density (n_{TCAD}), from this $(E_F)_{\mathrm{am}}$ is determined via inverting the expression for n_{am} and a backward Look-up Table. This is then fed into the Nenashev percolation mobility model to supply a μ_{TCAD} at each point which is fed back to the quasi-Fermi transport solver

In order to most closely match the TCAD model to the original compact model, which was found to accurately reproduce the experimental data of [8], a constant mobility of μ_0 was assumed everywhere in the system. In addition, Schottky contacts with a tunable barrier height were assumed at the contacts. Note that mobility is extracted from this model

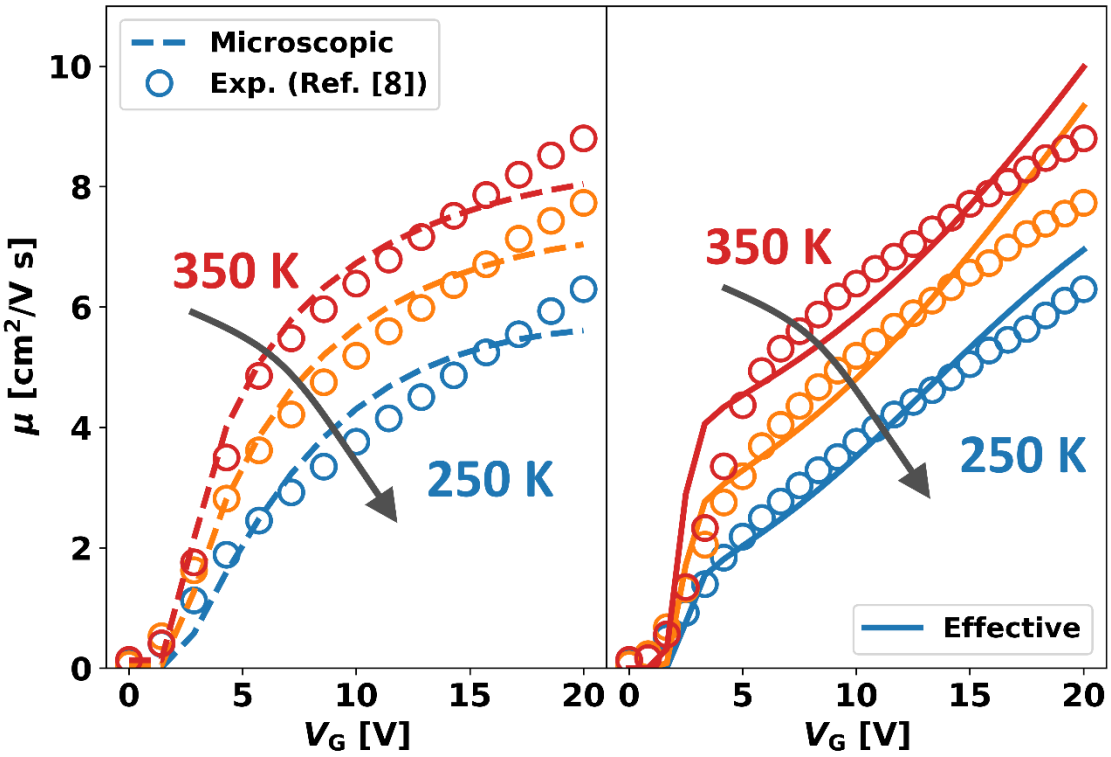

Figure 3: Mobility vs. gate voltage for different temperatures. The best-fit predictions of the Effective-Medium model are compared to the Microscopic model and to experimental results from [8]

by simulating an $I_D - V_G$ curve, taking the slope and applying the following expression:

$$\mu_{eff} = \frac{L}{W} \times \frac{1}{V_D C_{ox}} \times \frac{dI_D}{dV_G}$$

Given this it is worthwhile to reiterate the situation being simulated: there is a rolling landscape of hills and valleys and although at any given point in this landscape a constant mobility model is being used, and thus at any given point the mobility is voltage- and temperature- independent, the effective result of both the percolative flow through this landscape and the serial-resistance-effect of the Schottky contacts result in an effective mobility, μ_{eff}. This mobility is directly extracted from a $I_D - V_G$ curve in a manner analogous to what is done in real experiment and it is this mobility that has an emergent voltage- and temperature-dependence.

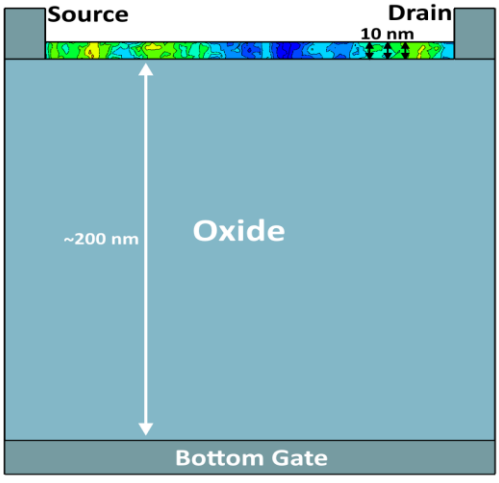

Figure 4: Simulated thin-film transistor device

A comparison of the predicted mobility of the Effective-Medium model versus that of the Microscopic TCAD model of [6] and experimental results of [8] is shown in Figure 3. The 3D simulated structure that was used is shown in cross-section in Figure 4. This thin-film transistor consisted of a 180 nm × 180 nm × 10 nm thick a-IGZO layer on a back-gated device with a 200 nm thick bottom SiO_2 oxide and Schottky source and drain contacts. The entire device was undoped, though for all but the lowest gate voltages the gate-induced carrier density far exceeds any a-IGZO intrinsic doping level, making doping a minor effect. The results in Figure 3 were generated using the best-fit parameters of 0.1125 eV for δ_c, 12.0 $cm^2/V{\cdot}s$ for μ_0 and an assumed Schottky source/drain contact barrier height of 0.4 eV.

Note that although the fits shown in Figure 4 for the effective model are quite good, in the original Nenashev paper ([8]) they were even better. The reason for this discrepancy is that in [8] a compact model is used where the carrier density is assumed to both be a single number and to have an exactly linear dependence on the gate voltage (i.e. $n_{am} = c(V_G - V_{th}(T))$. Furthermore, the threshold voltage used for each temperature curve is treated as a free parameter and fitted independently for each value of the temperature.

Conversely, in our "Effective" model a true TCAD simulation is performed and the model is applied at each site with the carrier density having a different value throughout the device. In addition, the same simulation parameters are used for all temperatures. Thus, these differences account for the discrepancy in fit.

Also note that the results for the Microscopic model here are somewhat worse than those shown in [9]. The reason for that is that in [9] the oxide thickness was treated as a fittable parameter where here it was fixed to be 200 nm.

Finally, to prove that the new model can be applied to large area devices we compare the root-mean-square (RMS) error between the results of very fine gridding (2.5 nm mesh size in the thin-film plane, 2.0 nm mesh size in the transverse in-film direction) for the same device versus a coarser gridding. As can be seen in Figures 5 and 6, the Effective model performs extremely well even for coarse meshes where the Microscopic model suffers substantial degradation in mobility predictions.

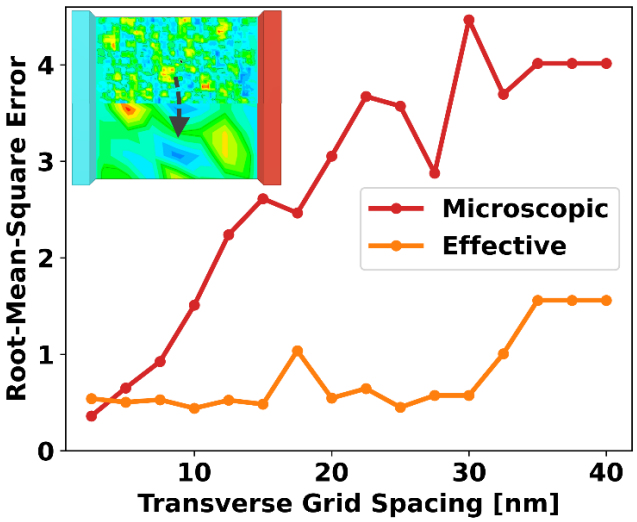

Figure 5: The root-mean-square (RMS) difference between the Microscopic and Effective-Medium models versus experimental results from [8] as the TCAD grid is made coarser

III. Conclusions

In this work an Effective-Medium model of a-IGZO was put forward which is accurate for large-devices and coarse gridding and its validity is proved relative to our previous Microscopic TCAD model and against experiment. Band-tails can also be easily included in this model depending on the density-of-states for bulk-carriers used.

Acknowledgements

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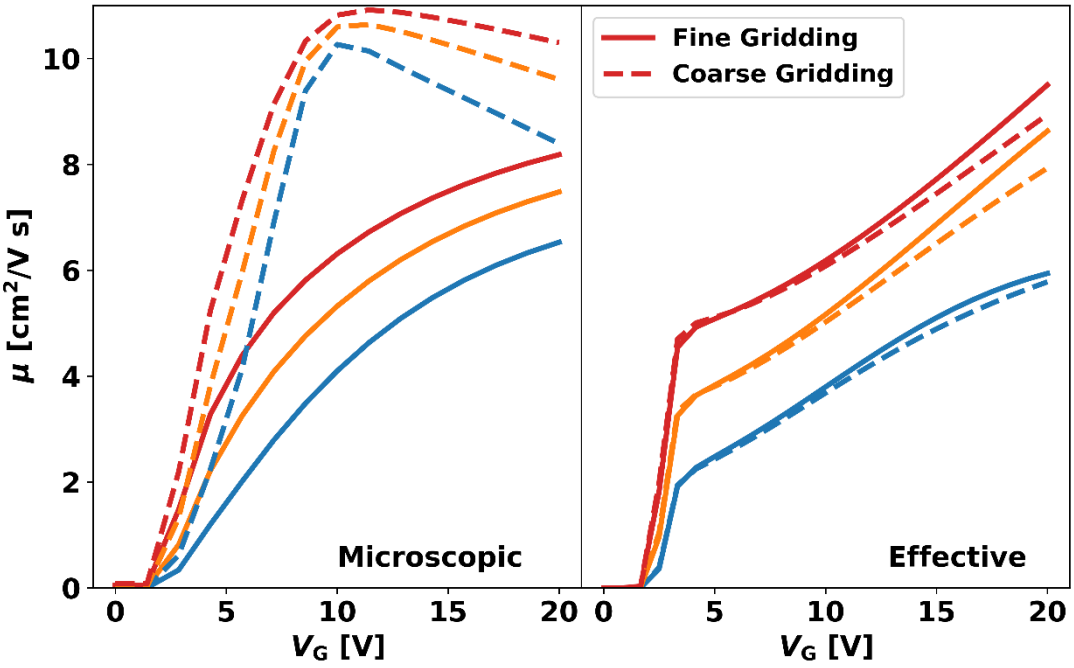

Figure 6: Mobility vs. gate voltage (identical to Fig. 3) for the case of fine- vs. coarse-gridding (2.5 nm vs 30 nm grid-size respectively) for the Microscopic vs. Effective-Medium model