

TCAD Simulation Models, Parameters, and Methodologies for β -Ga₂O₃ Power Devices

Hiu Yung Wong[†]

Department of Electrical Engineering, San Jose State University, California, U.S.A

Abstract: β -Ga₂O₃ is an emerging material and has the potential to revolutionize power electronics due to its ultra-wide-bandgap (UWBG) and lower native substrate cost compared to Silicon Carbide and Gallium Nitride. Since β -Ga₂O₃ technology is still not mature, experimental study of β -Ga₂O₃ is difficult and expensive. Technology-Computer-Aided Design (TCAD) is thus a cost-effective way to study the potentials and limitations of β -Ga₂O₃ devices. In this paper, TCAD parameters calibrated to experiments are presented. They are used to perform the simulations in heterojunction p-NiO/n-Ga₂O₃ diode, Schottky diode, and normally-off Ga₂O₃ vertical FinFET. Besides the current-voltage (I-V) simulations, breakdown, capacitance-voltage (C-V), and short-circuit ruggedness simulations with robust setups are discussed. TCAD Sentaurus is used in the simulations but the methodologies can be applied in other simulators easily. This paves the road to performing a holistic study of β -Ga₂O₃ devices using TCAD.

Keywords: Gallium Oxide, FinFET, Heterojunction, Power Devices, Short-Circuit Ruggedness, TCAD Simulation

1. Introduction

β -Gallium Oxide (β -Ga₂O₃) is an emerging material with an ultra-wide bandgap that has the potential to realize high breakdown and low loss power switching devices^{[1]-[3]}. Since the Baliga figure of merit (BFOM) scales as the sixth power of the bandgap, its BFOM is expected to be almost 9 times that of GaN^[1]. A low-cost substrate can also be obtained through various methodologies, such as the edge-defined film-fed growth (EFG) method^[1]. The two fundamental devices in power electronics systems, namely the diode^[4] and field-effect transistor (FET)^{[5][6]}, have been demonstrated using β -Ga₂O₃.

However, due to the absence of p-type doping in β -Ga₂O₃, forming a p-n diode is not possible and a Schottky diode needs to be used^[4]. It is also possible to create a heterojunction p-n diode. For example, in Reference [7], a high voltage heterojunction p-n diode is demonstrated by using p-type NiO and n-type Ga₂O₃. Due to the same reason, it is difficult to form a p-type substrate/body in a β -Ga₂O₃ n-type transistor. Therefore, β -Ga₂O₃ n-type transistors are usually normally ON^{[5][6]} (threshold voltage, $V_{TH} < 0$) which is not suitable for fail-safe operation. Innovative ideas have been proposed to form enhancement mode devices (normally off with $V_{TH} > 0$). For example, vertical β -Ga₂O₃ FinFET with a narrow fin is used to achieve normally-off devices by utilizing the difference between the gate workfunction and channel Fermi-level^{[8]-[10]}. Another example is by recessing a part of the channel of a cascode β -Ga₂O₃ MOSFET^{[11][12]}.

β -Ga₂O₃ is also known for its low thermal conductivity^[3]. Therefore, it is important to understand the effect of self-heating when designing novel β -Ga₂O₃ devices^[13].

[†] Correspondence to: H. Y. Wong, Email: hiuyung.wong@sjsu.edu

Technology Computer-Aided-Design (TCAD)^[14] is a very cost-effective tool for investigating novel ideals and structures of β -Ga₂O₃ devices^{[15][16]}, while the Ga₂O₃ technology is still expensive and not mature. TCAD can handle multi-physics including thermal effects. However, simulation of β -Ga₂O₃ is difficult due to the following reasons. Firstly, β -Ga₂O₃ is an emerging material and a widely-adopted and standardized set of models and parameters is not available. Secondly, like simulating wide-bandgap materials such as Gallium Nitride^[17], simulation convergence in UWBG is even more difficult due to its numerical underflow or overflow. Thirdly, to have useful and accurate simulations for high voltage applications in which self-heating is significant, models such as incomplete ionization, self-heating, and impact ionization which are notorious for causing convergence problems need to be included. Moreover, it is also important to include temperature-dependence parameters in the simulations.

Therefore, in this paper, we summarize a consistent set of models and parameters used for various types of β -Ga₂O₃ device simulations which are calibrated to experimental results. They are used in heterojunction p-NiO/n-Ga₂O₃ diode, Schottky diode, and normally-off Ga₂O₃ vertical FinFET simulations. Besides the IV simulations, breakdown, CV, and short-circuit ruggedness simulations with robust setups are discussed.

2. β -Ga₂O₃ TCAD Models and Parameters

2.1 Bandgap and other basics models

The basic material parameters are shown in Table 1. It includes the dielectric constant, thermal conductivity, and *temperature-dependent* bandgap parameters. The corresponding Sentaurus Device^[14] keywords are also shown. It should be noted that the thermal conductivity depends on the crystal orientation^{[3][18]} as β -Ga₂O₃ is anisotropic. While it is possible to perform anisotropic simulation in TCAD^[14], it is not recommended unless it is necessary, as this makes convergence more difficult.

For the bandgap parameters, the following models are used^{[14][19]}:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta} \quad (1)$$

$$\chi(T) = \chi_g(0) - \frac{\alpha T^2}{2(T + \beta)} \quad (2)$$

where T , $E_g(T)$, and $\chi(T)$ are the temperature, the bandgap, and electron affinity at temperature T , respectively. α and β are parameters. This gives a room temperature bandgap of 4.85eV. For electron affinity, there is a wide range of values in the literature from 3.5eV^[20] to 4eV^[21] at 300K. Table 1 shows the parameters that will make $\chi(300K) = 3.7eV$. Electron affinity value is less important in β -Ga₂O₃ as p-type doping is not available. However, for the Schottky device, oxide interface, and heterostructures, it is recommended to calibrate to the experimental value as Fermi-level pinning and interface traps will change the effective electron affinity.

The effective electron mass, m_e , is $0.28m_0$ ^[22], where m_0 is the electron rest mass. In TCAD simulation, what important is the density of state (DOS), N_c , which depends on m_0 . The following temperature-dependent equations are used. The parameter $N_c(300K)$ is chosen such that it gives $m_e = 0.28m_0$ at 300K.

$$N_c(T) = N_c(300K) \left(\frac{T}{300} \right)^{1.5} \quad (3)$$

$$\frac{m_e}{m_0} = \left(\frac{N_c(300K)}{2.5094 \times 10^{19}} \right)^{2/3} \quad (4)$$

2.2 Mobility and incomplete ionization models

In TCAD, phonon scattering limited mobility is calculated using the following equation,

$$\mu_L = \mu_{max} \left(\frac{T}{300} \right)^{-\theta} \quad (5)$$

For quick room temperature TCAD simulation, Eq. (5) is simplified to $\mu_L = \mu_{max}$ and one can use the value found in Reference [3] with $\mu_L = 300 \text{ cm}^2/(\text{Vs})$ without considering impurity scattering if the device is undoped. However, in most devices, the channel is doped. Therefore, it is necessary to include the doping-dependent mobility model. To model doping-dependent mobility, Reference [23] uses the Arora model, and Reference [24] uses the Masetti model. The Masetti model is not temperature-dependent and is not suitable for self-heating simulation. Although the Arora model is temperature dependent, the parameters have not been rigorously calibrated^[23]. The Philips Unified Mobility Model (PhuMob)^[25] is proposed to be used and will be discussed after the incomplete ionization model.

When the impurity scattering (Coulomb scattering) mobility model is used, it is also important to turn on the incomplete ionization model because the most commonly used dopants (such as Silicon and Germanium) in $\beta\text{-Ga}_2\text{O}_3$ are not shallow enough to assume complete ionization and the doping level is not high enough to form an impurity band^[26]. The impurity scattering depends on the percentage of ionization as only ionized dopants will contribute to mobility degradation. The following equation is used to model the doping-dependent ionization energy, E_D .

$$E_D = E_{D0} - \alpha N_D^{1/3} \quad (6)$$

For Silicon, the zero doping ionization energy of Si (E_{D0}) is set to 52meV with doping concentration (N_D) dependent ionization energy coefficient, α , being $3.398 \times 10^{-8} \text{ eVcm}$. For Germanium, E_{D0} is set to 17.5meV. N_D is not available for Germanium as doping-dependent experiments are available. The values extracted are consistent with the literature^{[27][32]}.

Fig. 1 shows the ionized dopant concentration as a function of temperature and doping in calibrated TCAD simulation and Hall measurement in refs. [27][28]. It shows that the ionization energy parameters are calibrated well.

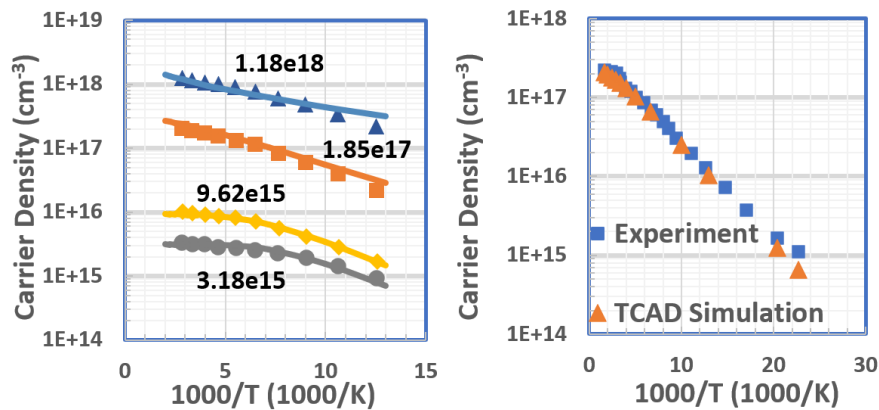


Fig. 1. Comparison of experimental^{[27][28]} and TCAD free carrier concentration data in Si-doped (left) and Ge-doped

(right) Ga₂O₃.

PhuMob model takes the screening of ionized impurities by charge carriers and temperature into account. In Reference [26], it has been demonstrated that it can be extended to cryogenic temperatures in a silicon device. The major PhuMob equations are the following and Table 2 shows the calibrated parameters.

$$\frac{1}{\mu} = \frac{1}{\mu_L} + \frac{1}{\mu_{DA}} \quad (7)$$

$$\mu_{DA} = \mu_N \left(\frac{N_{sc}}{N_{sc,eff}} \right) \left(\frac{N_{ref}}{N_{sc}} \right)^\alpha + \mu_c \left(\frac{n+p}{N_{sc,eff}} \right) \quad (8)$$

$$\mu_N = \frac{\mu_{max}^2}{\mu_{max} - \mu_{min}} \left(\frac{T}{300} \right)^{3\alpha-1.5} \quad (9)$$

$$\mu_c = \frac{\mu_{max}\mu_{min}}{\mu_{max} - \mu_{min}} \left(\frac{300}{T} \right)^{0.5} \quad (10)$$

The PhuMob model, μ , has two major parts, namely the phonon scattering due to lattice vibration, μ_L , and the impurity scattering part, μ_{DA} . They are combined through the Mathiessen rule in Eq. (7). The phonon scattering is temperature dependent as shown in Eq. (5) and the temperature sensitivity is determined by θ . μ_{DA} is also temperature dependent and determined by α . It also depends on a few parameters, namely, μ_{max} , μ_{min} , and N_{ref} . Note that μ_{max} is the same as the one in Eq. (5). In Eq. (8), n , p , N_{sc} , and $N_{sc,eff}$ are the electron, hole, scattering concentration, and effective scattering concentration with minority and electron-hole scattering effects, respectively. The model is calibrated against the experimental mobility data in refs. [27] and [28] with incomplete ionization turned on in Si and Ge^[29] (Table 2).

This calibrated PhuMob model has been used to simulate the Schottky diode^[29] and vertical FinFET^[30] and agrees with experimental data well after minor adjustments of μ_{max} and μ_{min} due to the difference in crystal qualities. Moreover, in Reference [29], it is demonstrated to match experimental Schottky diode IV with self-heating for Ga₂O₃ at various temperatures. It also shows a smooth trend up to 2000 K as shown in Fig. 2 which can be used for short-circuit simulation.

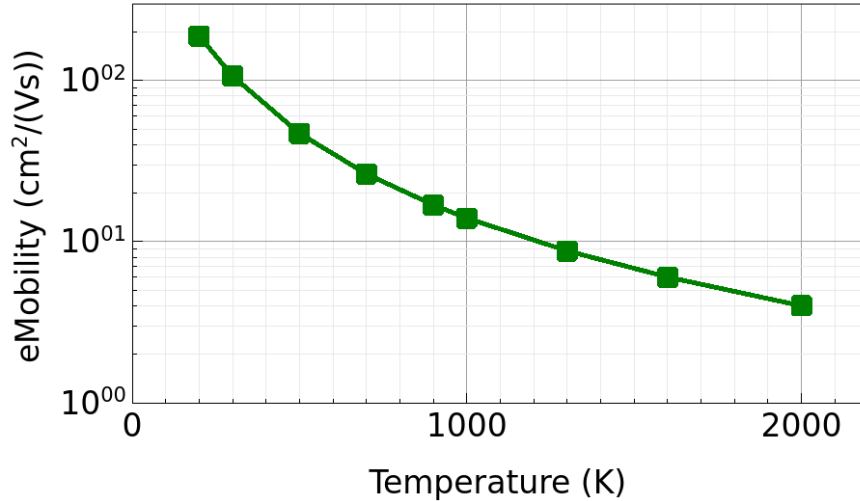


Fig. 2. Electron mobility as a function of temperature when the doping is $1.475 \times 10^{17} \text{ cm}^{-3}$.

Electron saturation velocity is found to be 2×10^7 cm/s based on Reference [31]. However, there is no experimental data on its temperature dependency. Therefore, the exponent, $v_{sat,exp}$, in the following equation is set to be 0.

$$v_{sat} = v_{sat,0} \left(\frac{300}{T} \right)^{v_{sat,exp}} \quad (11)$$

2.3 Impact ionization model

Since β -Ga₂O₃ is intended for high-power high-voltage electronics, it is important to include the impact ionization model in the simulation in the breakdown and short-circuit simulations. Although the convergence will be worse, it is also necessary to turn on the self-consistent impact ionization model, in which the generated carriers are included in the Poisson and carrier continuity equations for accurate simulations. The impact ionization coefficient is calculated using the van Overstraeten – de Man model[14]:

$$\alpha = ae^{\frac{-b}{F}} \quad (12)$$

where a and b are fitting parameters and F is the effective driving force in V/m. For good accuracy and convergence, the gradient of the electron quasi-Fermi level is used as the driving force. For the device breaks down in the (100) direction, the corresponding parameters, a and b , are 0.79×10^6 V/cm and 2.92×10^7 V/cm, respectively, based on Reference [33].

It should be noted that due to deep acceptor traps, very often impact ionization is not the cause of initial device breakdown because the hole generated are captured by the deep acceptors [34]. However, when the electric field is high enough, impact ionization of the deep traps will occur [34].

Table 1. Gallium Oxide Material Parameters Used in this Work.

Parameter	Keyword in SDevice	Value (unit)	Source
Dielectric Constant	Epsilon	10.0 (unitless)	[3]
Thermal Conductivity [100]	Kappa	0.11 (WK/cm)	[3]
Thermal Conductivity [010]	Kappa	0.27 (WK/cm)	[3]
Bandgap at 0K, $E_g(0)$	Eg0	5.0234(eV)	[19]
Bandgap parameter α	Alpha	4.45e-3 (eV/K)	[19]
Bandgap parameter β	Beta	2000 (K)	[19]
Electron Affinity at 0K, $\chi_g(0)$	chi0	3.6128(eV)	Within the range of [20] and [21]
Electron Density of State, $N_c(300K)$	Nc300	3.718e18 (cm ⁻³)	[22]
Constant Mobility, μ_L	mumax	300 (cm ² /(Vs))	[3]
Silicon Ionization Energy at zero concentration, E_0	E_Si_0	0.052 (eV)	[29]
Silicon Ionization Energy coefficient, α	alpha_Si	3.398e-8 (eV·cm)	[29]
Si dopant degeneracy, g	g_Si	2	[29]

Ge Ionization Energy at zero concentration, E_0	E_Ge_0	0.0172 (eV)	Fig. 1
Ge dopant degeneracy, g	g_Ge	2	Fig. 1
Saturation Velocity, v_{sat}	vsat0	2e7 (m/s)	[31]
Impact ionization pre-exponent, a	a(low), a(high)	7.9e5 (cm ⁻¹)	[33]
Impact ionization exponent, b	b(low), b(high)	2.92e7 (V/cm)	[33]

Table 2. Philips Unified Mobility Model Parameters for Si and Ge dopants in Ga₂O₃. * is either Si or Ge,

Parameter	Keyword in Sdevice	Si in Ga ₂ O ₃	Ge in Ga ₂ O ₃
μ_{max} (cm ² /V·s)	mumax_*	150	115
μ_{min} (cm ² /V·s)	mumin_*	80	0
θ	theta_*	1.8	1.65
N_{ref} (cm ⁻³)	n_ref_*	2×10 ¹⁷	5.68×10 ¹⁸
α	alpha_*	0.9	0.68

3. Simulations of β -Ga₂O₃ Devices

3.1. Heterojunction p-NiO/n-Ga₂O₃ diode

Since it is difficult to form p-type Ga₂O₃ and thus a Ga₂O₃ p-n diode, it has been proposed to form a heterojunction p-n diode with p-NiO and n-Ga₂O₃^[7]. Such novel structures usually have many non-idealities as the technologies of both materials and their interface are not mature. TCAD is very suitable to help understand its electrical properties. By using the parameters discussed in the earlier section except with $\chi(300K) = 4eV$ to achieve a better fitting to the experiment, it can be seen in Fig. 3 that the discontinuity at the valence band (3.69eV) is much higher than that of the conduction band (2.2eV). Therefore, electron current is expected to be dominating at forward bias.

In Reference [7], TCAD is also used to reverse engineer its properties by simulating its capacitance-voltage (CV) characteristics with various n-doping levels. It is found that when the doping is 4.5×10¹⁶cm⁻³, the TCAD CV matches the experimental CV the best (Fig. 3). This value is similar to the expected value based on the experimental design. It should be noted that, for the properties being studied, only 1D or pseudo-1D simulations are required. This will speed up the simulation and also improve the convergence. For the CV simulation, one may also turn off incomplete ionization to further speed up the simulation and improve the convergence as the result is expected to be the same. This is because all dopants are expected to be fully ionized in the depletion region.

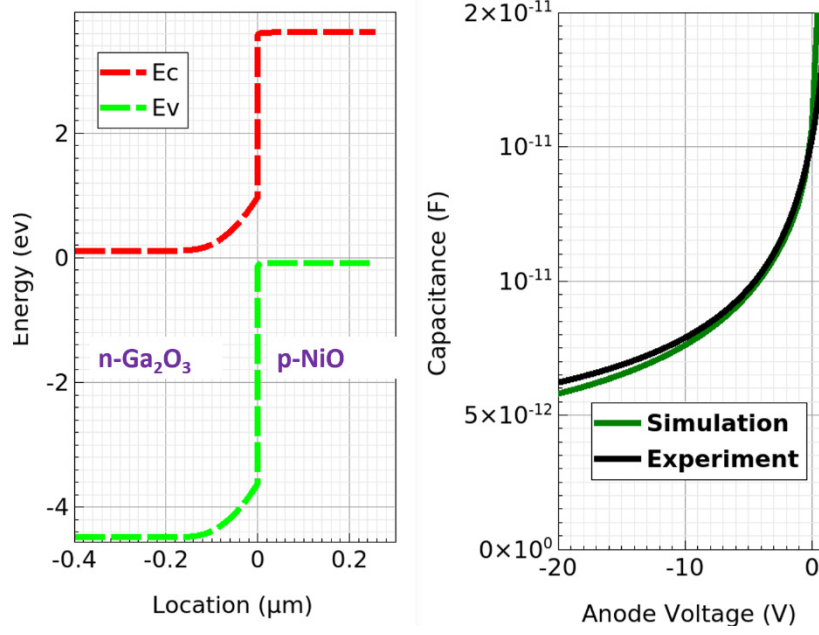


Fig. 3. TCAD simulated band diagram at zero bias (left) and comparison of simulated and experimental CV curves when the n-type doping is $4.5 \times 10^{16} \text{cm}^{-3}$ (right) of a heterojunction p-NiO/n-Ga₂O₃ diode.

3.2. Schottky $\beta\text{-Ga}_2\text{O}_3$ diode simulation

Schottky diode is the natural choice as a two-terminal rectifier in $\beta\text{-Ga}_2\text{O}_3$ technology since p-type $\beta\text{-Ga}_2\text{O}_3$ is not available. In ref [29], TCAD is calibrated by comparing the current-voltage current against experimental data at various temperatures in a Schottky diode (Fig. 4). The models and parameters in Section 1 are used except that μ_{max} is changed to $123 \text{cm}^2/\text{V}\cdot\text{s}$ in Table 3 from $150 \text{cm}^2/\text{V}\cdot\text{s}$ in Table 2. This can be justified by the possibility that the crystal quality in this experiment may be worse than the one in Reference [27].

Since $\beta\text{-Ga}_2\text{O}_3$ has a low thermal conductivity, it is necessary to turn on self-heating for accurate simulation. It is thus also important to include the substrate in the simulation domain to properly account for heat transfer. Usually, to speed up the simulation, one may use an effective thermal resistance. However, this needs careful calibration. Fortunately, power Schottky diodes usually have cylindrical symmetry. Therefore, one can create a 2D slice of the structure and perform a 3D simulation using cylindrical coordinates. By using coarse mesh in the substrate, an IV curve can be obtained in a few minutes with a full domain of 3.3mm (Fig. 4). Indeed, the simulation speed is fast enough to generate tens of thousands of data for machine learning^{[35][36]}.

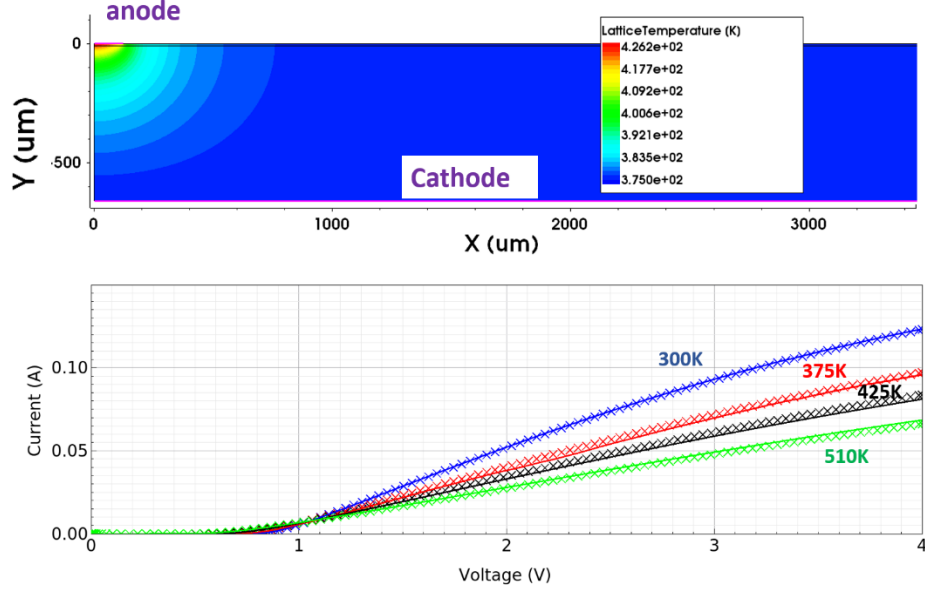


Fig. 4. Temperature distribution when the Schottky diode is under 4V forward bias (top) and TCAD vs. experimental forward IV at various ambient temperatures (bottom). The cylindrical coordinate is used and rotated about $X = 0\mu\text{m}$.

Table 3. Philips Unified Mobility Model Parameters used in Schottky diode [29]

Parameter	Keyword in Sdevice	Si in Ga_2O_3
μ_{max} ($\text{cm}^2/\text{V}\cdot\text{s}$)	mumax_*	123
μ_{min} ($\text{cm}^2/\text{V}\cdot\text{s}$)	mumin_*	80
θ	theta_*	1.8
N_{ref} (cm^{-3})	n_ref_*	2×10^{17}
α	alpha_*	0.9

3.3. Vertical $\beta\text{-Ga}_2\text{O}_3$ FinFET simulation

Vertical $\beta\text{-Ga}_2\text{O}_3$ FinFET is a very promising power device that can be normally off for fail-safe operations as long as it has a narrow enough fin and appropriate gate workfunction^{[8]- [10] [16][30][37]}. However, since the fin is narrow and is formed after etching, the effective mobility can be substantially reduced. By using the model presented earlier, it is found that the mobility in the fin needs to be recalibrated. Fig. 5 shows the structure of the FinFET and the TCAD and experimental $I_D V_G$ comparison. To match the $I_D V_G$, the Fin channel mobility is reduced by changing μ_{max} and μ_{min} of PhuMob model to $18.45\text{cm}^2/\text{V}\cdot\text{s}$ and $12\text{cm}^2/\text{V}\cdot\text{s}$, respectively (Table 4) to account for the degradation of the crystal quality due to etching and the narrow fin.

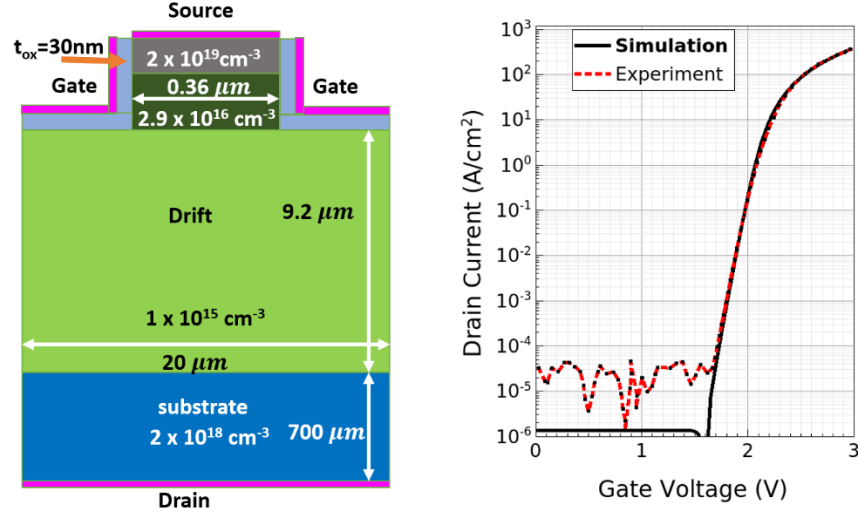


Fig. 5. Illustration of the vertical Ga₂O₃ FinFET structure (left) and TCAD vs. experimental $I_D V_G$ (right)

Table 4. Philips Unified Mobility Model Parameters used in Ga₂O₃ FinFET [30][37]

Parameter	Keyword in Sdevice	Si in Ga ₂ O ₃
μ_{max} (cm ² /V·s)	mumax_*	123 (bulk)/ 18.45 (Fin)
μ_{min} (cm ² /V·s)	mumin_*	80 (bulk)/ 12 (Fin)
θ	theta_*	1.8
N_{ref} (cm ⁻³)	n_ref_*	2 × 10 ¹⁷
α	alpha_*	0.9

Simulation of β -Ga₂O₃ simulation does not present much more convergence challenges compared to the Schottky diode. However, when performing breakdown and short circuit simulations, it is necessary to turn on background carrier generation to stabilize the numeric to avoid underflow or overflow. As shown in Reference [37], a background carrier generation of 10⁵ cm⁻³s⁻¹ to 10¹² cm⁻³s⁻¹ is required to obtain a correct breakdown value and this will also improve convergence^[17].

4. Conclusion

In this paper, we present a comprehensive set of TCAD models and parameters for β -Ga₂O₃ power device simulations. Most of the parameters are temperature-dependent and calibrated to various experiments. We demonstrated their applications in heterojunction p-NiO/n-Ga₂O₃ diode, Schottky diode, and normally-off β -Ga₂O₃ vertical FinFET simulations. The setup is robust and accurate. It is expected that, with the setup, β -Ga₂O₃ devices can be designed and optimized before the technology is matured.

Acknowledgments

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