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Modeling, simulations, and optimizations of gallium oxide on gallium–nitride Schottky barrier diodes

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With technology computer-aided design (TCAD) simulation software, we design a new structure of gallium oxide on gallium–nitride Schottky barrier diode (SBD). The parameters of gallium oxide are defined as new material parameters in the material library, and the SBD turn-on and breakdown behavior are simulated. The simulation results reveal that this new structure has a larger turn-on current than Ga_2O_3 SBD and a larger breakdown voltage than GaN SBD. Also, to solve the lattice mismatch problem in the real epitaxy, we add a ZnO layer as a transition layer. The simulations show that the device still has good properties after adding this layer.

Keywords: technology computer-aided design (TCAD), gallium oxide (Ga_2O_3), gallium nitride (GaN), Schottky barrier diode (SBD)

PACS: 73.40.Kp, 64.70.kg, 61.72.uj, 85.30.–z **DOI:** 10.1088/1674-1056/abc0dd

1. Introduction

β-gallium oxide (β-Ga_2O_3) is a wide-bandgap semiconductor with potential applications in high-frequency and high-power devices.[1–3] Among the five polymorphs of Ga_2O_3, the β-Ga_2O_3 is the most stable.[4] It has a monoclinic structure and belongs to the space group $C2/m$.[5] For simplicity, Ga_2O_3 denotes β-Ga_2O_3 in the following text. With the development of Ga_2O_3 epitaxy techniques, two-inchsized Ga_2O_3 substrates have been commercialized,[6] and the n-type doping technique using Sn or Si has been matured.[1] The Ga_2O_3 device fabrication and p-type doping technique are the two major problems in current Ga_2O_3 research.

It is quite hard to isolate the different phases in pure Ga_2O_3 crystalline form.[7] As a result, simulations and calculations have been used to forecast Ga_2O_3 crystal and device properties. For example, He *et al.* calculated the band structure by density functional theory (DFT).[5] Osipov *et al.* calculated the structural and elastoplastic properties, including Young's modulus and linear compressibility.[8] However, the Ga_2O_3 device simulations based on the finite element method have been scarce until now, which is mainly because the Ga_2O_3 is not a well-defined semiconductor material in major device simulation software and wide-bandgap semiconductor simulations are difficult to converge.[9]

In this work, we first conduct a thorough survey of available literature material parameters of Ga_2O_3 and make careful selections and estimations of these parameters.[9,10] We then update the material library of APSYS^{TM} developed by Crosslight Software for our simulations. Also, we select suitable recombination models for gallium oxide and gallium nitride separately. Based on these new definitions, parameter calibrations are performed to fit the available experimental data of gallium–oxide–metal–semiconductor field-effect transistor (MESFET)[11] and gallium–oxide Schottky barrier diode (SBD).[12] The experimental data are fitted well. With the selected models and calibrated parameters, we design a new SBD structure, which is composed of a gallium–oxide layer on a gallium–nitride substrate. Our simulations show that this new SBD device has a larger turn-on current than Ga_2O_3 SBD and a higher breakdown voltage than GaN SBD, making it more suitable to the high-power applications. To our knowledge, our work has been the first systematic study of important material parameters of Ga_2O_3 up to now, which is an indispensable step for future Ga_2O_3 TCAD simulations and device design.

2. Parameters and models

In this work, two finite element analysis-based device simulation tools are used: Silvaco Atlas by Silvaco (2019 version) and APSYS by Crosslight Software (2019 version). While GaN material parameters are well-defined in the two simulators, the properties of Ga_2O_3 are still lacking in both of them. As a result, we need to define them manually. To define a new material in the software, we first need to select a material that is the most close to the new material. Here we choose GaN. The minimum set of material parameters to define a new material in Silvaco Atlas is listed in Table 1.

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Table 1. Basic parameters for defining a new material in APSYS.

Names	Symbols	Values
Material name	material	Ga_2O_3
Default material	user.default	GaN
Material type	user.group	semiconductor
Electron affinity (eV)	affinity	4.0
Bandgap (eV)	eg300	4.8
Effective density of states in the conduction band/valance band (cm^{-3})	nc300, nv300	3.72×10^{18}, 3.72×10^{18}
Relative permittivity	permittivity	10
Electron/hole mobility ($cm^2/(V{\cdot}s)$)	mun, mup	118, 50
Thermal conductivity (W/(m·K))	tc.const	0.13

The actual code can be found in the supplementary material.

However, in order to obtain more accurate and reliable simulation results, we need to examine the full material database and find all the parameters in the material library. Also, there are some differences between Silcavo and Crosslight material libraries. Table 2 shows the comparison between the data of Silcavo and Crosslight material libraries and Ga_2O_3 parameters used in our simulation.

These parameters are selected from Refs. [5–8] separately to the best of our knowledge. For the values not reported, we use the value of GaN. Luckily, these parameters, such as the hydrostatic deformation potential and the shear deformation potential just have a minor effect on our simulations, for these mechanical parameters do not affect the current flow significantly.

After the new material is defined, we need to choose a suitable model for the current calculations. The well-known drift-diffusion current model, which is the default model in the software, is oversimplified. The reason is that for the wide-bandgap semiconductors, especially for the Ga_2O_3, the drift component of conductivity is very tiny, so the current iterations are hard to converge. Hence, we must consider the recombination process in the semiconductor. Generally speaking, there are three kinds of recombination processes, and these models are all available in the software.

Table 2. Ga_2O_3 parameters defined in Silvaco and Crosslight material libraries.

Parameters	Symbols	Ga_2O_3 values	Silvaco Atlas	APSYS
Electron effective mass (m/m_0)	MZZ, MTT	0.13, 0.124	Yes	Yes
Hole effective mass (m/m_0)	A1, A2, A3, A4, A5, A6	larger than GaN but not reported	Yes	Yes
Valance band reference	N/A	–2.2	Yes	N/A
Spin–orbit split energy (eV)	DELTA1	not reported	Yes	Yes
Crystal-field split energy (eV)	DELTA2	not reported	Yes	Yes
Direct band gap (eV)	Eg300	4.8	Yes	Yes
Electron affinity (eV)	Affinity	4.0	Yes	Yes
Relative permittivity	Permittivity	10.0	Yes	Yes
Electron mobility ($cm^2/(V{\cdot}s)$)	Mun	118	Yes	Yes
Hole mobility ($cm^2/(V{\cdot}s)$)	Mup	50	Yes	Yes
Thermal conductivity (W/(m·K))	tcon.const tc.const	0.13	Yes	Yes
Lattice constant (Å)	ALATTICE	not the same lattice-type	Yes	Yes
Elastic constant (N/m)	$C33$, $C31$, $C11$, $C12$, $C44$	318, 146, 208, 118, 50	not complete	Yes
Hydrostatic deformation potential (eV)	AC	not reported	Yes	Yes
Shear deformation potential (eV)	$D1$, $D2$, $D3$, $D4$	not reported	Yes	Yes
Compliance tensor	$S11$, $S12$, $S13$, $S22$, $S23$, $S33$	not reported	No	Yes
Specific heat (J/(mol·K))	Spec_heat value	490	No	Yes

2.1. Direct recombination

Direct recombination refers to electrons dropping from the conduction band to the valance band directly. Photon is emitted in direct recombination, so direct recombination is also called as radioactive recombination. It often occurs in the direct bandgap semiconductors, and it is important for light-emitting devices.

2.2. Shockley–Read–Hall recombination

The SRH recombination is also called trap-assisted recombination. Electrons and holes recombine through traps between the valance band and the conduction band. The traps are often caused by energy levels of impurities in the semiconductor. The SRH recombination is a dominant process in the indirect bandgap semiconductor materials, such as silicon.[13]

2.3. Auger recombination

Auger recombination is a three-particle process. Electrons and holes recombine and give energy to the third particles, which is often an electron instead of a photon. Auger recombination is a non-radiative process and occurs mostly in direct bandgap materials.[14,15]

For GaN, we use the Auger recombination model as a primary recombination model because GaN has direct bandgap, and several experiments and simulations have focused on that before.[16] For Ga_2O_3, we use the SRH recombination model as a dominant model because it is an indirect bandgap semiconductor. The formula involving the SRH recombination is

$$R_{\mathrm{SRH}} = \frac{pn - n_i^2}{\mathrm{TAUP0}\left(n + n_i \exp\left(\frac{\mathrm{ETRAP}}{kT}\right)\right) + \mathrm{TAUN0}\left(p + n_i \exp\left(\frac{-\mathrm{ETRAP}}{kT}\right)\right)}, \tag{1}$$

where TAUP0, TAUN0, and ETRAP correspond to the hole lifetime, electron lifetime, and energy level for trap. They can be adjusted to fit the experimental data in the calibration process below.

3. Calibration with experimental data from the literature

Since our material Ga_2O_3 is newly defined, we need to check whether the parameters and models could fit or explain the available experimental results. To the best of our knowledge, we find two suitable experimental studies. One is the Ga_2O_3 MESFETs in Ref. [11], and the other is the Ga_2O_3 SBDs in Ref. [12]. Figure 1 shows the device structures in these two references respectively.

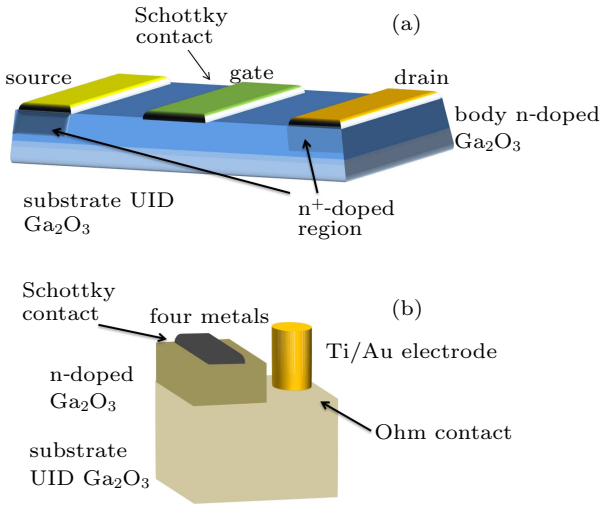


Fig. 1. Schematic structure of (a) Ga_2O_3 MESFET in Ref. [11], and (b) Ga_2O_3 SBDs in Ref. [12]. UID: unintentionally doped.

In the Ga_2O_3 MESFET, the work function is determined to be 5.23 eV in the gate material Ti/Au.[11] In Ga_2O_3 SBD, four different metals (Pd, Ni, Pt, and Au) are used in the Schottky contact. Different metal has different work function.[12] In this calibration process, the carrier lifetime and the trap energy level are tuned to fit the experimental data. From formula (1), the minority carrier lifetime TAUP0 is more critical than TAUN0, since n $\gg$ p in n-Ga_2O_3. Also, ETRAP will greatly influence the recombination rate since it appears in the exponential index. The TAUP0 value is fitted between 10^{-8} s and 10^{-9} s, and slightly different between two experiments. This value is similar to that in GaN. The n-type trap energy level is about 0.4 eV.

Figure 2 below shows the comparison between simulation results and the experimental data. The scale is suitably converted to make the plot placed in the same graph.

From Fig. 2, we can see that the difference between currents from the experiment and the simulation is minimal. Therefore, our parameters and models for Ga_2O_3 are reasonable, based on which we can proceed to design new Ga_2O_3 structures.

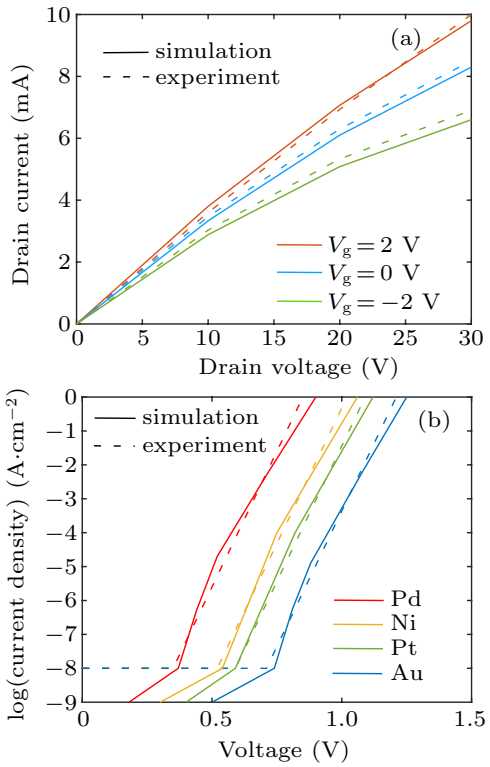


Fig. 2. Comparisons between currents from experiment and simulation for (a) Ga_2O_3 MESFET and (b) Ga_2O_3 SBD.

4. Design of Ga_2O_3 on GaN SBDs

There are lots of researches on the GaN SBD,[17–19] and Ga_2O_3 SBDs have attracted much attention recently.[20] In Ref. [20], the recent progress in the Ga_2O_3 SBD is reviewed and some methods are provided to improve the Ga_2O_3 SBD performance. These methods include increasing the doping concentration and using a p-Cu_2O layer. Here, we propose another strategy and design a new structure of the Schottky barrier diode, which is the n-type gallium oxide on an unintentionally doped gallium–nitride substrate. The metal contact is defined as titanium and gold (Fig. 3(a)). Following a similar procedure to the procedure shown later, we simulate the turn-on current behavior and compare it with the result obtained in the case of using the Ga_2O_3 substrate. Moreover, we change the gate length and the doping concentration to find the current trend (see Fig. 3).

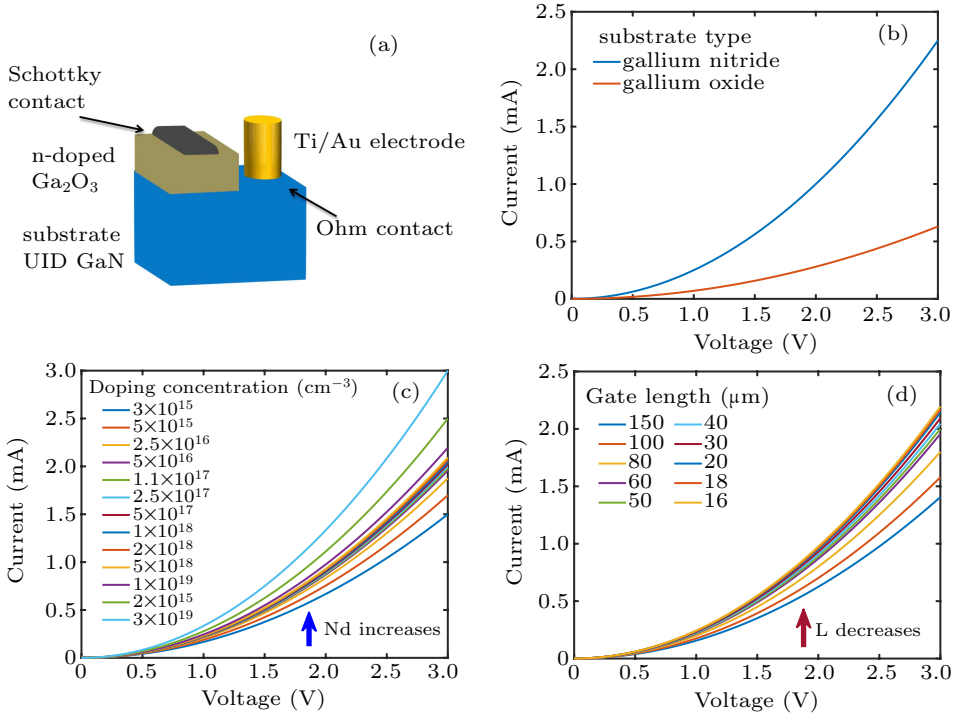


Fig. 3. (a) Structure, variations of turn-on current with voltage for using (b) GaN substrate and Ga_2O_3 substrate, (c) different doping concentrations, and (d) different gate lengths, of gallium oxide on gallium–nitride substrate SBD.

From Fig. 3(b) we can see that the current increases by three times after changing the substrate, which is good for application since the small current is difficult to detect. Figures 3(c) and 3(d) show the changing trend of current for different doping concentrations and the gate lengths, respectively. The n-type Ga_2O_3 doping concentration changes from 3×10^{15} cm^{-3} to 3×10^{19} cm^{-3}. The current grows steadily at first, but increases rapidly when it is above 1×10^{19} cm^{-3}. The gate length is varied between 16 μm and 150 μm, and the current changes as expected.

An essential problem in the real application is the lattice mismatch in the epitaxy process. Gallium oxide is monoclinic, while gallium nitride is hexagonal. It is hard to grow gallium oxide on gallium nitride directly. An important strategy to solve this problem is to add a transition layer.[21] Here, we add a zinc oxide (ZnO) layer as a transition layer in between. Zinc oxide is a perfect transition layer since zinc oxide is also hexagonal so that it can be grown on the gallium–nitride substrate. Moreover, zinc oxide can form a solid solution with gallium oxide,[22] and it is feasible to stack a layer of gallium oxide on it. In the real molecule beam epitaxy (MBE) process, we can use Ga, Zn, and O atoms, and block the Ga source first. After some time, we open the Ga source and block the Zn source. We may have a ZnO–Ga_2O_3 solid solution, and it is more feasible than stacking Ga_2O_3 directly since Ga_2O_3 and GaN have different lattice types.

Figure 4(a) shows the updated structure. After adding this new layer, the current decreases, but it is still larger than the current in the original Ga_2O_3 on Ga_2O_3 SBD (see Fig. 4(b)).

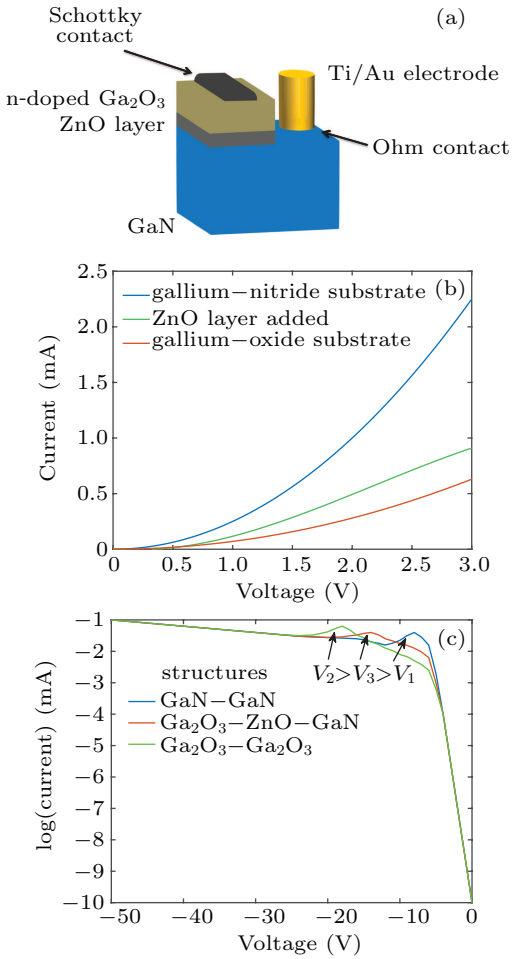


Fig. 4. (a) Structure of SBD after adding transition layer, and breakdown behaviors for (b) different substrates and (c) different structures of SBD.

Another important property of the SBD is the breakdown

voltage. Here, our definition of breakdown voltage is the same as that of the GaN SBD breakdown voltage in Ref. [23], which corresponds to the voltage where the current suddenly drops or rises. Generally speaking, a Ga_2O_3 device has a larger breakdown voltage than a GaN device, so this new structure should have a larger breakdown voltage than GaN SBD, which is confirmed through further simulating the breakdown behavior. After adding a transition layer, the breakdown voltage decreases, but it is still better than GaN SBD (see Fig. 4(c)).

In summary, the design of adding a ZnO transition layer is successful. Its advantage is still over the original designs, though it is not so good as that without the transition layer. To make the device easily fabricated in experiment, this price is acceptable.

5. Conclusions

We designed a gallium oxide on gallium–nitride substrate SBD in this paper by TCAD simulations. We started this design by defining the new material Ga_2O_3 in the software database since Ga_2O_3 is not included in the material library. After that, the calibration simulation shows that our new definition accords well with the experiment data in Ga_2O_3 MESFET and Ga_2O_3 substrate SBD. We proceeded with this simulation and designed a new Ga_2O_3 on GaN substrate SBD. This new SBD has a better turn-on property and a higher breakdown voltage than the original SBD. To solve the lattice mismatch problem in real fabrication, we added a transition layer ZnO. More simulations show that the SBD still maintains these good properties after adding this transition layer. Our simulation is the first systematic simulation of Ga_2O_3, which is of great significance for further conducting simulations.

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