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Electrical Properties of GaN/Ga_2O_3 P-N Junction: A TCAD Study

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ABSTRACT

Ga_2O_3 and GaN are promising candidates for the fabrication of high-power semiconductor devices due to their wide range of band gap from 3.0 eV to 4.9 eV. Heterostructure of p-type GaN and n-type Ga_2O_3 (GaN/Ga2O3 p-n junction) is expected to have an excellent performance for high-power semiconductor device applications at high temperature. In this work, effects of GaN thickness and its doping concentration in GaN/Ga_2O_3 p-n junction are studied using (TCAD) simulations, aiming at optimizing the junction performance. It was found that the current-voltage (IV) characteristic of the diode decreases as the thickness of GaN layer increases. To achieve a high current output, the optimized thickness is determined to be 500 nm. Furthermore, the doping concentration within the diode strongly influences the output current. The highest current is obtained for an un-doped GaN sample, and the increase in the doping concentration leads to a decrease in the obtained current.

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1. Introduction

β-Ga_2O_3 is a potential wide bandgap semiconductor with several potential applications such as power devices, UV photodetectors, photocatalysts, gas sensors, solar cells, and sometimes works as the transparent conducting materials in optoelectronic devices [1], [2]. Ga_2O_3 has gained attention due to its intriguing properties such as ultra-wide band-gap (4.6 - 4.9 eV), high critical field of 8 MV/cm, high saturation electron velocity of 2×10^7 cm/s, and high electron mobility up to 200 cm^2/Vs at room temperature [3]. Ga_2O_3 has an advantage over other wide band-gap materials such as SiC and GaN because of its low fabrication cost using Czochralski (CZ) [4], floating zone (FZ) or edge-defined film-fed (EFG) methods [5]. In order to utilize Ga_2O_3 in high power applications, it is crucial to improve the Baliga's Figure of Merit (BFOM) in metal-oxide semiconductor field-effect transistors (MOSFETs) [6]. This figure of merit is determined by two key factors: dielectric breakdown ($E_{ox,\ br}$) and maximum surface electric field ($E_{SURF\ max}$). Previous study reported the $E_{SURF\ max}$ values for SiO_2 and HfO_2 are 1.56 MV/cm and 2.60 MV/cm, respectively [7].

Despite many promising applications in electronic devices, the further development of Ga_2O_3 are still limited due to the lack of p-type β-Ga_2O_3 based materials, which is mainly the massive acceptor ionization energy, low hole activation efficiency, hole-trapping effect, and self-compensation effects of cation [8]. On the other hand, large band gap p-type semiconductor can be easily achieved in GaN with the band gap up to 3.4 eV makingit becomes a potential p-type material for the next generation of power devices [9]-[15]. Therefore, the combination of β-Ga_2O_3 and GaN in bipolar devices is expected to to mitigate the drawbacks of Ga_2O_3 while leveraging the properties of p-type GaN. S. Leone et al. grew epitaxial GaN/Ga_2O_3 heterostructures by MOCVD. A strong oxygen inter-diffusion has been observed at GaN/Ga_2O_3 interface leads to reduce the quality of GaN layer [16]. Ga_2O_3/GaN diode was reported to be used as a light emitting diode (LED) in Yang Zhao's study [17]. Deep ultraviolet (UV) photodiodes based on a heterojunction between β-Ga_2O_3 and GaN were demonstrated to have the highest sensitivity to the light with $\lambda < 260$ nm and the response time in the order of milliseconds [18]. Recently, Ga_2O_3/NiO_x p-n junction was fabricated with extremely high breakdown voltage (8.32 kV) and power figure-of-merit (13.2 GW/cm^2) [19].

This study aims to contribute to the development of a GaN/Ga_2O_3 diode that can be utilized in high-power device applications. The simulated device is calibrated against experimental GaN and Ga_2O_3 diodes, considering the effect of thickness of GaN layer and its doping concentration on the performance of GaN/Ga_2O_3 diodes. The band structures of devices are investigated to revial which factors that affect the properties of GaN/Ga_2O_3 diode.

2. Methodology and Settings

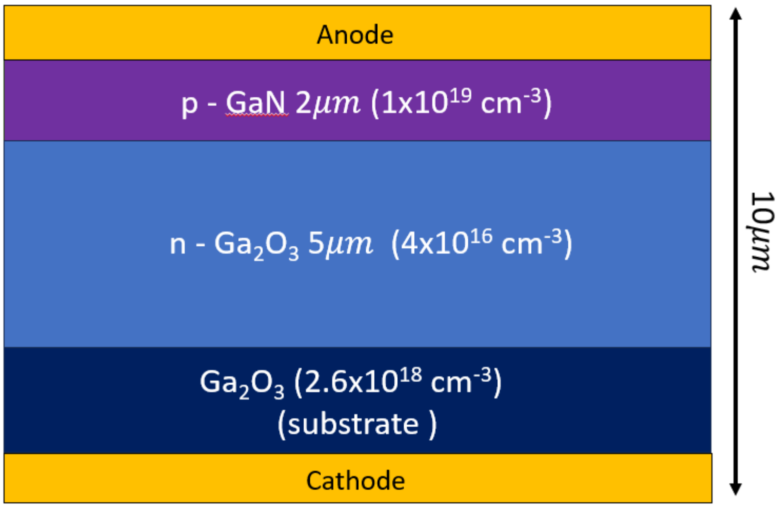

Figure 1. *Schematic cross section of GaN/Ga_2O_3 p-n diode.*

Table 1. *The details of material parameters of Ga_2O_3 and GaN used for simulation*

Parameters	**n-type Ga_2O_3[7]**	**p-type GaN***
Band Gap (eV)	4.85	3.43
Eletron Affinity (eV)	3.9	4.31
Effective electron mass	0.28	0.20
Relative dielectric constant	10	8.9
Room-temperature electron mobility (cm^2/Vs)	200	-
Room-temperature hole mobility (cm^2/Vs)	-	16
Saturation electron velocity (cm/s)	2.00×10^7	-
Saturation hole velocity (cm/s)	-	1.91×10^7

*These parameters are default from TCAD.

The GaN/Ga_2O_3 p-n junction was theoretically studied using the 2-D device simulation tool. The device structure is illustrated in Fig. 1. All devices have the same n-type doping concentration of 2.6×10^{18} cm^{-3} in Ga_2O_3 substrate, and initial p-type doping concentration of 1×10^{19} cm^{-3} in GaN drift layer was used in the calibration process. To investigate the properties of the diodes, the thicknesses of the GaN layer were varied at 10 nm, 20 nm, 50 nm, 100 nm, 500 nm and 2 µm. The simulated parameters of Ga_2O_3 and GaN are shown in Table 1. In order to consider the impact of carrier concentration and high electrical field on the mobility, a concentration-dependent lifetime model and a high field model were used. The Auger recombination model was adapted to consider the influence of high electron concentration, and a thermal model was used to examine the self-heating effect.

3. Results and Discussion

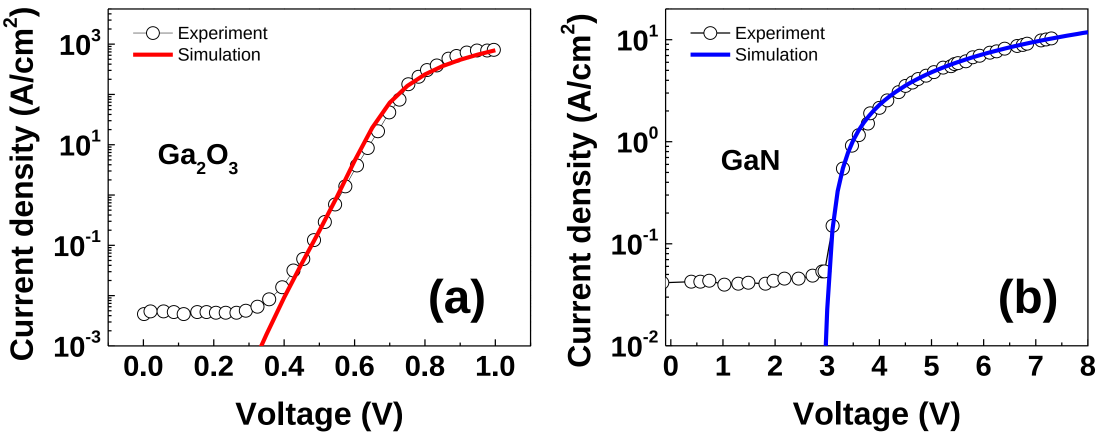

Figure 2. *The I-V characteristics of (a) the Ga_2O_3 diode and (b) the GaN diode as compared to the experimental results obtained from the same devices [20], [21].*

TCAD parameters are calibrated against experimental Ga_2O_3 and GaN diodes. The I-V characteristics, which are illustrated in Fig. 2(a) for Ga_2O_3 diode and in Fig. 2(b) for GaN diode, show that both I-V curves fit well with the experimental date [20], [21]. The calibrated parameters are used in simulation of all GaN/Ga_2O_3 p-n diodes, including the investigation of impacts of GaN drift layer thickness and the doping concentration of this layer on the behaviors of diodes. The electron mobility of Ga_2O_3 was extracted to be 115 cm^2/Vs, which is in good agreement with experimental report [22].

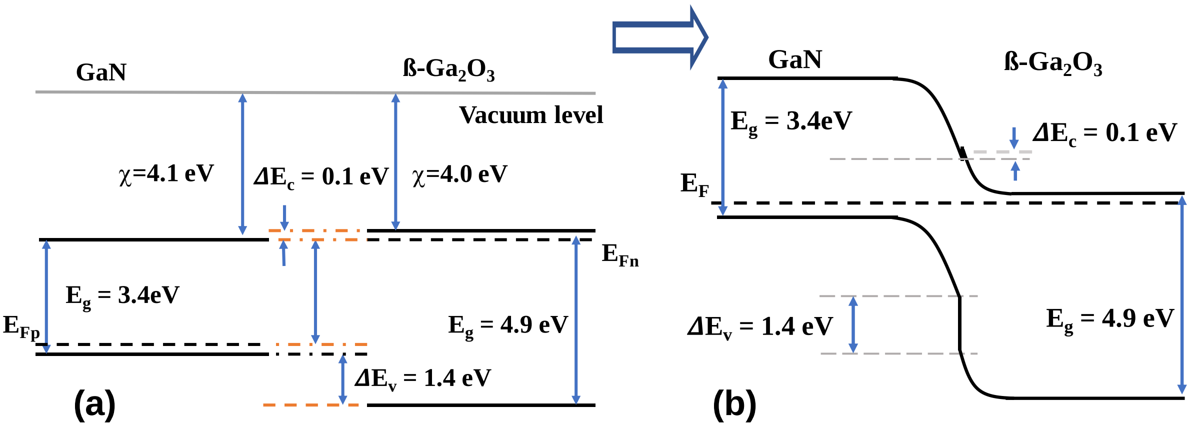

Figure 3. *Band-diagram of GaN/Ga_2O_3 p-n junction diode (a) before and (b) after forming the p-n junction simulated by TCAD.*

The band diagram of the GaN/Ga_2O_3 p-n junction is illustrated in Fig. 3. Before the formation of the p-n junction, the energy levels of the conduction band (CB) minimum in both GaN and Ga_2O_3 are nearly identical. However, a depletion region is observed after the junction region is formed, having a CB offset of 0.1 eV and a valence band (VB) offset of 1.4 eV. The CB and VB offsets values are consistent with the findings of a previous report [23].

Fig. 4 (a) shows the I-V characteristics of the GaN/Ga_2O_3 p-n junction as a function of GaN thickness. It is found that as the thickness of GaN increases the current density decreases because the deleption region is broadened in the p-type region. However, the reduction in current density is not linear with respect to the GaN thickness as shown in Fig. 4(b). The threshold voltage of the diode, namely the knee voltage, is found to decrease significantly for small thicknesses (<100 nm) of GaN, affecting the on-voltage of the diode significantly. However, as the GaN thickness exceeds 100 nm, the slope of the Kee voltage – GaN thickness curve decreases, indicating the less dependence of knee voltage on GaN thickness.

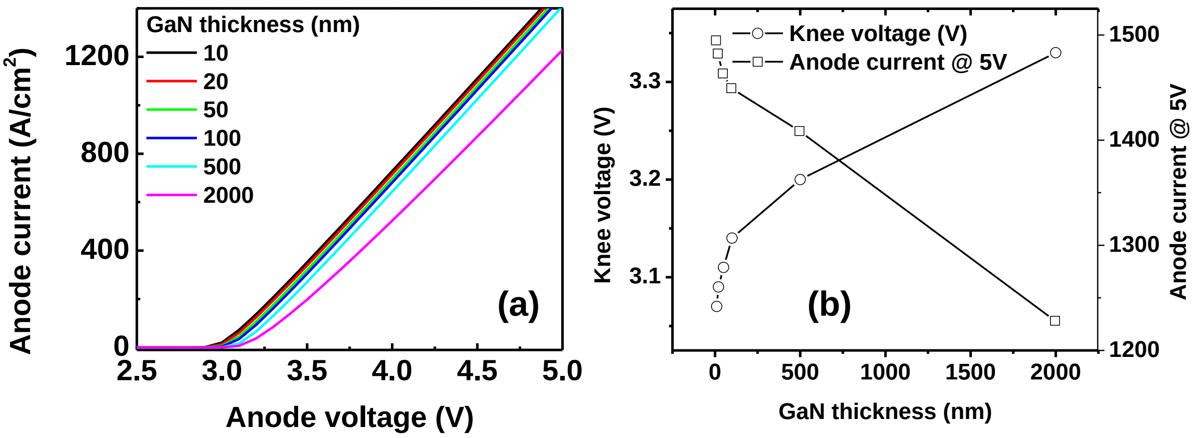

Figure 4. *(a) I-V characteristics of GaN/Ga_2O_3 p-n junction as a function of GaN thickness, and (b) knee voltage and current density at V_{anode} = 5 V as a function of GaN thickness*

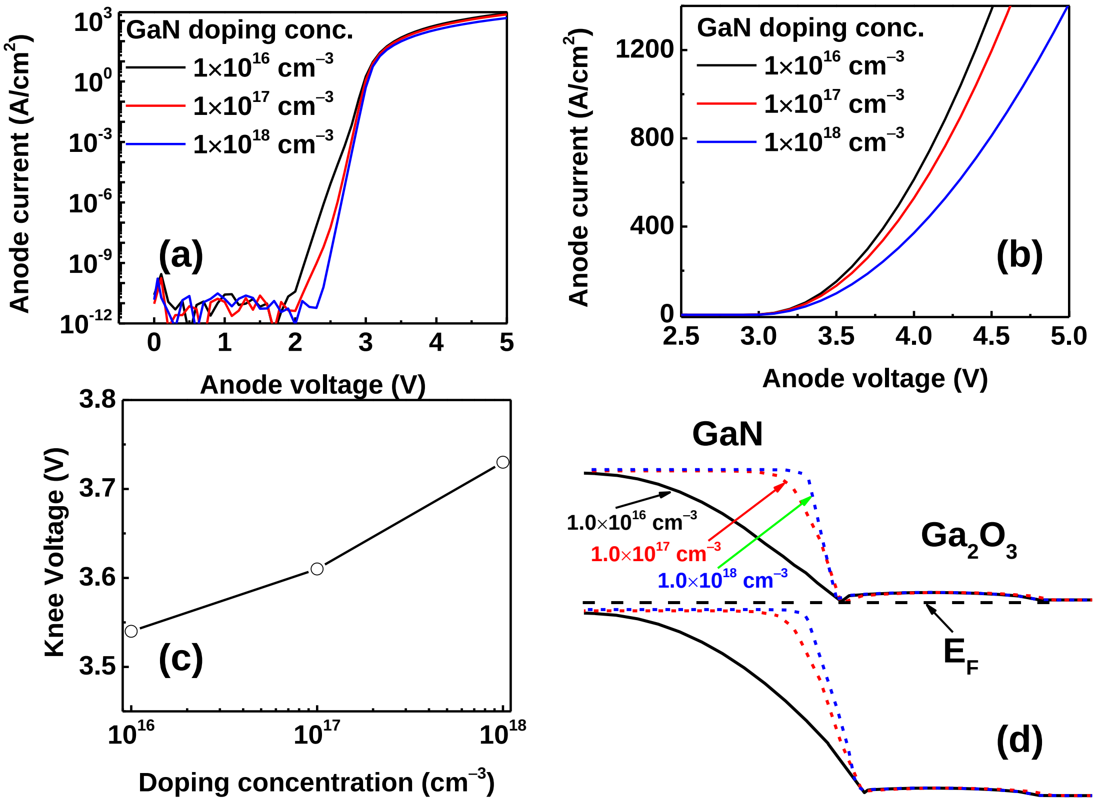

Figure 5. *I-V characteristics of GaN/Ga_2O_3 p-n junction as a function of doping concentration in GaN, presenting in (a) log scale, and (b) linear scale. (c) Knee voltage as a function of doping concentration in GaN. (d) Band diagram at GaN/Ga_2O_3 junction when the doping concentration in GaN is changed from 1.0×10^{16} cm^{-3} to 1.0×10^{18} cm^{-3}.*

The impacts of doping concentration of GaN layer on GaN/Ga_2O_3 p-n junction are investigated in Fig. 5. We obtained the ratio of I_{on}/I_{off} greater than 1.0×10^{15}. This high ratio indicates that GaN/Ga_2O_3 is a highly promising candidate for the applications of high-power devices with low leakage current. Fig. 5(b) indicates that the current tends to decrease as the doping concentration in GaN increases. This reduction can be attributed to the changes occurring within the band structure of the diode. Fig. 5(c) illustrates a slight change in the knee voltage, from 3.54 V to 3.73 V, when the doping concentration is increased from 1.0×10^{16} cm^{-3} to 1.0×10^{18} cm^{-3}. The electrical properties of the diode can be explained by simulating their band diagram. Figure 5(d) shows a change in the shape of the GaN/Ga_2O_3 junction, varying from a linear-junction (represented by the black solid line) to an abrupt-junction (represented by the blue dashed line). This change results in an increase of Schottky barrier within the depletion region, which explains the decrease of the observed I-V characteristic.

4. Conclusions

In conclusion, the GaN/Ga_2O_3 p-n junction was investigated using TCAD simulations. The impacts of GaN thickness and its doping concentration on I-V characteristics of GaN/Ga_2O_3 diodes was conducted. It is observed that the knee voltage is strongly dependent on the thickness of GaN when its thickness is less than 100 nm. The dependence becomes little when the GaN thickness increases. It was observed that a change in the shape of the GaN/Ga_2O_3 junction when the doping concentration is increased from 1.0×10^{16} cm^{-3} to 1.0×10^{18} cm^{-3}, moving from a linear-junction to an arupt-junction. This change leads to an increase in the Schottky barrier within the depletion region. The study provides thorough guidance for fabricating GaN/Ga_2O_3 p-n junction, which is applicable in high power device applications.

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Conflict of Interest

The authors declare no conflict of interest.

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