

Self-screening of the polarized electric field in wurtzite gallium nitride along [0001] direction

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Self-screening of the polarized electric field in wurtzite gallium nitride along [0001] direction

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The strong polarization effect of GaN-based materials is widely used in high-performance devices such as white-light-emitting diodes (white LEDs), high electron mobility transistors (HEMTs), and GaN polarization superjunctions. However, the current researches on the polarization mechanism of GaN-based materials are not sufficient. In this paper, we studied the influence of polarization on electric field and energy band characteristics of Ga-face GaN bulk materials by using a combination of theoretical analysis and semiconductor technology computer-aided design (TCAD) simulation. The self-screening effect in Ga-face bulk GaN under ideal and non-ideal conditions is studied respectively. We believe that the formation of high-density two-dimensional electron gas (2DEG) in GaN is the accumulation of screening charges. We also clarify the source and accumulation of the screening charges caused by the GaN self-screening effect in this paper and aim to guide the design and optimization of high-performance GaN-based devices.

Keywords: gallium nitride, polarized electric field, self-screening effect, surface states, donor doping, intrinsic thermal excitation

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1. Introduction

High-density two-dimensional electron gas (2DEG) could be induced by the strong spontaneous and piezoelectric polarization in wurtzite GaN materials.[1] It is widely used in the manufacture of high electron mobility transistors (HEMTs), Schottky diodes, Gunn diodes, and many other excellent radio frequency (RF) or power switching devices. Chaudhuri *et al*. used the negative polarization charges of GaN/Al(Ga)N interface to generate two-dimensional hole gas (2DHG) and formed a p-channel GaN HEMT with the lowest sheet resistance.[2] Simon *et al*. achieved high-conductivity p-type doping through polarization-induced technology, which improved the light emission efficiency in UV LEDs.[3] Combining with n-channel and p-channel GaN MOS-HEMTs structures on the same wafer, Chu *et al*. first demonstrated the GaN complementary metal–oxide–semiconductor (CMOS) field-effect-transistor technology. They successfully fabricated an integrated inverter and provided new feasibility for the GaN-integrated circuit.[4] In addition, AlGaN/GaN HFETs,[5] MOSFETs,[6] GaN tunnel junction LEDs,[7] GaN polarization superjunction,[8] and many other high-performance devices were also developed using the polarization characteristics of GaN materials.

The polarization charges on the GaN surface generate the polarized electric field inside GaN. Carriers would be redistributed to compensate the polarized electric field. The process mentioned above is known as the self-screening effect. Zhang *et al*., Nanyang Technological University, first proposed the polarization self-screening effect. They demonstrate that the quantum confined Stark effect (QCSE) in LEDs can be self-screened by bulk charges induced by InGaN quantum barrier with graded indium composition.[9] Mishra *et al*., the University of California, has discussed the phenomenon of screening of polarized electric field in n-type GaN bulk materials with donor-like surface states and n-type impurities.[10] However, they did not systematically explain the self-screening effect and the origin of screening charges. So far, the self-screening effect under the polarized electric field in GaN bulk materials has not been discussed in-depth and studied comprehensively. In this work, we used a combination of theoretical analysis and semiconductor technology computer-aided design (TCAD) simulations to study this effect. We systematically study the self-screening effect of the polarized electric field in GaN bulk materials under different situations such as ideal intrinsic GaN, intrinsic GaN with donor-like surface states, n-type GaN, and actual bulk GaN. After that, we clarify the source and accumulation of the screening charges caused by the self-screening effect. It can be considered that the essence of 2DEG in GaN is the accumulation of screening

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charges influenced by the self-screening effect of the polarized electric field. Therefore, this research will provide the accurate guidance for the structural design and the characteristic analysis of GaN devices.

2. TCAD experiment

The experimental conditions are determined by the following actual situations.

Wurtzite GaN has two polarities along the *c*-axis direction, Ga-polar and N-polar. The high densities of negative polarization charges and positive polarization charges are concentrated on the Ga-face and N-face of GaN material respectively. Ga-polar GaN epitaxy technology is more developed than N-polar GaN and the Ga-polar GaN-based devices have been put into commercial production and widely used. In order to be realistic, GaN bulk materials are all grown along with the [0001] direction in this paper. We assume that the ideal GaN bulk materials are relaxed, that is, there is only spontaneous polarization in GaN. If the spontaneous polarization intensity P_{sp} is 2.9×10^{-6} C/cm^{-2},[11] the surface polarization charges density n_π would be 1.8×10^{13} cm^{-2}.

GaN materials are generally grown on heterogeneous substrates[12,13] by MOCVD, MBE or HVPE. The material quality is greatly affected by growth parameters such as temperature, V/III ratio or the lattice parameters of heterogeneous substrates. So the concentration or density of the impurities, defects or surface states in GaN materials would generally be quite high.[14,15] Many studies have shown that actual GaN materials are n-type due to the existence of silicon doping,[16] oxygen impurity,[17,18] and surface states (such as nitrogen vacancies[19,20]). Therefore, in this work, we analyze the self-screening effect of the polarized electric field in the ideal intrinsic Ga-face GaN bulk materials. Then intrinsic bulk GaN with donor-like surface states and with n-type doping are discussed respectively. Finally, we analyze a complex case about GaN bulk materials with both surface states and n-type doping. So that we could clarify the self-screening effect of the polarized electric field in an actual GaN bulk materials.

3. Result and discussion

The simplified symbols used in all figures are shown in Table 1, and the physical terms in all equations are described in Table 2.

Table 1. The definition of simplified symbols used in all figures.

Symbol	Definition	Symbol	Definition
t_{GaN}	the thickness of bulk GaN	W_d	width of depletion region formed by donor impurity ionization
t_{cr}	the critical thickness of the ideal intrinsic GaN	$-Q_i$	electrons excited by the intrinsic thermal excitation
E_c	conduction band	$+Q_i$	holes excited by the intrinsic thermal excitation
E_f	fermi level	Q_π	surface polarization charge
E_v	valence band	Q_s	screening charges provided by surface state ionization
E_{DD}	donor-like surface state level	Q_d	screening charges provided by the donor impurity ionization

Table 2. The physical terms defined or described in all equations.

Symbol	Definition	Symbol	Definition
ε_π	the polarized electric field in bulk GaN	n_{s-cr}	the critical density of donor-like surface states
σ	charge surface density	D_{ss}	the density of donor-like surface states
ε	the dielectric constant of GaN material	D_{ss}^+	the density of ionized donor-like surface states
E_g	the bandgap of GaN	n_{s-i}	the charge density provided by intrinsic thermal excitation
e	the elementary charge	V_{bi}	the built-in potential difference
ε	total electric field in bulk GaN	N_d	the concentration of donor doping
σ_n	the density of screening charges	N_c	the effective state density of conduction band
t_{DDcr}	the critical thickness of GaN with Ga-face donor-like surface states	δ	the difference between Fermi level and the bottom of the flat region of conduction band

3.1. Intrinsic GaN on Ga-face

The direction of ε_π in bulk GaN is from N-face to Ga-face, and the intensity of ε_π can be calculated by Poisson equation: $|\varepsilon_\pi| = n_\pi/\varepsilon \approx 3.45$ MV/cm.

If the polarization charges cannot be screened, there will be a strong constant polarized electric field of an order of MV/cm inside GaN, which slopes the energy band of GaN. There is a significant energy difference between the top of the Ga-face valence band and the Fermi level in thin bulk GaN. In this case, the intrinsic thermal excitation hardly occurs and its influence on the polarized electric field can be ignored. The electric field in GaN should be constant, as shown in Fig. 1(a). As the thickness of GaN increases, the energy difference between the top of Ga-face valence band and Fermi level gradually decreases. When the top of the Ga-face valence

band is quite close or getting to the Fermi level, the probability of intrinsic thermal excitation increases sharply, and many electron–hole pairs are excited, as shown in Fig. 1(b). The electrons and holes drift to N-face and Ga-face respectively to screen a part of the polarized electric field. The total electric field inside the GaN reduces and the slope of energy band begins to decrease. With the thickness of GaN increasing further, like Fig. 1(c), the Fermi level is clamped at the Ga-face valence band. The intrinsic thermal ionization is promoted, excites more screening charges and the polarized electric field is getting screened further.

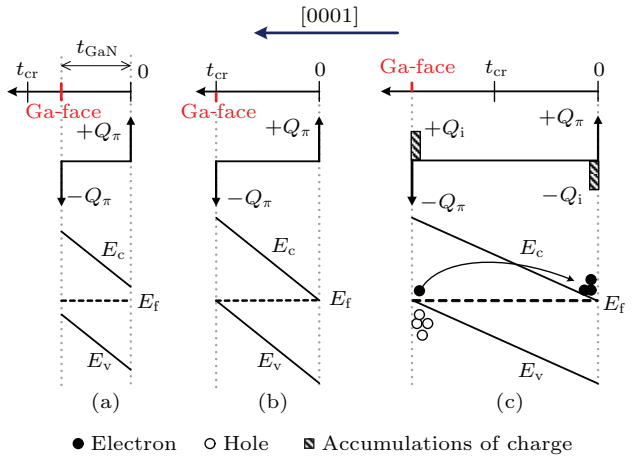


Fig. 1. The material structure, charges block diagram, and energy band diagram during the epitaxial growth of intrinsic bulk GaN: (a) the case when t_{GaN} is less than t_{cr}, (b) the case when t_{GaN} is equal to t_{cr}, and (c) the case when t_{GaN} is greater than t_{cr}.

When the Ga-face valence band is equal to the Fermi level, the GaN thickness is called the critical thickness of GaN. In this case, assuming that the intensity of the polarization electric field is almost constant, the uniform electric field intensity in GaN should be approximately equal to

$$|\epsilon_\pi| = \frac{E_g}{e \cdot t_{cr}}. \tag{1}$$

Under the symmetry principle, formula (2) is given Gauss's theorem.

$$|\epsilon_\pi| = \frac{\sigma}{\varepsilon}. \tag{2}$$

Combining formulas (1) and (2), the t_{cr} can be approximately considered to be related to the material's bandgap and the intensity of polarized electric field[10]

$$t_{cr} = \frac{E_g}{e\,|\epsilon_\pi|}. \tag{3}$$

For GaN bulk materials, t_{cr} is about 10 nm. If t_{GaN} is greater than t_{cr}, the electric field inside GaN is roughly inversely proportional to thickness:

$$|\epsilon| = \frac{E_g}{e \cdot t_{GaN}}. \tag{4}$$

According to Poisson's equation, we can get

$$|\epsilon| = \frac{n_\pi - \sigma_n}{\varepsilon}. \tag{5}$$

Combining formulas (4) and (5), the relationship between σ_n and t_{GaN} is approximately

$$\sigma_n = n_\pi - \frac{\varepsilon E_g}{e t_{GaN}}. \tag{6}$$

We simulate intrinsic GaN bulk materials with different thicknesses by TCAD simulations. The energy band of intrinsic bulk GaN is shown in Fig. 2(a) and it is basically the same as our analysis. The E_f is clamped at the Ga-face valence band and the N-face conduction band. The carrier distribution in the 3-μm bulk GaN is extracted and shown in Fig. 2(b), and it is also consistent with our analysis.

The σ_n and intensity of ε obtained by simulations are compared with theoretical analysis results, as shown in Fig. 3. The error is less than 5% about σ_n and less than 15% about ε. Figure 3(a) shows the ε and σ_n as a function of GaN thickness. It can be found that as the t_{GaN} increases, σ_n gradually increases, which promotes the screening of polarized electric field. So that the net charges on the Ga-face and N-face of the GaN decreases and then the internal electric field decreases. It is worth noticing that although σ_n is close to the n_π, it still cannot fully compensate the polarization charges. Figure 3(b) shows that as the bulk GaN thickness increases from 10 nm to 10 μm, Ga-face net charge density reduces from 1.8×10^{13} cm^{-2} to 4.1×10^{10} cm^{-2}, and electric field intensity reduces from 3.4 MV/cm to 3 kV/cm but the ϵ_π is still not completely screened.

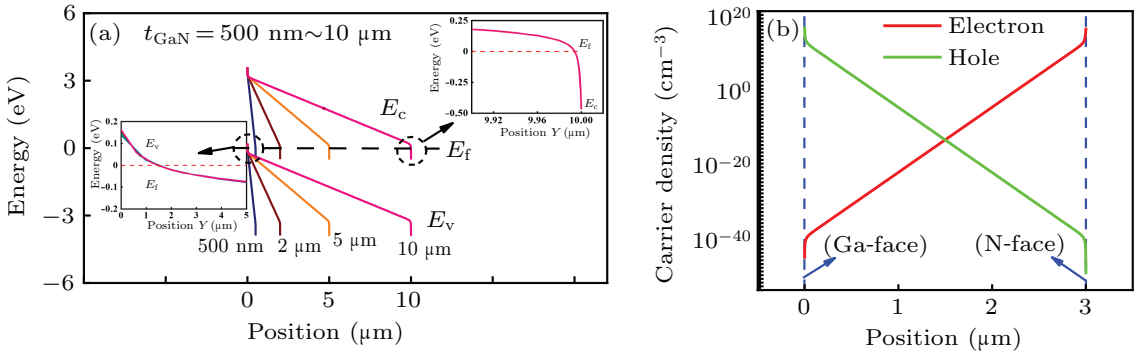


Fig. 2. (a) Band diagram of 500 nm–10 μm GaN, (b) spatial distribution of charges in 3-μm GaN bulk material.

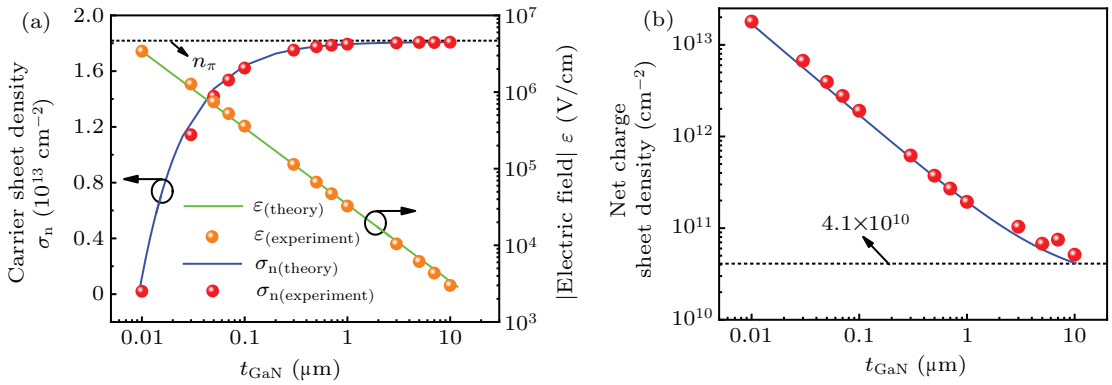


Fig. 3. Comparison of theoretical results of the self-screening effect of the polarized electric field in intrinsic bulk GaN with the TCAD simulation results. (a) The relationship between the screening charge density and the electric field of the GaN material as a function of GaN thickness, (b) Ga-face net charge density as a function of GaN thickness.

3.2. Intrinsic GaN with Ga-face donor-like surface states

The self-screening effect of the polarized electric field in intrinsic GaN with Ga-face donor-like surface states is like that in intrinsic bulk GaN. As a thin GaN, a large energy difference is between the surface state energy level and Fermi level. The ionization probability of the donor-like surface states is extremely low, as shown in Fig. 4(a). As t_{GaN} increases, the difference between E_{DD} and Fermi level gradually decreases. When δ is small enough, the probability of donor-like surface state ionization increases and electrons are ionized to screen a part of the polarized electric field, leaving positive ionized donor-like surface states, as shown in Fig. 4(b). Analogously, when Ga-face Fermi level is equal to E_{DD}, we call this GaN thickness as the critical thickness. Same method as formula (3), the t_{DDcr} approximately depends on E_{DD},

$$t_{DDcr} = \frac{E_{DD}}{e|\epsilon_\pi|}. \tag{7}$$

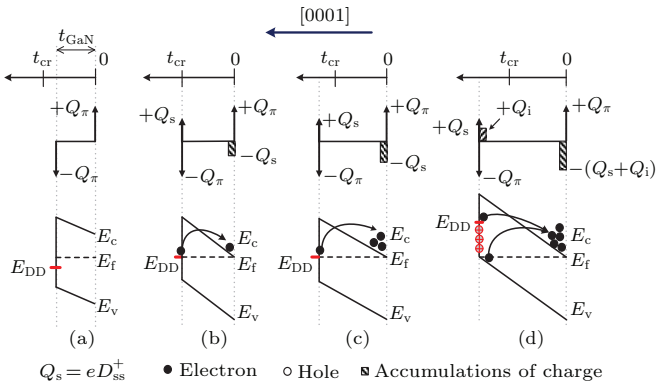


Fig. 4. The material structure, charges block diagram, and energy band diagram of intrinsic bulk GaN with Ga-face donor-like surface states: (a) the case when $t_{GaN} < t_{DDcr}$, (b) the case when $t_{GaN} = t_{DDcr}$, (c) the case when $t_{GaN} > t_{DDcr}$ and $D_{ss} > n_{s-cr}$, (d) the case when $t_{GaN} > t_{DDcr}$, but $D_{ss} < n_{s-cr}$.

When t_{GaN} is greater than t_{DDcr}, the Fermi level will be clamped at E_{DD}. The Ga-face donor-like surface states will be further ionized, more electrons will be ionized and concentrate on N-face to screen polarized electric field, as shown in Fig. 4(c). However, when D_{ss} is less than n_π, with the increase of t_{GaN}, the intrinsic thermal excitation occurs after the donor-like surface state is completely ionized and continues to screen polarized electric field. So, the Fermi level will be clamped at Ga-face valence band instead of E_{DD}, as shown in Fig. 4(d). Therefore, with a certain t_{GaN} (greater than t_{DDcr}) and E_{DD}, there is a critical donor-like surface state density resulting in the Fermi level being clamped at the transition from E_{DD} to Ga-face valence band. From formula (6) the specific mathematical relationship of n_{s-cr} in this case is

$$n_{s-cr} = n_\pi - \frac{\varepsilon E_{DD}}{et_{GaN}}. \tag{8}$$

The ε is related to t_{GaN}, energy level, and D_{ss}, as follows:

$$|\epsilon| = \begin{cases} \dfrac{E_{DD}}{et_{GaN}}, & D_{ss} \geq n_{s-cr}, \\ \dfrac{E_g}{et_{GaN}}, & D_{ss} < n_{s-cr}. \end{cases} \tag{9}$$

The corresponding σ_n should be

$$\sigma_n = \begin{cases} eD_{ss}^+ = n_\pi - \dfrac{\varepsilon E_{DD}}{et_{GaN}}, & D_{ss} \geq n_{s-cr}, \\ eD_{ss}^+ + n_{s-i} = n_\pi - \dfrac{\varepsilon E_g}{et_{GaN}}, & D_{ss} < n_{s-cr}. \end{cases} \tag{10}$$

We simulated the GaN bulk material with Ga-face donor-like surface states and the energy band of 3-μm GaN with different D_{ss} at $E_{DD} = 1$ eV.[21] The results are shown in Fig. 5(a). When D_{ss} is higher than 5×10^{13} cm^{-2}, the Fermi level is always clamped at E_{DD}. When D_{ss} is lower than 1×10^{13} cm^{-2}, the Fermi level is always clamped at the Ga-face valence band. That means the n_{s-cr} is between 1×10^{13} cm^{-2} and 5×10^{13} cm^{-2}. Figure 5(b) shows the n_{s-cr} under different t_{GaN} and E_{DD}. The n_{s-cr} shows a decreasing trend with the increase of the donor energy level. As GaN thickness increases, n_{s-cr} gradually approaches n_π. These results are consistent with our theoretical analysis.

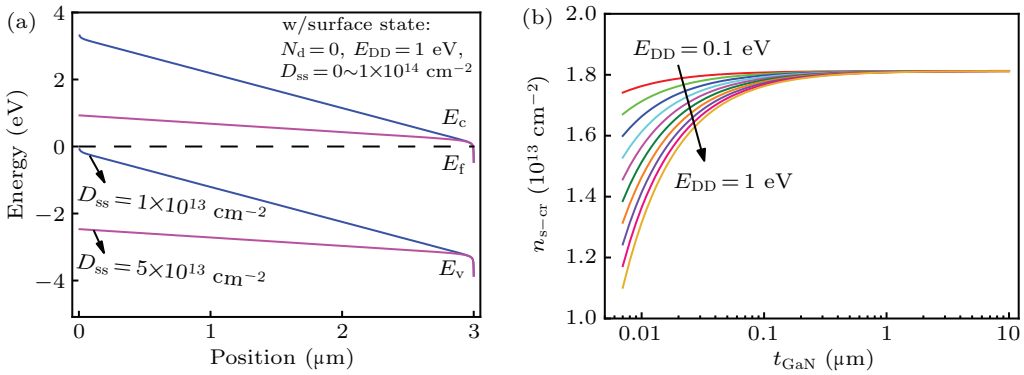


Fig. 5. (a) Energy band diagrams of bulk GaN with different D_{ss}, (b) the corresponding n_{s-cr} at different t_{GaN} and E_{DD}.

3.3. The n-type GaN without surface states

For bulk GaN with only n-type doping, the electrons are ionized by impurities and directionally drift to the N-face of GaN under the polarized electric field, leaving the positive ionized impurities which forms a depletion region, playing a certain role in screening polarized electric field. If t_{GaN} is greater than t_{cr}, the surface potential (ϕ_s) of GaN can be considered approximately equal to E_g, and the W_d should be

$$W_d = \sqrt{\frac{2\varepsilon}{eN_d}V_{bi}}, \tag{11}$$

$$V_{bi} = E_g - \delta, \tag{12}$$

$$\delta = E_c - E_f = -kT\ln\left(\frac{N_d}{N_c}\right). \tag{13}$$

Combining formulas (11)–(13), the W_d formed by donor impurity ionization is mainly affected by N_d and V_{bi}, but not by GaN thickness. As N_b increases, the bottom of the conduction band gets closer to the Fermi level. It is worth noticing that although N_b is quite low (10^{15} cm^{-3} in our simulations and calculations), δ is only about 0.2 eV, calculated by formula (13), which is negligible compared with E_g (about 3.4 eV). So that the formula (11) can be approximated as

$$W_d = \sqrt{\frac{2\varepsilon}{eN_d}E_g}. \tag{14}$$

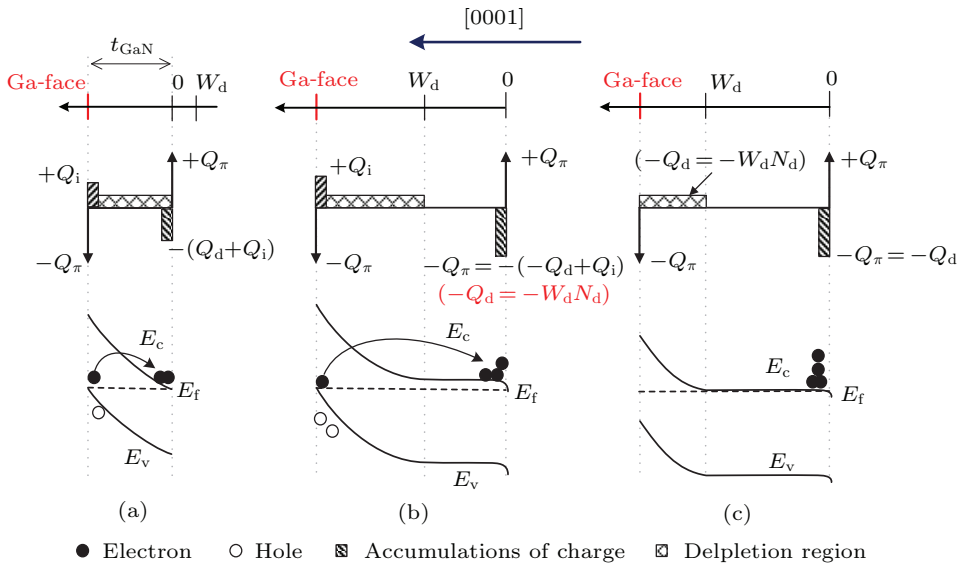


Fig. 6. The material structure, charges block diagram, and the energy band diagram of bulk GaN with donor impurities: (a) the case when $t_{GaN} < W_d$, (b) the case when $t_{GaN} > W_d$ and $N_d < 10^{19}$ cm^{-3}, (c) the case when $t_{GaN} > W_d$ and $N_d \geq 10^{19}$ cm^{-3}.

By further analysis we know that if t_{GaN} is less than W_d, the donor impurity in the GaN material will be completely ionized, as shown in Fig. 6(a). The screening charge density provided is $N_d \cdot t_{GaN}$, which should be less than n_π. In this case, a part of screening charges should be provided by intrinsic thermal excitation, so that the Fermi level will be clamped at the Ga-face valence band. As t_{GaN} increases to be greater than W_d, a flat energy band region appears, which means that the polarized electric field is completely screened in that region like Fig. 6(b). Figure 6(b) shows a condition about the N_d is lower than 10^{19} cm^{-3} (a critical value of N_d in our simulation. When N_d is 10^{19} cm^{-3}, the electron density provided by donor impurity ionization is exactly equal to n_π in Fig. 7(a)), the electron density provided by donor impurity ionization is

$N_d \cdot W_d$ and it is still less than n_π. So that the Fermi level is clamped at the Ga-face valence band to complement screening charges. However, when N_d is greater than or equal to 10^{19} cm^{-3}, the electron density provided by donor impurity ionization is already greater than n_π. Due to the self-stability of charges in a balanced system, the Fermi level would not be clamped at the Ga-face valence band and no obvious intrinsic thermal excitation occurs. The W_d will also decrease because the ϕ_s of GaN decreases, ensuring $N_d \cdot W_d$ is exactly equal to n_π. In this case, the polarized electric field inside GaN would be completely screened and the internal energy band gets flat, as shown in Fig. 6(c).

Figure 7(a) shows the energy band characteristics of bulk GaN with various donor doping concentrations from 10^{15} cm^{-3} to 10^{19} cm^{-3} obtained by TCAD simulations. With the increase of N_d, W_d gradually decreases. The flat region of the energy band indicates that the electric field is 0 and the polarized electric field is completely screened. As N_d is about 10^{15} cm^{-3}–10^{18} cm^{-3}, the Fermi level is clamped at the Ga-face valence band. When N_d is equal to 10^{19} cm^{-3}, the Fermi level is no longer clamped at the Ga-face valence band.

Figure 7(b) shows the electron density provided by the donor impurity ionization, total screening charge density, and W_d from simulation and theoretical analysis results. With the increase of the doping concentration, σ_n gradually increases, while the remaining electrons provided by intrinsic thermal excitation gradually decreases and the total screening charge density is still equal to n_π, which means the polarized electric field inside GaN is always completely screened.

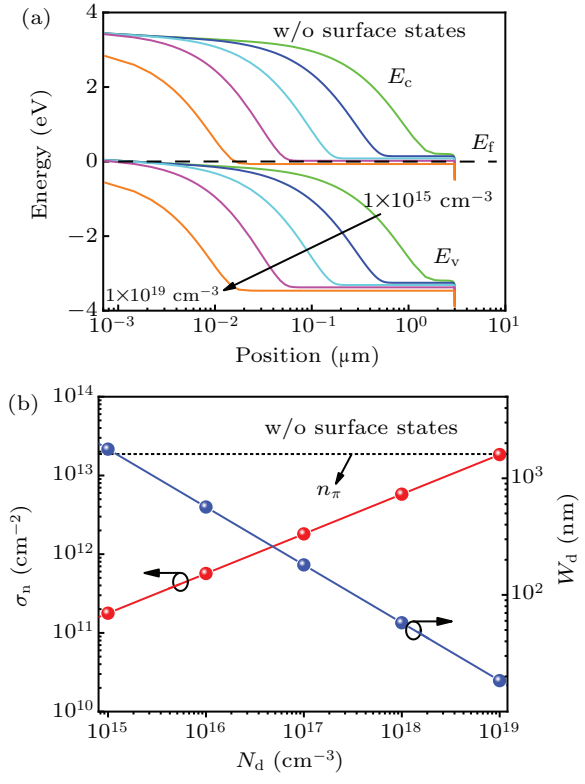


Fig. 7. (a) Energy band diagram of bulk GaN with different n-type doping concentrations (semi-logarithmic coordinates), (b) σ_n and W_d provided by donor impurity ionization under different doping concentrations.

3.4. The n-type GaN without surface states

Generally, there are both donor-like surface states and shallow-level donor impurities[21] in actual GaN materials, and the two factors together impact the polarized electric field inside GaN. The W_d is generally from tens of nanometers to several microns and the t_{DDcr} is only several nanometers, which is much smaller than W_d. If t_{GaN} is less than t_{DDcr}, the charges from impurity ionization, donor-like surface states ionization, and intrinsic thermal excitation together still cannot completely screen the polarized electric field, the energy band characteristics would be just like Fig. 4(a) and have little practical significance. So, the following analysis assumes that the thickness of GaN is always greater than t_{DDcr}.

When D_{ss} is greater than n_{s-cr}, Fermi level will be clamped at E_{DD}, as shown in Figs. 8(a) and 8(b). When t_{GaN} is less than W_d, as shown in Fig. 8(a) and donor impurities are completely ionized but cannot completely screen the polarized electric field. The t_{GaN} in Fig. 8(b) is greater than W_d and a part of donor impurities are ionized. The electrons from donor impurities and donor-like surface states screen the polarized electric field and form a flat energy band region. The screening charges in Figs. 8(a) and 8(b) come from ionizing donor impurities and donor-like surface states.

As D_{ss} is less than n_{s-cr}, donor-like surface states are completely ionized and the Fermi level is clamped at Ga-face valence band, which means a part of screening charges are provided by intrinsic thermal excitation like Figs. 8(c) and 8(d). Like the analysis above, figure 8(c) shows that when t_{GaN} is less than W_d, the donor impurities are completely ionized and the polarized electric field cannot be completely screened. Figure 8(d) shows that when t_{GaN} is greater than W_d, the polarized electric field is completely screened and a flat energy band region appears. The screening charges in Figs. 8(c) and 8(d) come from ionization of donor impurities, donor-like surface states, and intrinsic thermal excitation which is different from the case in Figs. 8(a) and 8(b).

Generally, in GaN with both donor-like surface states and donor impurities, the density of the donor-like surface states first determines the position where the Fermi level is clamped and the V_{bi}. Then it determines the W_d and the density of screening charges that can be provided. The sources of screening charges are summarized in Fig. 9. If t_{GaN} is greater than W_d, the polarized electric field can be completely screened. The sources of screening charges mainly include the electrons provided by the ionization of the donor-like surface states and the donor impurity ionization. When the surface state density is low, the intrinsic thermal excitation occurs and provides screening charges. But if t_{GaN} is greater than W_d and heavily doped (over 10^{19} cm^{-3}), the intrinsic thermal excitation would rarely occur. That case can be comprehended uncomplicatedly following the analysis in Subsection 3.3, Fig. 6(c).

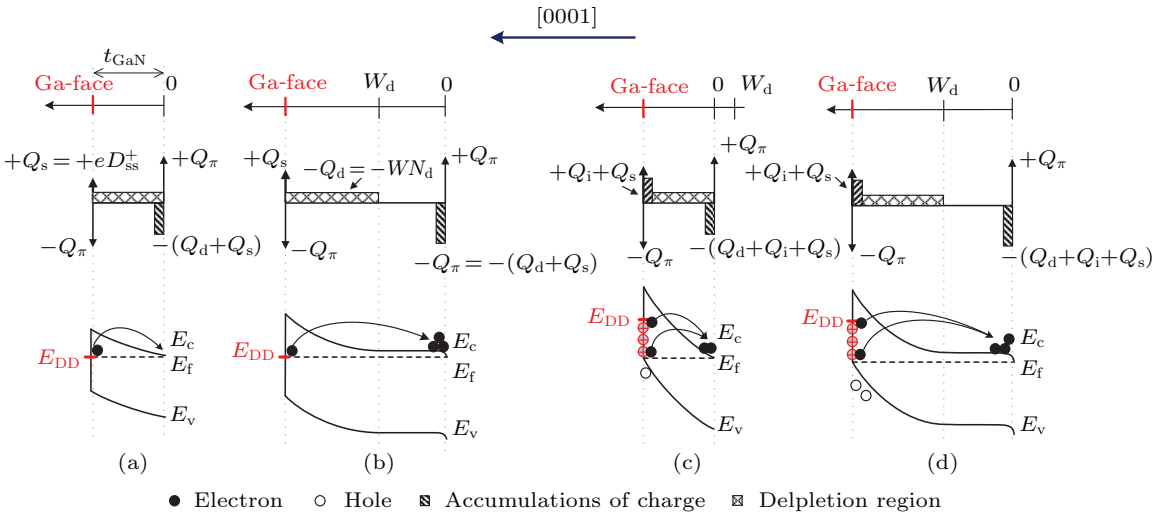


Fig. 8. The material structure, charges block diagram, and energy band diagram of bulk GaN with both donor-like surface states and donor impurities: (a) the case when $D_{ss} > n_{s-cr}$, $t_{GaN} < W_d$, and $N_d < 10^{19}$ cm^{-3}; (b) the case when $D_{ss} > n_{s-cr}$, $t_{GaN} > W_d$, and $N_d < 10^{19}$ cm^{-3}; (c) the case when $D_{ss} < n_{s-cr}$, $t_{GaN} < W_d$, and $N \geq 10^{19}$ cm^{-3}; (d) the case when $D_{ss} < n_{s-cr}$, $t_{GaN} > W_d$, and $N \geq 10^{19}$ cm^{-3}.

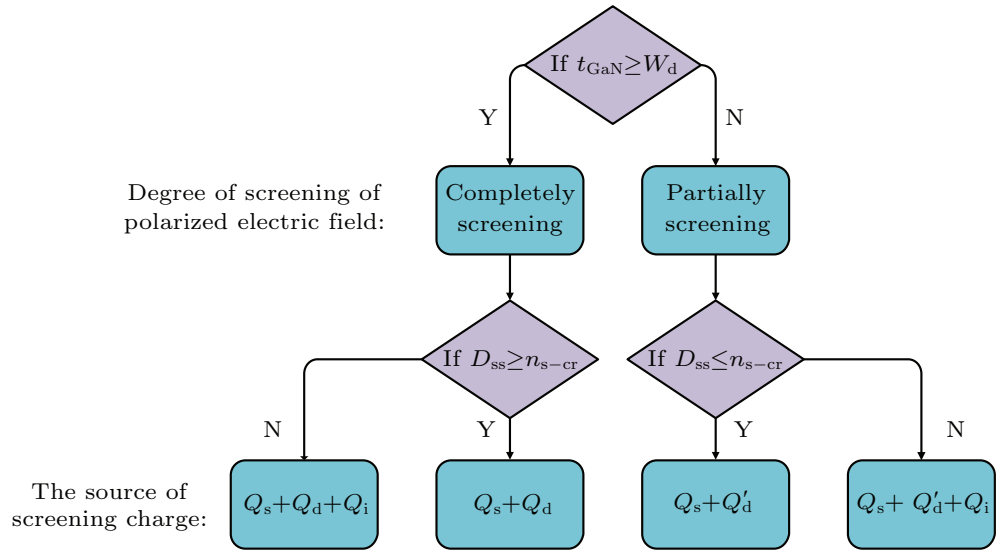


Fig. 9. The source of screening charges in bulk GaN. In the figure, Q'_d is the screening charges provided by the ionization of donor impurities when $t_{GaN} < W_d$ and $Q'_d = t_{GaN} \cdot N_d$.

For GaN with various values of D_{ss} and N_d, figure 10 shows their TCAD simulation results of the band structure. The t_{GaN} is greater than W_d in simulations. The energy band has a flat region and the polarization electric field is completely screened. When D_{ss} is 10^{14} cm^{-2}, the Fermi level is clamped at E_{DD}, the built-in potential should be $V_{bi} = E_{DD} - \delta$ in this condition. The W_d and electron density provided by donor impurity ionization are determined by V_{bi}. The remaining electrons are provided by the ionization of the donor-like surface states. When D_{ss} is 10^{13} cm^{-2}, the Fermi level is clamped at the Ga-face valence band and the built-in potential should be $V_{bi} = E_g - \delta$ in this condition. Donor-like surface states are completely ionized and the remaining electrons are provided by donor impurity ionization and intrinsic thermal excitation, which can be seen to be consistent with our theoretical analysis.

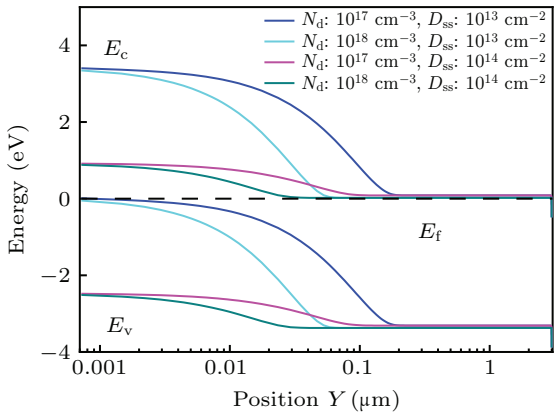


Fig. 10. Energy band diagram of bulk GaN with both donor surface states and donor impurities.

4. Conclusion and perspectives

In summary, this work uses TCAD simulations to study the self-screening effect of the polarized electric field in Ga-

face bulk GaN and the source of screening charges with several conditions: (i) The electric field in intrinsic bulk GaN is inversely proportional to GaN thickness, screening charges provided by intrinsic thermal excitation. (ii) In intrinsic GaN with Ga-face donor-like surface states, there is a critical donor-like surface state density which decides where the Fermi level is clamped. And it determines the density of screening charges and the degree of screening of the polarized electric field in GaN. (iii) In bulk GaN with donor impurities, if GaN thickness is greater than the width of the depletion region, the polarized electric field inside the GaN can be completely screened. In this condition, the screening charges are provided by donor impurity ionization and intrinsic thermal excitation. However, they are only provided by donor impurity ionization when GaN is heavily doped. (iv) As GaN with both Ga-face donor-like surface states and donor impurities, only when the thickness of GaN is greater than the width of the depletion region, can the polarization electric field in GaN be completely screened. And the donor-like surface state density determines the surface potential of the GaN, determining the width of the depletion region and density of screening charges provided by donor impurities in that condition. The sources of screening charges are mainly donor impurity ionization and donor-like surface states ionization. The intrinsic thermal excitation could participate in the screening effect when the surface state density is lower than the critical value.

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References

[1] Ambacher O, Smart J, Shealy J R, Weimann N G, Chu K, Murphy M, Schaff W J and Eastman L F 1999 *J. Appl. Phys.* **85** 3222
[2] Chaudhuri R, Bader S J, Chen Z, Muller D A, Xing H G and Jena D 2019 *Science* **365** 1454
[3] Simon J, Protasenko V, Lian C, Xing H and Jena D 2010 *Science* **327** 60
[4] Chu R, Cao Y, Chen M, Li R and Zehnder D 2016 *IEEE Electron Dev. Lett.* **37** 269
[5] Zhou Q, Wei D, Zhu R P, *et al.* 2018 *Superlattices & Microstructures* **122** 85
[6] Zhang J L, He L, Li L A, Ni Y Q, Que T T, Liu Z X, Wang W J, Zheng J X, Huang Y F, Chen J, Gu X, Zhao Y W, He L, Wu Z S and Liu Y 2018 *IEEE Electron Dev. Lett.* **39** 1720
[7] Zhang Y T, Deng G Q, Yu Y, Wang Y, Zhao D G, Shi Z F, Zhang B L and Li X H 2020 *ACS Photon.* **7** 1723
[8] Unni V, Long H, Sweet M, Balachandran A, Narayanan E M S, Nakajima A and Kawai H 2014 *IEEE 26th ISPSD*, June 15–19, 2014, Waikoloa, Hawaii, p. 245
[9] Zhang Z H, Liu W, Ju Z, Tan S T, Ji Y, Kyaw Z, Zhang X L, Wang L C, Sun X W and Demir H V 2014 *Appl. Phys. Lett.* **104** 243501
[10] Mishra U K and Singh J 2008 *Semiconductor device physics and design* (Netherlands: Springer), pp. 388–392
[11] Bernardini F, Fiorentini V and Vanderbilt D 1997 *Phys. Rev. B* **56** 10024
[12] Lahrèche H, Vennéguès P, Tottereau O, Laügt M, Lorenzini P, Leroux M, Beaumont B and Gibart P 2000 *J. Crystal Growth* **217** 13
[13] Korbutowicz R, Dumiszewska E and Prażmowska J 2007 *Crystal Research and Technology* **42** 1297
[14] Popovici G, Kim W, Botchkarev A, Tang H P and Morkoç H 1997 *Appl. Phys. Lett.* **71** 3385
[15] Koleske D D, Wickenden A E, Henry R L and Twigg M E 2002 *J. Crystal Growth* **242** 55
[16] Nakamura S, Mukai T and Senoh M 1992 *Jpn. J. Appl. Phys.* **31** 2883
[17] Slack G A, Schowalter L J, Morelli D and Freitas J A Jr 2002 *J. Crystal Growth* **246** 287
[18] Zywietz T K, Neugebauer J and Scheffler M 1999 *Appl. Phys. Lett.* **74** 1695
[19] Smorchkova I P, Elsass C R, Ibbetson J P, Vetury R, Heying B, Fini P, Haus E, DenBaars S P, Speck J S and Mishra U K 1999 *J. Appl. Phys.* **86** 4520
[20] Bogusławski P, Briggs E L and Bernholc J 1995 *Phys. Rev. B* **51** 17255
[21] Nidhi, Rajan S, Keller S, Wu F, DenBaars S P, Speck J S and Mishra U K 2008 *J. Appl. Phys.* **103** 124508
[22] Freitas Jr. J A, Moore W J, Shanabrook B V, Braga G C B, Koleske D D, Lee S K, Park S S and Han J Y 2003 *Phys. Stat. Sol. (b)* **240** 330