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GaN-based heterostructures: electric–static equilibrium and boundary conditions*

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In the GaN-based heterostructures, this paper reports that the strong electric fields induced by polarization effects at the structure boundaries complicate the electric–static equilibrium and the boundary conditions. The basic requirements of electric–static equilibrium for the heterostructure systems are discussed first, and it is deduced that in the application of the coupled Schrödinger–Poisson model to the heterostructures of electric–static equilibrium state, zero external electric field guarantees the overall electric neutrality, and there is no need to introduce the charge balance equation. Then the relation between the screening of the polar charges in GaN-based heterostructures and the possible boundary conditions of the Poisson equation is analysed, it is shown that the various boundary conditions are equivalent to each other, and the surface charge, which can be used in studying the screening of the polar charges, can be precisely solved even if only the conduction band energy is correctly known at the surface. Finally, through the calculations on an AlGaN/GaN heterostructure with typical structure parameters by the coupled Schrödinger–Poisson model under the various boundary conditions, the correctness of the above analyses are validated.

Keywords: GaN-based heterostructures, electric–static equilibrium, boundary conditions, coupled Schrödinger–Poisson model

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1. Introduction

The polarization effects strongly modulate the energy band structures of the GaN-based heterostructures, thereby strengthen the confinements and raise the sheet densities of the two-dimensional electron gases (2DEG).[1] But the polarization effects also complicate the picture of the electric–static equilibrium of the GaN-based heterostructures. When the one-dimensional coupled Schrödinger–Poisson model[2] is adopted to solve the energy band and carrier density distributions of the AlGaN/GaN heterostructures, the polarization effects introduce polar charges at the surface of AlGaN, AlGaN/GaN interface and the bottom of GaN. But according to the measured conduction band energy at the surface (denoted as $E_{\rm Cs}$ below) of AlGaN/GaN heterostructures[3] and the plentiful experimental results of 2DEG densities AlGaN/GaN heterostructures, the polar charges added at the structure boundaries (the surface of AlGaN and the bottom of GaN) induce such strong electric fields that the self-consistent iteration often diverges or converges at the wrong solutions.

So the screening of polar charges at the boundaries of GaN-based heterostructures needs to be considered, but it is difficult to measure quantitatively the degree of screening at present. Jogai assumed that the density of the surface charge (denoted as $\sigma_{\rm s}$ below) including the polar charge and the screening charge, implants the charge balance equation into the coupled Schrödinger–Poisson model to force the heterostructure systems to realize overall electric neutrality, and add $\sigma_{\rm s}$ into the charge balance equation and the Poisson equation to consider its effects.[4] In iteration $\sigma_{\rm s}$ is modified repeatedly to obtain a reasonable $E_{\rm Cs}$ value, and at last the energy band and carrier density distributions accompanied by $\sigma_{\rm s}$ are obtained. However, the charge balance equation needs to be solved additionally, and as for physical parameters the relatively unknown factors such as $\sigma_{\rm s}$ are modified to satisfy the relatively obvious factors such as $E_{\rm Cs}$, so the calcu-

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lation cost is larger and the application is less convenient.

In this paper, the basic requirements of electric–static equilibrium for the heterostructure systems are discussed at first, and the equivalence between zero external electric field and the overall electric neutrality is deduced. So it is unnecessary to consider the charge balance equation in the application of the coupled Schrödinger–Poisson model to the heterostructures of electric–static equilibrium state. Then the screening of polar charge in GaN-based heterostructures is analysed and the possible boundary conditions of the Poisson equation are presented. At last, through the calculations on an AlGaN/GaN heterostructure by the self-consistent model, the feasibility of solving $\sigma_{\rm s}$ is validated from the calculation results with only $E_{\rm Cs}$ known and $\sigma_{\rm s}$ totally unconsidered in the boundary conditions, and the equivalence of various boundary conditions of the Poisson equation.

2. GaN-based heterostructures: electric–static equilibrium and boundary conditions

2.1. Basic requirement of electric–static equilibrium for the heterostructure systems

Ridley *et al* have suggested that a heterostructure system in equilibrium satisfies overall electric neutrality, zero external fields and zero voltage drop.[5] These requirements can be analysed by the one-dimensional Poisson equation as follows:

$$\begin{aligned}\frac{\mathrm{d}(\varepsilon_0\varepsilon(z)F(z))}{\mathrm{d}z} &= \rho(z)\\ =\rho_{\rm e}(z) - \frac{\mathrm{d}P(z)}{\mathrm{d}z} &= \rho_{\rm e}(z) + \rho_{\rm pol}(z),\end{aligned} \tag{1}$$

$$F(z) = -\frac{\mathrm{d}V(z)}{\mathrm{d}z}, \tag{2}$$

where $\varepsilon(z)$ is the static dielectric constant, $F(z)$ the electric field, and $V(z)$ the static electric potential, $\rho(z)$ is the sum of the charges in the system, including the polar charge $\rho_{\rm pol}(z)$ and the non-polar charge $\rho_{\rm e}(z)$, $\rho_{\rm pol}(z)$ is induced by the spatial change of the polarization strength $P(z)$, and is zero in the systems where there are no polarization effects.

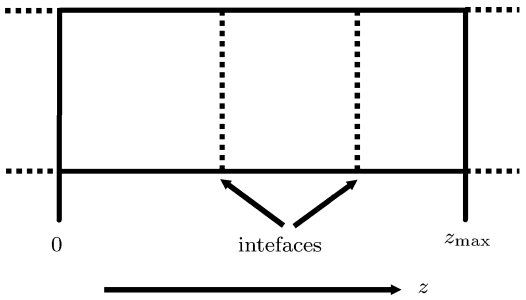


Fig.1. A semiconductor system in electric–static equilibrium state. The boundaries 0 and $z_{\max}$ can be natural one or contrived ones.

For a heterostructure system in equilibrium, whose charge exchange with the surroundings reaches the balance state, zero external fields is natural. Suppose the external sides of the system boundaries are 0^- and $z^+_{\max}$, and we have

$$F(0^-) = F(z^+_{\max}) = 0. \tag{3}$$

Integrating both sides of Eq.(1) from 0^- to $z^+_{\max}$, and considering Eq.(3), we have

$$\begin{aligned}&\varepsilon_0(\varepsilon(z^+_{\max})F(z^+_{\max}) - \varepsilon(0^-)F(0^-))\\ &= \int_{0^-}^{z^+_{\max}} \rho(z)\mathrm{d}z = 0.\end{aligned} \tag{4}$$

From Eq.(4) we can see that overall electric neutrality is not independent and can be deduced by zero external fields. Extending this issue to three-dimensional space we will reach the same conclusion by the Gauss theorem.

Zero voltage drop across the system is right when it means that the Fermi level is continuous and aligned, but it should not be explained as equal electric potentials at both ends of the system. In Ref.[5], it is supposed that (i.e. $E_1a + E_2b$=0 in Eq.(2) of Ref.[5])

$$\int_{0^+}^{z^-_{\max}} F(z)\mathrm{d}z = 0. \tag{5}$$

This means that $V(0^+)$ should equal to V $(z^-_{\max})$, and such a requirement is not satisfied even in the simplest p-n junction, so it is not necessary for electric–static equilibrium. From another related paper of Ridley,[6] it is explained that this assumption is based on the introduction of an imaginary electrode at the bottom of the structure, so it holds only in this case.

All in all, in a heterostructure system in equilibrium, the Fermi level is aligned, the external electric field is zero, and overall electric neutrality is thereby realized. So when the coupled Schrödinger–Poisson

model is applied to solve the energy band and carrier density distributions of the heterostructures, zero external electric field guarantees the overall electric neutrality, and there is no need to solve the charge balance equation additionally.

2.2. Screening of the polar charge/ field in GaN-based heterostructures

Through the transformation of Eq.(1) as below,

$$\frac{\mathrm{d}(\varepsilon_0\varepsilon(z)F(z)+P(z))}{\mathrm{d}z}=\rho_{\mathrm{e}}(z), \tag{6}$$

we can see that if there is no non-polar charge for a semiconductor surface/interface at $z = z_0$ it holds that

$$\begin{aligned}&\varepsilon(z_0^-)\varepsilon_0F(z_0^-)+P(z_0^-)=\varepsilon(z_0^+)\varepsilon_0F(z_0^+)+P(z_0^+)\\&\varepsilon(z_0^-)\varepsilon_0F(z_0^-)+\sigma_{\mathrm{pol}}=\varepsilon(z_0^+)\varepsilon_0F(z_0^+).\end{aligned} \tag{7}$$

Where $\sigma_{\mathrm{pol}}=P(z_0^-)-P(z_0^+)$ is the sheet polar charge, and Eq.(7) shows the electric displacement continuity at the abrupt hetero-interface.

For the AlGaN/GaN heterostructure shown in Fig.2, if σ_{pol} at the structure boundaries is totally unscreened and the external field is zero, the internal electric field near the structure boundaries induced by σ_{pol} would cause in both the layers such great band bending that it can reach the energy gap in each layer in less than 10 nm.

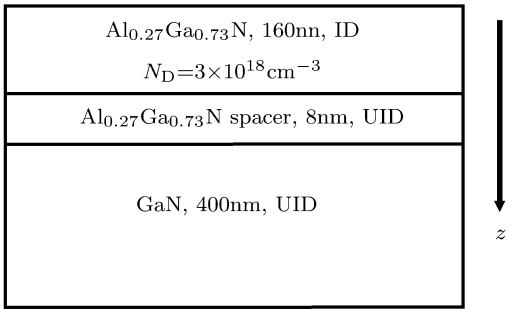


Fig.2. The simulating structure of AlGaN/GaN.

In fact these high fields are screened by various mechanisms in GaN-based heterostructures. At present GaN-based heterostructures are grown mostly by epitaxy techniques, and the nuclear region near substrate features high density of lattice defects. Polarization is sensitive to lattice parameters and their changes, so σ_{pol} or more possibly ρ_{pol} is reduced in the nuclear region, whose thickness is usually tens of nanometres. Meanwhile, the region accumulates charged defects and impurities, which screen ρ_{pol} to some extent. At the surface, the surface states and the external charges adsorbed screen σ_{pol}. At internal interfaces σ_{pol} causes the break of electric field, quantum wells of conduction band or valence band are often formed and electrons or holes accumulated to screen σ_{pol}.

So in the modelling of the polarization effects, σ_{pol} or ρ_{pol} at the boundaries of the heterostructures is usually omitted, or considered appropriately as needed to explain some experimental results or physical mechanisms, and σ_{pol} at the internal interfaces is totally taken into consideration.

2.3. The boundary conditions of GaN-based heterostructures

In the application of the one-dimensional coupled Schrödinger–Poisson model to the GaN-based heterostructures, the boundary condition of Schrödinger equation, i.e. the wave function is zero at the boundaries, is not affected, while the boundary conditions of Poisson equation are relevant to the screening degree of σ_{pol} or ρ_{pol} at the structure boundaries.

In order to solve Poisson equation there must be a boundary with the known static electric potential, there are three combinations of the boundary conditions and illustrated by AlGaN/GaN heterostructures as follows:

$\mathbf{B_1}$ The electric potential is known at the surface of AlGaN and electric field known at the bottom of GaN. Since E_{Cs} can be measured and the conduction band energy is directly related to the electric potential, so at the surface there is

$$E_{\mathrm{C}}\,|_{z=0}=E_{\mathrm{Cs}}. \tag{8}$$

In device simulation it is usually assumed that at the boundary far from the active area of device, the electric field is zero, or

$$F_{\mathrm{b}}=\frac{\mathrm{d}V}{\mathrm{d}z}\,|_{z=z\mathrm{max}}=0. \tag{9}$$

$\mathbf{B_2}$ The electric potential is known at both the surface of AlGaN and the bottom of GaN. At the surface of AlGaN Eq.(8) is still adopted. The conduction band energy at the bottom of GaN can be determined by the background carrier density n_{bg} as follows:

$$E_{\mathrm{C}}\,|_{z=z\mathrm{max}}=-k_{\mathrm{B}}T\ln\left(\frac{n_{\mathrm{bg}}}{N_{\mathrm{C}}}\right)+E_{\mathrm{F}}, \tag{10}$$

where k_B is the Boltzmann constant, T is the temperature, N_C the effective density of state and E_F the Fermi level.

B_3 The electric field is known at the surface of AlGaN and electric potential known at the bottom of GaN. At the bottom of GaN Eq.(10) is still adopted, and at the surface of AlGaN it is set as below allowing for zero external field,

$$\varepsilon_{\mathrm{AlGaN}}\varepsilon_0 F|_{z=0} = \sigma_s. \tag{11}$$

At the boundaries the sheet charges, if present, are related to the electric field directly and to the electric potential indirectly. So if the boundary conditions B_1 and B_2 are used, though no σ_s considered in the charge distribution (or $\rho(z)$ in Eq.(1)), the surface electric field can be solved and a precise σ_s can be obtained by Eq.(11) with the measured E_{Cs}. While the boundary conditions B_3 assumed plausibly the screening degree of σ_{pol} at the structure surface by σ_s, the correctness of σ_s can only be validated by the calculation results. That is likely a trial-and-error procedure. In the boundary conditions B_1, that at the GaN bottom boundary both of the internal and the external field are zero means that there is no sheet charge at the boundary, or it is assumed that σ_{pol} or ρ_{pol} at the interface between the heterostructure and the substrate is completely screened. In the boundary conditions B_2 and B_3, if it is assumed that n_{bg} is equal to the background doping density N_{DB}, the local electric neutrality is reached at the GaN bottom boundary, thus at this boundary the electric field is approximately zero. So these boundary conditions are equivalent to each other, but B_1 and B_2 are more practical.

3. The calculation results under various boundary conditions

The calculation is carried out for the structure shown in Fig.2 through a one-dimensional coupled Schrödinger–Poisson model,[7] and under the boundary conditions B_1–B_3 the results are obtained. The unintentional doping (UID) is assumed to be presented throughout the whole structure with N_{DB}=$10^{16}\,\mathrm{cm}^{-3}$. The temperature is 300K. The polarization effects are calculated with the nonlinear models.[8] The other relevant model parameters can be found in Ref.[9]. It is assumed that E_F=0, and E_{Cs}=1.2eV for the boundary conditions B_1 and B_2, and $n_{bg} = N_{DB}$ for B_2 and B_3.

Some physical quantities derived by the solved conduction band energy and carrier density distributions are listed in Table 1. The sheet densities n_{s2D} of the 2DEG and n_{s3D} of the bulk electrons, and the 2DEG energy levels show the difference between the calculation results in the internal part of the heterostructure, while σ_s and F_b show the difference between the results at the boundaries of the heterostructure. $\int \rho$ is the integral of all the charges in the structure, and it shows to what a degree the charge distribution deviates from the overall electric neutrality ($\int \rho$=0). As for the calculation results R_1 and R_2 obtained under the boundary conditions B_1 and B_2, the calculated σ_s is also considered in $\int \rho$.

Table 1. The calculation results for all the boundary conditions. n_{s2D} is the 2DEG sheet density. $E_0 - E_2$ are the 2DEG energy levels. n_{s3D} is obtained by the integral of bulk electron densities along z direction throughout the structure. The values of σ_s are calculated by Eq.(11) in R_1–R_4, and assumed as boundary conditions to be $-5.4618\times10^{12}\,\mathrm{cm}^{-2}$ in R_3 and $-9.8697\times10^{12}\,\mathrm{cm}^{-2}$ in R_4. The values of $\int \rho$ are calculated by the integral of all the charges throughout the structure, and reflect the overall electric neutrality.

Results	Boundary conditions	n_{s2D} /$10^{12}\mathrm{cm}^{-2}$	n_{s3D} /$10^{12}\mathrm{cm}^{-2}$	E_0 /meV	E_1 /meV	E_2 /meV	σ_s /$10^{12}\mathrm{cm}^{-2}$	F_b /$10^{-2}\mathrm{Vcm}^{-1}$	$\int \rho$ /$10^{8}\mathrm{cm}^{-2}$
R_1	B_1	9.0267	0.6300	–96.6	23.6	64.3	–5.4618	–0.0002	–0.4401
R_2	B_2	9.0267	0.6309	–96.6	23.6	64.3	–5.4618	1.7494	–0.4136
R_3	B_3	9.0332	0.6312	–96.6	23.6	64.3	–5.4550	1.9757	–0.4197
R_4	B_3	4.6801	0.5837	–45.7	41.4	73.9	–9.8574	1.9758	–0.0782

From R_1 and R_2 it is shown that the calculation results obtained under B_1 and B_2 are almost completely the same no matter in the internal part or at the boundaries of the heterostructure. The results R_3 obtained under B_3, whose σ_s value is deduced with Eq.(11) by the surface electric field from R_1 and R_2, are also in good agreement with R_1 and R_2. So the equivalence of various boundary conditions of the

Poisson equation is validated. While in the results R_4 obtained under B_3, whose absolute value of σ_s is assumed to equal σ_{pol} at the AlGaN/GaN interface, the conduction band energy at the surface of AlGaN reaches 3.4493 eV, and the values of the physical quantities for the internal part of the heterostructure differ very much from R_1–R_3. All these results are caused by the too large absolute value of σ_s for R_4.

In all the results, the electric potential or field at the boundaries shows a very weak deviation with their set value in the boundary conditions, which is caused by the error of the numerical algorithms. Allow for the unavoidable error, it is obvious that all the results in Table 1 reach the overall electric neutrality.

4. Conclusion

The polarization effects of the nitride materials raise greatly the 2DEG sheet density of the GaN-based heterostructures, but the induced strong electric fields at the structure boundaries make it very hard to analyse the electric–static equilibrium and the boundary conditions of GaN-based heterostructures. So it is necessary to consider the screening of the polarization effects, thus introduce the polar charges at the structure boundaries of reasonable values into the overall electric neutrality, and apply the correct boundary conditions to guarantee the agreements between the quantitative calculation results of the energy band and carrier density distributions with the experimental results. Through the analysis of the basic requirements of the electric–static equilibrium for the heterostructure systems, we show that zero external electric field guarantees the overall electric neutrality. So the charge balance equation is unnecessary when the heterostructures of electric–static equilibrium state are studied by the coupled Schrödinger–Poisson model. The analysis of the possible boundary conditions of the Poisson equation shows their equivalence. At the boundary where the electric potential is given, the sheet charge if exists can be obtained form the solved boundary electric field. This can serve as a theoretical approach to research into the screen of the polar charge in the GaN-based heterostructures. The above deductions are validated by the application of the coupled Schrödinger–Poisson model on an AlGaN/GaN heterostructures under the various boundary conditions.

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