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Electron distribution in polar heterojunctions within a realistic model

Nguyen Thanh Tien [a,*], Dinh Nhu Thao [b], Pham Thi Bich Thao [a], Doan Nhat Quang [c]

[a] College of Natural Science, Can Tho University, 3-2 Road, Can Tho City, Vietnam
[b] Center for Theoretical and Computational Physics, College of Education, Hue University, 34 Le Loi Street, Hue City, Vietnam
[c] Institute of Physics, Vietnamese Academy of Science and Technology, 10 Dao Tan Street, Hanoi, Vietnam

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ABSTRACT

We present a theoretical study of the electron distribution, i.e., two-dimensional electron gas (2DEG) in polar heterojunctions (HJs) within a realistic model. The 2DEG is confined along the growth direction by a triangular quantum well with a finite potential barrier and a bent band figured by all confinement sources. Therein, interface polarization charges take a double role: they induce a confining potential and, furthermore, they can make some change in other confinements, e.g., in the Hartree potential from ionized impurities and 2DEG. Confinement by positive interface polarization charges is necessary for the ground state of 2DEG existing at a high sheet density. The 2DEG bulk density is found to be increased in the barrier, so that the scattering occurring in this layer (from interface polarization charges and alloy disorder) becomes paramount in a polar modulation-doped HJ.

1. Introduction

Recently, electronic transport and intersubband optical transition in polar heterostructures (HSs), such as gallium nitride (GaN) (or zinc oxide (ZnO)), and their compounds have been intensively investigated [1,2]. These properties are characteristic of the quality and performance of electronic and optical devices [3]. The quoted semiconductors possess unique features that make them important to fabricate electronic and optical devices in view of their promising potential for high-voltage, high-power, and high-temperature microwave applications.

The electronic transport in a HS is characterized by a high mobility of two-dimensional electron gas (2DEG) in the sample, and its optical absorption by a narrow spectral linewidth. Both properties in question are determined by various scattering processes taking place with 2DEG. The effect of a scattering process in the lateral plane is determined by its mechanism, but this also depends on the electron distribution along the growth direction (quantization direction). Thus, the effect of an electron scattering process in the lateral plane depends on the envelope function, i.e., on confinement sources.

As is well known [1,2], polarization is an important property of a nitride and oxide-based HS. The HS possesses a very high (areal) density of polarization charges bound on the interface ($\sigma \sim 10^{13}$ cm^{-2}). For formation of 2DEG in a polar HS, interface polarization charges take a double role: they are a source to supply carriers (electrons) into the sample, but they also are a source to confine the carriers along the growth direction. It is worth noting that for formation of 2DEG in a modulation-doped HS, ionized impurities take such a double role as well [3,4].

Therefore, the aim of this paper is to present a theoretical study of the electron distribution (2DEG) in a polar modulation-doped HS, where the above double role of both interface polarization charges and ionized impurities is reasonably taken into account. Especially, we want to compare the role of the interface polarization charges and the ionized impurities which has not be done so far.

For simple illustration, we deal with a two-layer HS, i.e., single heterojunction (HJ) based on GaN. In Section 2, the 2DEG in a HJ is assumed to occupy the ground subband. The corresponding electron state is approximately described by a variational wave function in a triangular quantum well (QW). Within this realistic model, the QW has a finite potential barrier and a bent band.

In Section 3, parameters figuring the variational wave function are determined for a polar modulation-doped HJ by all confining potentials, especially from interface polarization charges and ionized impurities. Numerical results illustrating the electron distribution in HJ are also presented in Section 3. Lastly, a summary is given in Section 4.

* Corresponding author.
E-mail address: thanhtienctu@gmail.com (N.T. Tien).

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2. Theory

2.1. Variational wave function for HJ of finite potential barrier

We are now dealing with wurtzite III-nitride-based HJs, e.g., an AlGaN/GaN sample, which is composed of an AlGaN layer grown on a GaN layer. The system is featured with the z-axis along and opposite to the growth direction [0001], and $z=0$ being the interface plane between the GaN channel ($z>0$) and the AlGaN barrier ($z<0$). It is assumed that the channel layer (large thickness) is relaxed, while the barrier one (small thickness) is under tensile strain and modulation-doped.

At low temperature, the 2DEG is assumed to primarily occupy the lowest subband. It was shown [4–6] that in the realistic model of triangular QWs with a finite potential barrier, the electron state may be well described by a Fang–Howard wave function modified by Ando [5]:

$$\zeta(z)=\begin{cases} A\kappa^{1/2}\exp(\kappa z/2) & \text{for } z<0,\\ Bk^{1/2}(kz+c)\exp(-kz/2) & \text{for } z>0.\end{cases} \tag{1}$$

Here, κ and k are half the wave numbers in the barrier and channel layers, respectively. A, B, and c are dimensionless parameters given in terms of k and κ through the boundary and normalization conditions, as follows [4,6]:

$$\begin{aligned} &A\kappa^{1/2}=Bk^{1/2}c,\\ &A\kappa^{3/2}/2=Bk^{3/2}(1-c/2),\\ &A^2+B^2(c^2+2c+2)=1. \end{aligned} \tag{2}$$

The wave function of the lowest subband (its wave vectors k and κ) is to minimize the total energy per electron, which is fixed by the Hamiltonian

$$H=T+V_{\text{tot}}(z), \tag{3}$$

where T is the kinetic energy, and $V_{\text{tot}}(z)$ is the overall confining potential.

2.2. Confining potentials in a polar modulation-doped HS

Carrier confinement in a polar modulation-doped HS is determined by all confining sources located along the growth direction (z-axis): potential barrier, interface polarization charges, and Hartree potential induced by ionized impurities and 2DEG:

$$V_{\text{tot}}(z)=V_{\text{b}}(z)+V_{\sigma}(z)+V_{\text{H}}(z). \tag{4}$$

We are to specify the individual confining potentials in Eq. (4). First, for the potential barrier of a finite height V_0 located at the interface plane $z=0$, it holds

$$V_{\text{b}}(z)=V_0\,\theta(-z), \tag{5}$$

with $\theta(z)$ as a unity step function. The potential barrier height is fixed by the conduction band offset between the AlGaN and GaN layers: $V_0=\Delta E_{\text{c}}(x)$, with x as the alloy (Al) content in the AlGaN barrier.

It is well known [7–10] that due to piezoelectric and spontaneous polarizations in a nitride-based strained HS there exist positive polarization charges bound on the interface. These charges create a uniform normal electric field with the potential given by [11]

$$V_{\sigma}(z)=\frac{2\pi}{\varepsilon_{\text{a}}}e\sigma|z|, \tag{6}$$

with σ as their total density. Here $\varepsilon_{\text{a}}=(\varepsilon_{\text{b}}+\varepsilon_{\text{c}})/2$ is the average value of the dielectric constants of the barrier (ε_{b}) and channel (ε_{c}).

Next, we calculate the Hartree potential induced by the ionized donors and 2DEG in the HS. This is determined according to Poisson's equation [6,12]

$$\frac{d^2}{dz^2}V_{\text{H}}(z)=\frac{4\pi e^2}{\varepsilon_{\text{a}}}\big[N_{\text{I}}(z)-n(z)\big], \tag{7}$$

where $N_{\text{I}}(z)$ is the bulk density of donors along the growth direction, and $n(z)$ the one of electrons.

Hereafter, we are concerned with such samples that are modulation-doped in the barrier [13–15]:

$$N_{\text{I}}(z)=\begin{cases} N_{\text{I}} & \text{for } -z_{\text{d}}\le z\le -z_{\text{s}},\\ 0 & \text{elsewhere},\end{cases} \tag{8}$$

where $z_{\text{s}}=L_{\text{s}}$ and $z_{\text{d}}=L_{\text{s}}+L_{\text{d}}$, with L_{s} and L_{d} as the thicknesses of the spacer and doping layers, respectively.

The bulk density of electrons along the z-axis is determined by the envelope wave function in Eq. (1):

$$n(z)=n_{\text{s}}|\zeta(z)|^2, \tag{9}$$

with n_{s} as their sheet density.

We solve the Poisson equation for the Hartree potential $V_{\text{H}}(z)$ induced by the above distributions of the donors and 2DEG in combination with the boundary conditions at $z=\pm\infty$. For a non-polar HS, the subsystem composed of the donors and the 2DEG is neutral, so its electric field is vanishing at $z=\pm\infty$ [4,6,16]:

$$\partial V_{\text{H}}/\partial z(\pm\infty)=0. \tag{10}$$

However, in a polar HS the 2DEG originates not only from donors, but also from polarization charges, the neutrality condition is not claimed on the donor-2DEG subsystem. Hence, the boundary condition at $z=-\infty$ must be different, given as follows [12]:

$$\partial V_{\text{H}}/\partial z(-\infty)=0 \quad\text{and}\quad V_{\text{H}}(-\infty)=E_{\text{I}}, \tag{11}$$

with E_{I} as the binding energy of an ionized donor.

As a result, the Hartree potential may be represented in the form

$$V_{\text{H}}=V_{\text{I}}+V_{\text{s}}. \tag{12}$$

Here the first term is the potential due to remote donors, determined by the doping profile, viz., the donor sheet density ($n_{\text{I}}=N_{\text{I}}L_{\text{d}}$) and the thicknesses of the doping and spacer layers, given by

$$V_{\text{I}}(z)=E_{\text{I}}+\frac{4\pi e^2 n_{\text{I}}}{\varepsilon_{\text{a}}}\begin{cases} 0 & \text{for } z<-z_{\text{d}},\\ (z+z_{\text{d}})^2/2L_{\text{d}} & \text{for } -z_{\text{d}}<z<-z_{\text{s}},\\ z+(z_{\text{d}}+z_{\text{s}})/2 & \text{elsewhere}.\end{cases} \tag{13}$$

The second term is the potential due to 2DEG, determined by the electron sheet density n_{s} and its z-axis distribution, i.e., the electron wave function, given by

$$V_{\text{s}}(z)=-\frac{4\pi e^2 n_{\text{s}}}{\varepsilon_{\text{a}}}\begin{cases} f(z) & \text{for } z<0,\\ g(z)+z+f(0)-g(0) & \text{for } z>0.\end{cases} \tag{14}$$

The auxiliary functions in Eq. (14) are defined in terms of the variational parameters entering Eq. (1), as follows:

$$f(z)=\frac{A^2}{\kappa}e^{\kappa z} \tag{15}$$

and

$$g(z)=\frac{B^2}{k}e^{-kz}\big[k^2z^2+2k(c+2)z+c^2+4c+6\big]. \tag{16}$$