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Analysis of energy states where electrons and holes coexist in pseudomorphically strained InAs HEMTs

Yui Nishio, Takato Sato, Naomi Hirayama, Tsutomu Iida, and Yoshifumi Takanashi[1]
[1] Tokyo University of Science
Department of Materials Science and Technology, Faculty of Industrial Science and Technology
6-3-1, Niijuku, Katsushika-ku, Tokyo 125-8585, Japan
Phone: +81-3-5876-1417(1815) E-mail: j8213703@ed.tus.ac.jp

Abstract

For a system where electrons and holes co-exist, we establish the theory that takes into account the non-parabolicity only for the conduction band of the InAs channel layer in strained InAs-HEMTs (InAs-PHEMTs). This theory enables us to rigorously determine not only the energy states and the concentration profiles for both carriers but the shift of the threshold voltage of PHEMTs due to the holes accumulate in the channel. The calculation is made by solving the Schrödinger and Poisson equations self-consistently for both carriers.

1. Introduction

High-electron-mobility transistors with a pseudomorphically strained InAs channel (InAs-PHEMTs) have attracted much attention because of their high-speed operation and their applicability to high-speed ICs.[1)] We have recently used an energy-dependent effective mass to calculate the energy states of the two-dimensional electron gas (2DEG) in the InAs channel of InAs-PHEMTs.[2,3)] The purpose of this paper is to provide the theory describing the 2DEG and the two-dimensional hole gas (2DHG) energy states required for understanding characteristics of InAs-PHEMTs. In this theory the nonparabolic relation between the energy and the wavenumber was taken into account for the conduction band, but the parabolic relation was taken into account for the valence band.

2. Analytical method

We chose the z-direction perpendicular to the quantum-well plane. For the conduction band, the nonparabolic dependence of the energy E on the wavenumber vector $\mathbf{k}$ is taken into account by defining the following energy-dependent effective mass based on the $\mathbf{k}\cdot\mathbf{p}$ perturbation theory:

$$m^*(z,E) = m_c^*(z)\left[1+\alpha(z)\left(E-E_c(z)\right)\right], \quad (1)$$

where z is the distance from the surface, m_c*(z) is the effective mass at the bottom of the conduction band, and E_c(z) is the conduction band energy. In addition, α(z) is a nonparabolicity parameter equal to $1/E_g$, E_g being the bandgap energy of the channel. The analytical method and equations for electrons is described in detail elsewhere.[2)] For the valence band, both heavy hole (*hh*) and light hole (*lh*) are taken into account in the following calculation. Also, the parabolic dependence of E on $\mathbf{k}$ for holes is for simplicity assumed to be isotropic. As a result, the Schrödinger equations for electrons and holes in the n[th] subband are expressed as follows:

$$\left\{\begin{array}{l} -\dfrac{\hbar^2}{2m_c^*(z)\left[1+\alpha(z)\left(E_{n\mathbf{k}}-E_c(z)\right)\right]}\dfrac{\partial^2}{\partial z^2} \\ +E_c(z)+\dfrac{\hbar^2k^2}{2m_c^*(z)\left[1+\alpha(z)\left(E_{n\mathbf{k}}-E_c(z)\right)\right]} \end{array}\right\}\psi_{n\mathbf{k}}(z) = E_{n\mathbf{k}}\psi_{n\mathbf{k}}(z)$$

(*electrons*) (2)

and

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_i^*(z)}\frac{d}{dz}\right)+E_{vi}(z)\right]\psi_{ni}(z) = E_{ni}\psi_{ni}(z)\ ,$$

(*holes* : i=*hh*,*lh*) (3)

where $E_{n\mathbf{k}}$ and $\Psi_{n\mathbf{k}}$(z) represent the energy and the wavefunction of electrons, respectively, and where E_{ni}, Ψ_{ni}, E_{vi}(z), and m_i(z) are the energy, wavefunction, valence-band energy, and effective mass of holes. The Schrödinger equation (2) for electrons was solved using a standard perturbation theory approach. That is, we regarded the terms including α as the perturbed Hamiltonian and regarded the rest of the terms as the unperturbed Hamiltonian.[2)] The electron density is provided by the following equation: [2)]

$$n(z) = \sum_n \int_{E_n}^{\infty} \frac{\rho_n(E)}{1+exp\left(\dfrac{E-E_{Fe}}{kT}\right)}\left|\psi_{n\mathbf{k}}(z)\right|^2 dE, \quad (electron)\ (4)$$

where $\rho_n(E)$ is the density of states and E_{Fe} is the quasi-Fermi energy for electrons. The heavy-hole and light-hole densities are given by

$$p_i(z) = \sum_n \frac{m_i^*(z)kT}{\pi\hbar^2}\ln\left[1+exp\left(\frac{E_{ni}-E_{Fh}}{kT}\right)\right]\left|\psi_{ni}(z)\right|^2,$$

(*holes* : i=*hh*,*lh*) (5)

where E_{Fh} is the quasi-Fermi energy for holes.

Using the distribution profiles for both carriers, we can estimate the exchange-correlation energy included in the Schrödinger Eqs. (2) and (3).[2,4)] By letting φ(z) be the electrostatic potential, the Poisson equation is written as

$$\frac{d}{dz}\left[\varepsilon(z)\frac{d}{dz}\varphi(z)\right] = -e\left[N_D^+(z)+p(z)-n(z)\right], \quad (6)$$

where ε(z) is the dielectric constant, N_D^+(z) the ionized donor density, n(z) the electron density, and p(z) = p_{hh}(z) + p_{lh}(z) the hole density. The potential energies E_c(z) in Eq. (2) and E_{vi}(z) in Eq. (3) were estimated using φ(z) in addition to the exchange-correlation and the band discontinuity.[2,4)]

3. Results and discussion

The cross section of PHEMTs assumed in the

calculation of quantum states for InAs PHEMTs, which corresponds to that of an InAs PHEMT reported in Ref. 1, is shown schematically in Fig. 1. The epitaxial layers consist of an undoped InAlAs layer, an undoped $In_xGa_{1-x}As/InAs/In_xGa_{1-x}As$ composite channel layer (10 nm), and an InAlAs barrier layer with a Si-doping density of 2 x 10^{12} cm^{-2} (4 nm).

Figure 2(a) is the energy band diagram for the conduction band and the carrier concentration of 2DEG at a gate-to-source voltage V_{GS} of 0 V for the case where p_s is zero. Here the sheet electron density of 2DEG, n_{s0}, in p_s= 0 is 3.0×10^{12} cm^{-2}. The surface potential energy was set to 0.655 eV, which corresponds to a V_{GS} of 0 V. The E_{Fe} lies near the 2nd subband energy because of the high doping level and the large conduction band discontinuity ΔE_c (about 0.74 eV). Figure 2(b) shows the energy band diagram for the conduction and valence bands as well as the carrier concentrations of 2DEG and 2DHG for the case where p_s was 2.0×10^{12} cm^{-2} comparable to the n_{s0} of 2DEG. As a result, n_s is increased to 5.0×10^{12} cm^{-2} (n_s=n_{s0} +p_s) because of the effect of the hole accumulation. The E_{Fe} is measured from the bottom of the conduction band on the surface side of the InAs channel. The E_{Fe} is larger than that for p_s= 0 by ΔE_{Fe} = 0.04 eV, where ΔE_{Fe} is defined as the shift of E_{Fe} due to an increase in the electron concentration. This implies that the threshold voltage V_{TH} of PHEMT shifts by ΔE_{Fe} because of the effect of the hole accumulation. Figure 3 shows the p_s dependence of ΔV_{TH}; where ΔV_{TH} varies in proportion with p_s in a lower p_s region. This result is consistent with the so-called photo-voltaic effect observed in solar-cells. Their open-circuit voltage is known to increase logarithmically with the irradiated optical power. Our theory may explain the dependence of ΔV_{TH} on the irradiated optical power in InAs-PHEMTs.[4] In this way, for a system where electrons and holes co-exist, self-consistently solving the Schrödinger and Poisson equations for both carriers enabled us to rigorously determine not only the energy states and the concentration profiles for both carriers but the shift of V_{TH} of PHEMT due to the holes accumulated in the channel as a function of p_s.

4. Conclusions

In summary, for a system where electrons and holes co-exist, we established the theory that takes into account the nonparabolicity only for the conduction band of the InAs channel layer. This theory enables us to rigorously determine not only the energy states and the concentration profiles for both carriers but the shift of V_{TH} of PHEMT due to the holes accumulated in the channel. The calculation was made by solving the Schrödinger and Poisson equations self-consistently for both carriers.

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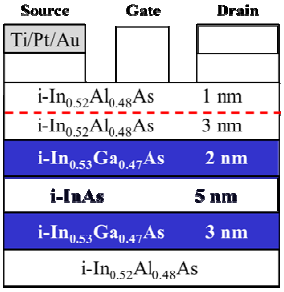


Figure 1: Schematic cross section of pseudomorphically strained InAs HEMTs assumed in the calculation.

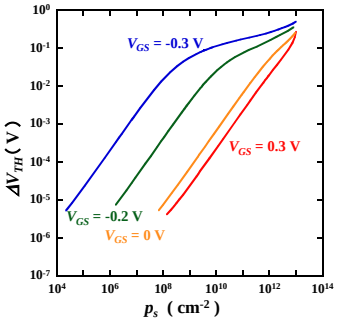
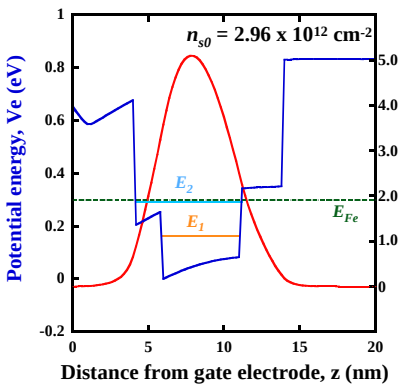
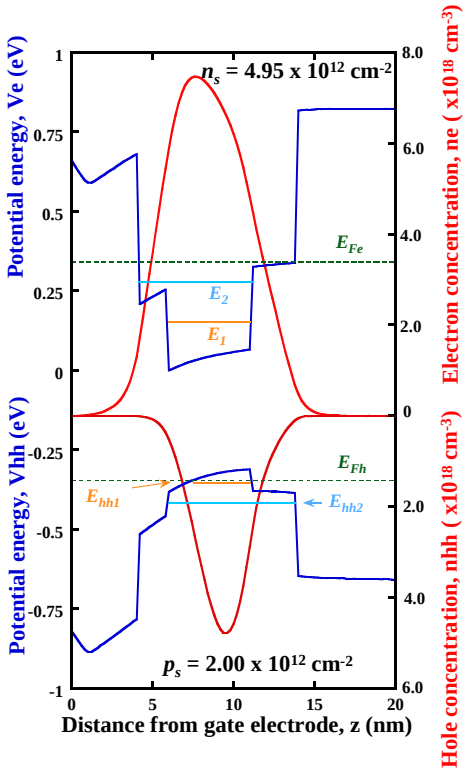


Figure 3: p_s dependence of the V_{TH} shift of HEMTs.



(a)

Figure 2: (a) Energy band diagram insource region for conduction band and carrier concentration of 2DEG (p_s=0); (b) Energy band diagram insource region for conduction and valence bands and carrier concentrations of 2DEG and 2DHG for p_s=2.01×10^{12} cm^{-2}.



(b)