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Tunneling current in w-GaN/AlN(0001) structures with deep-level defects

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ABSTRACT

The influence of the interface deep-level defects on the tunneling current of a double-barrier w-AlN/GaN (0001) structure is studied. It is shown that the peculiarities of the current essentially depend on the positions of deep-levels, concentrations and spatial distribution of defects. At high concentrations of defects comparable to those of polarization charge, partial compensation of polarization charges near the contacts of the structure occurs and a resonance level in the triangular well can arise. Defective structures can possess a huge peak-to-valley ratio higher than 100 due to the small value of the valley current. The results of the simulations are consistent with some experimental dependences of the tunneling current in double-barrier structures.

1. Introduction

The features of the tunneling current (asymmetry, bistability, jumps, hysteresis, sweep rates, etc.) in the polar nitride w-GaN/AlGaN (0001) structures are essentially related to the internal electric fields and defects. The deep-level defects cause a depletion of the 2DEG in the transistors channel [1], instability of the negative-differential-resistance (NDR), a current collapse, and a leakage current [2]. These can give the dominant contribution to the tunneling current [3] and lead to the self-charging effects [4]. Interface defects play a special role in properties of the resonant tunneling diodes (RTDs). Due to the high density ($\geq 10^{13}\,cm^{-2}$), such defects cause band tilting on the Ga-face and N-face and change the properties of RTDs [2]. Their sources can be roughness, deformations, dislocations, and point defects localized near the heteroboundaries. The detailed nature of such traps has not yet been established, but there are some data on their energy levels and spatial distribution. So, the deep level transient spectroscopy measurements reveal three traps with the energy levels of 0.11, 0.17, and 0.22 eV in AlGaN/GaN [5] and the levels of interface traps located ~ 0.2 eV below the conduction band bottom in GaN [6]. Recent calculations show [7] that the traps in GaN can be been nitrogen vacancies having low formation energy and deep levels localized slightly below the conduction band bottom.

A lot of efforts have been made to enhance NDR of double barrier structures (DBS). The highest value of the peak-to-valley current ratio (PVCR ~ 32) was obtained for the structures grown on a sapphire substrate and having high dislocation density [8]. The instabilities and steepness of the peak current indicate that it is rather due to the defects, than to the resonance state of the GaN quantum well (QW). The structures grown on GaN substrates have stable I-V characteristics due to the low dislocation density, but they exhibit low value of PVR (~2) [9]. An obstacle to the increase of PVR can be interface defects induced by large lattice relaxation [10].

Some simulations of defective RTDs were performed in Refs. [3,4,11–13]. In particular, it was established that the current degradation is related to the traps with long time constants [14] and the polarization-matched RTDs have a great defect tolerance

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[15]. New experimental and theoretical studies are required to identify the defects [16]. Especially, it is necessary to clarify the influence of the spatial distribution and position of deep levels of defects on the DBS properties.

In the previous work [17], we investigated the features of tunneling current in the w-GaN/AlN (0001) DBS caused by the resonance in a triangular quantum well (TQW) formed by the polarization charges and amphoteric interface traps (AITs). Such model allowed to explain band tilting as a result of partial compensation of polarization charges by charged deep centers at the contacts of DBS with the spacer layers.

In this paper, we investigate the influence of the defect concentration, spatial distribution, and position of energy levels on the QW and TQW current peaks and NDR characteristics of the double barrier w-AlN/GaN/AlN (0001) structures.

2. Method of calculation

The two-barrier structures w-AlN (0.5 nm)/GaN (0.5 nm)/AlN (0.5 nm) (0001) with spacer layers of *i*-GaN with the thickness $d = 10$ nm, similar to [18], were investigated. The contact regions of *n*-GaN were doped by silicon atoms with the concentration $N_i = 10^{19}\ \mathrm{cm}^{-3}$ and an ionization energy of $E_i = 30.8$ meV [19]. The current density *j(V)* was calculated on the basis of a self-consistent solution of the Poisson and Schrödinger equations in the single-valley (Γ) model of the band spectrum. Polarization charges with the surface density $\sigma = \pm e \times n_0$ were introduced according to [20] near the hetero-boundaries in thin layers with the thickness $\delta = 0.26$ nm and $n_0 = 5.6 \times 10^{13}\ \mathrm{cm}^{-2}$. Amphoteric defects were introduced into the spacer layers. Their concentration exponentially decreased with distance from the heteroboundaries. The AIT levels were located under the bottom of the conduction band of GaN at energies $E_d^\alpha = (E_d^0 + \alpha \times 0.05)$ eV for three charge states $\alpha = \{-1, 0, +1\}$.

The volume concentration of deep defects in different charge states near the DBS boundaries with the spacer layers (left - z_{b1}, right - z_{b2}) was determined using the Fermi-Dirac function:

$$n_d^\alpha(z) = \frac{\frac{n_{ds}}{\lambda} \times \exp\left(-\frac{z - z_{bi}}{\lambda}\right)}{1 + g_\alpha \times \exp\left[\alpha \times \frac{E_F - E_d^\alpha - W(z)}{kT}\right]}; z \le z_{b1}, z \ge z_{b2}$$

Here, n_{ds} is the surface concentration of AITs, g_α is the degeneration factor, λ is the distribution depth of AIT, E_F is the energy of the Fermi level in the depth of the *n*-GaN contacts, and *W(z)* is the potential energy. Taking into account the band tilting [2], the density of defects should be of the same order as $\sigma = \pm e \cdot n_0$. Besides, the interface nature of the defects requires that the depth should be comparable with the thickness δ. Therefore, the concentration varied within the interval $(1 - 9) \times 10^{13}\ \mathrm{cm}^{-2}$, and the distribution depth was assumed to be equal to $\lambda = 0.25$, 0.5, and 0.75 nm. The energy of the defects E_d^0 varied within 0.15–0.35 eV in accordance with [5–7].

The electron concentration in the DBS was calculated using the probability density determined from the solution of the Schrödinger equation. In the spacer layers, the electron concentration was determined quasi-classically, similarly to [21]. The calculations were carried out for room temperature, so the Fermi level E_F is located 0.007 eV below the conduction band bottom of *n*-GaN.

It was assumed that electrons tunnel through DBS, if their energies are higher than the value of the potential energy E_m at the interface between the *n*-GaN contact and spacer layer in the emitter. Then, electrons are captured by AITs in the collector, if their energies fall into the interval 2kT near the energies of the defect levels E_d^α. Other details of the calculation method are given in Ref. [17].

3. Dependence of the tunneling current on the distribution of deep centers

The results of calculating the current density *j(V)* are given in Fig. 1(a) for DBS with various distributions of AITs. The surface

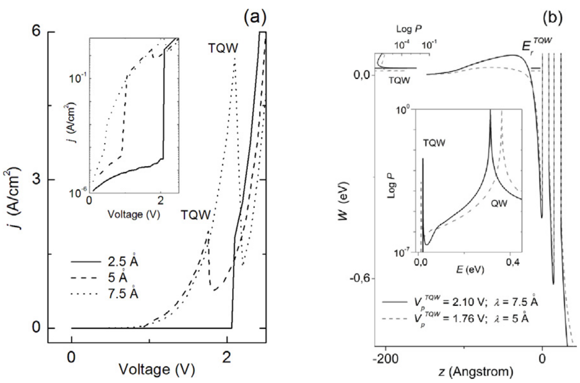

Fig. 1. Density *j(V)* of the tunneling current (a), potential energies *W*, and transmission coefficients *P* at the voltages V_p^{TQW} of the corresponding TQW- peaks of current (b) in the two-barrier structure w-AlN/GaN for various depths λ and surface concentration $n_{ds} = 3 \times 10^{13}\ \mathrm{cm}^{-2}$.