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On the tunnel mechanism of current flow in Au–TiB_x–*n*-GaN–*i*-Al_2O_3 Schottky barrier diodes

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Abstract. We investigated a current flow mechanism in the Au–TiB_x–*n*-GaN–*i*-Al_2O_3 Schottky barrier diodes, in which the space-charge region width is much over the de Broglie wavelength in GaN. An analysis of the temperature dependences of the *I–V* curves of forward-biased Schottky barriers showed that, in the temperature range 80–380 K, the current flow occurs as a tunneling one along dislocations crossing the space-charge region. The dislocation density ρ estimated from the *I–V* curves (in accordance with the model of tunneling along the dislocation line) was ≈ 1.7×10^7 cm^{-2}. This value is close to that obtained with x-ray diffraction technique.

Keywords: gallium nitride, Schottky barrier, tunnel current, dislocation density.

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1. Introduction

In recent years, an interest of the developers of microwave devices in wide-gap semiconductor compounds of the trinitride group has increased considerably. This interest is dictated by a real possibility to develop various devices for extreme electronics. Gallium nitride is the most advanced material in this area. Its electrical characteristics are most suitable for the development of heat- and radiation-resistant microwave diodes and transistors [1, 2]. However, in spite of many advantages of GaN, there is no native (gallium nitride) substrate material with the area sufficient for mass production. GaN epitaxy on foreign substrates is accompanied by the appearance of a considerable (predominantly misfit) dislocation density [3, 4]. It was shown in a number of works by Evstropov *et al.* [5-8] dealing with III–V heterojunctions that the current flow in them, even at room temperature, is due predominantly to dislocation-aided multiple tunneling, despite the fact that the heteropairs are formed with nondegenerate semiconductors. No such investigations have been made on GaN.

The object of our work was to investigate, in a wide (80–600 K) temperature range, the current flow mechanism in the forward-biased Schottky barrier diodes (SBDs) made on the basis of the *n*-GaN–*i*-Al_2O_3 heterostructure.

2. Samples and experimental procedures

We studied Au–TiB_x–*n*-GaN–*i*-Al_2O_3 SBDs. The *n*-GaN epitaxial layers (~1 μm thick) with donor concentration ~$(1\ldots3)\times10^{17}$ cm^{-3} were grown at the Closed Corporation "Elma-Malakhit" (Russia). At first, an n^+-GaN buffer layer ~3 μm thick was grown on single-crystalline Al_2O_3 (0001) substrates using metal-organic vapor-phase epitaxy, and then an *n*-GaN layer was grown on it. The perfection of the structure of *n*-GaAs layers was studied with x-ray diffraction (XRD) technique. The ohmic contacts were made on the basis of Au–TiB_x–Al–Ti–n^+-GaN metallization. The Au–Ti metallization was formed on a semiinsulating sapphire substrate for diode structure packaging. A diode structure chip is shown in Fig. 1. Multilayer contacts were prepared with the use of the magnetron sputtering of atomic metals and quasiamorphous TiB_x alloy. The layer thicknesses were as follows: for the barrier contact – Au (3000 nm)–TiB_x (100 nm); for the ohmic contact – Au (2500 nm)–TiB_x

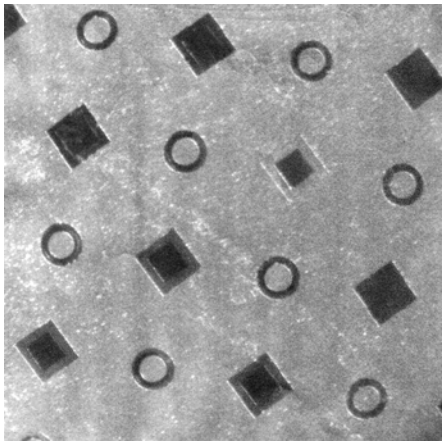


Fig. 1. A wafer section with diode structures.

(100 nm)–Al (500 nm)–Ti (50 nm); for the sapphire metallization – Au (3000 nm)–Ti (50 nm). The distribution of contact metallization components was studied with Auger electron spectroscopy (AES). The physico-chemical properties of contact systems with a TiB_x diffusion barrier were described in [9]. The diode chips (100 μm in diameter) were made as forward mesas using plasma-chemical etching. To investigate the current flow mechanisms, the diode chips were packaged, and the forward branches of SBD *I–V* curves were taken in the temperature range 80–600 K. The SBD *C–V* curves were taken at a temperature of 300 K. The main SBD parameters were calculated from the experimental *I–V* and *C–V* curves.

3. Experimental results and discussion

3.1. Some model concepts

According to the dislocation model for tunnel current in the barrier structures made on the basis of nondegenerate semiconductors (*p-n* junctions, SBDs, *p-n* hetero-junctions), their *I–V* curves can be presented as [8]

$$I = I_0\left(\exp qV/\eta - 1\right). \tag{1}$$

Here,

$$I_0 = q\rho\nu_D \exp\left(-qV_K/\varepsilon\right) \tag{2}$$

is the saturation current density; q – elementary charge; $qV_K = \varphi_b - \mu_n$ is the diffusion potential for Schottky barriers (SBs); φ_b – SB height; $\mu_n \cong kT\ln\dfrac{N_C}{N_d}$ – chemical potential; $N_C = 2.23\times10^{18}$ cm^{-3} is the effective level density in the GaN conduction band [10]; $\nu_D \approx 1.5\times10^{13}$ s^{-1} is the Debye frequency for GaN; ρ is the dislocation density; $\eta = nkT$ is the characteristic tunneling energy; n is the ideality factor; k is the Boltzmann constant; T – temperature; N_d is the concentration of ionized donors in GaN (in our case, it equals ~3×10^{17} cm^{-3}).

Knowing the values of I_0, η, and V_K from the experimental *I–V* curves, one can calculate the dislocation density ρ from Eqs. (1) and (2) as

$$\rho = \frac{I_0(0)}{q\nu_D}\exp\frac{qV_K(0)}{\eta(0)}. \tag{3}$$

Here, $I_0(0)$ and $\eta(0)$ are obtained from the temperature dependences of I_0 and η by extrapolation to zero temperature. According to the empirical dependence of φ_b on the GaN gap E_g ($\varphi_b \approx \dfrac{1}{3}E_g$), $qV_K(0)$ can be determined as

$$qV_K(0) = \varphi_b(0) - \mu_n(0) \cong \frac{1}{3}E_g^{\mathrm{GaN}}(0) - \mu_n(0) \cong$$

$$\cong \frac{1}{3}E_g(0) \cong \frac{1}{3}\cdot 3.47 \approx 1.15 \text{ eV}.$$

3.2. Experimental results

In Fig. 2, we show the forward branches of the *I–V* curves of Au–TiB_x–*n*-GaN SBDs measured in the temperature range 80–600 K, as well as the temperature dependences of I_0 and η. The *C–V* curve of this diode

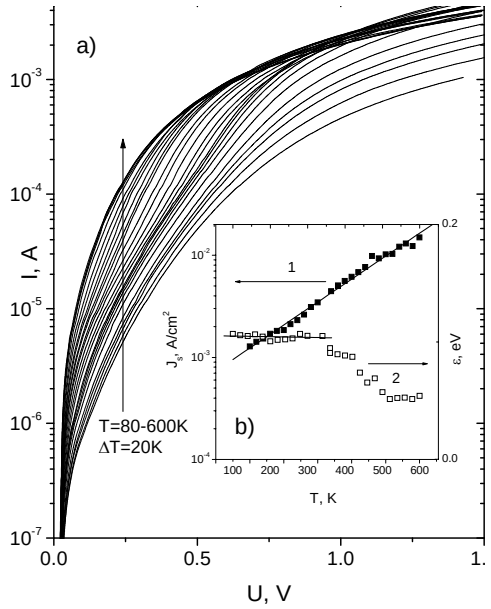


Fig. 2. Forward branches of Au–TiB_x–*n*-GaN SBD *I–V* curves taken in the temperature range 80–600 K (a); I_0 and η as functions of temperature (b).

is presented in Fig. 3. One can see that, in the temperature range 80–350 K, the current flow mechanism is the tunnel one. This is evidenced by the absence of temperature dependence of the characteristic tunneling energy in the temperature range under consideration and a weak temperature dependence of the saturation current density. A decrease of the characteristic tunneling energy in the temperature range 350–600 K is due to a considerable contribution from the over-barrier current to the current flow. Since the dependence $(1/C^2) = f(U)$ (Fig. 3) is linear, one can calculate the dopant concentration from its slope. In our case, it was equal to 3.2×10^{17} cm^{-3}, while φ_b calculated from the *C–V* curve was 1.15 eV.

Taking the $I_0(0)$, $\eta(0)$, and $qV_K(0)$ values into account, the dislocation density calculated from Eq.(3) is

$$\rho = \frac{7.35\times10^{-4}\ \text{A/cm}^2}{1.6\times10^{-19}\,\text{C}\cdot1.5\times10^{13}\,\text{s}^{-1}}\exp\left(\frac{1.15\ \text{eV}}{0.105\,\text{eV}}\right)\approx1.7\times10^{7}\,\text{cm}^{-2}.$$

This agrees rather well with the results of [4], where the dislocation density in the GaN layers (grown at the Closed Corporation "Elma-Malakhit" (Russia) on sapphire using metal-organic vapor-phase epitaxy) determined by XRD technique was $(1\ldots3)\times10^8$ cm^{-2} for different samples. A difference between the two ρ values is due to the fact that XRD technique allows one to determine the total density of structural defects in a sample, while only those defects (dislocations) which cross the space-charge region (SCR) take part in the current flow.

Though it is possible to describe the tunnel current in terms of multiple tunneling, a question appears concerning a realization of such mechanism in those SBs where SCR width W at $N_d \approx 3\times10^{17}$ cm^{-3} is much over the characteristic tunneling length λ (the de Broglie wavelength) in GaN. Indeed, it is known that W is determined as [11]

$$W = \left[\frac{2\varepsilon_0}{q}\left(\frac{\varepsilon}{N_d}\right)(V_K - U)\right]^{1/2},$$

where ε_0 (ε) is the vacuum (GaN) permittivity. In our case, at $U = 0$ and $V_K = 1.15$ V, $W \approx 7\times10^{-5}$ cm. An estimation of the characteristic tunneling length according to [10] [$\lambda = \dfrac{\hbar}{\sqrt{2m^* q(V_K - U)}}$, where $\hbar = h/2\pi$ (h is the Planck's constant) and $m^* = 0.2\,m_0$ is the electron effective mass in GaN] gives $\lambda \approx 0.4\times10^{-7}$ cm.

Such a process in the surface-barrier structures on the basis of III–V compounds (GaAs, GaP) has been studied earlier by Evstropov *et al.* [7], with $W/\lambda \approx$ 200…500 for different structures. Increasing the tunneling probability was related in [7] to the tunneling current flow along the dislocation line. Such current flow mechanism can be understood if one introduces a scale factor r which increases the characteristic tunneling length. This becomes apparent in the experiment as the increase of the characteristic tunneling energy as compared to its theoretical value η_t calculated from the expression [12]

$$\eta_t = \frac{\hbar q}{2}\left[\frac{1}{\varepsilon_0 m^*}\left(\frac{N_d}{\varepsilon}\right)\right]^{1/2}.$$

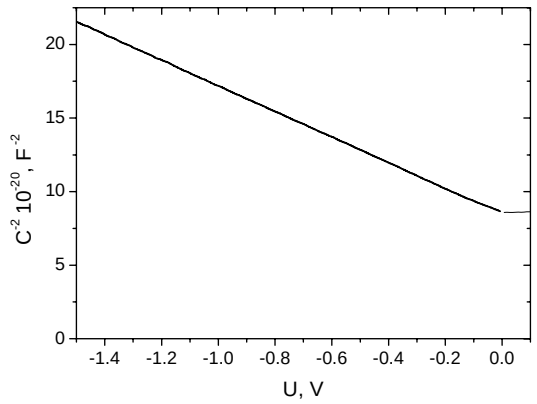
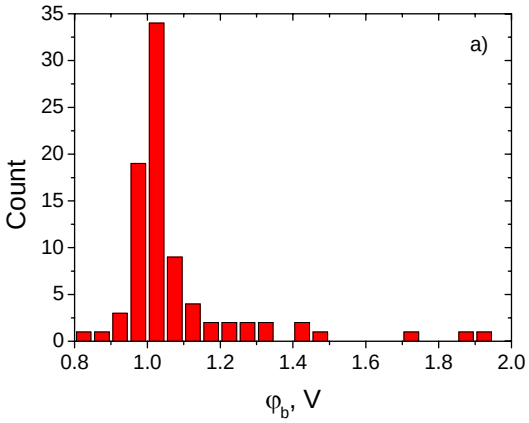


Fig. 3. *C–V* curve of the Au–TiB$_x$–*n*-GaN SBD whose *I–V* curves are presented in Fig. 2a.



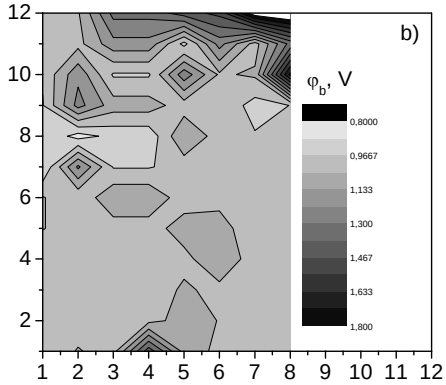


Fig. 4. A histogram (a) and a topogram (b) of the SB height distribution over the 8×12-mm wafer section.

In our case, it equals ~7 meV, so

$$r = \frac{\eta}{\eta_t} \approx \frac{0.105\ \text{meV}}{0.007\ \text{meV}} \approx 15\ .$$

The current flow in the temperature range 350–600 K occurs with predominance of the over-barrier current. This is indicated by a decrease of η as the temperature grows from 350 up to 600 K.

The feature of the diode structures under study is a considerable spread of SB parameters (φ_b, n, and I_0) over the wafer. This is illustrated with a histogram (Fig. 4a) and a topogram (Fig. 4b) of the SB height distribution over the 8×12-mm wafer section. However, the reason for the planar nonuniformity of the distribution of SB parameters is not related to the morphological and structural variations of the Ti (TiB_2)−GaN interface as one might assumed primarily. Indeed, a special rapid thermal annealing (RTA) of the diode structures on the wafer at the temperature T = 700 ºC did not change substantially the statistical distribution of the SB parameters. According to the AES results, RTA of the Au−TiB_2−Al−Ti−GaN test structures did not affect the layer structure of the ohmic contact metallization (Fig. 5).

Our earlier XRD investigation [13] of thermal stability of the Au−TiB_x−GaN SB contact showed that the contact system was stable. No phase changes were detected, even after RTA at T = 870 ºC. At the same time the distribution of dopant concentration N_d calculated from the C−V curves (Fig. 6a), as well as the topogram of N_d distribution over the wafer section (Fig. 6b), indicated the impurity nonuniformity of the n-GaN heteroepitaxial film, and the XRD results for the initial n-GaN/Al_2O_3 heterostructures showed a high density of structure defects in GaN. They were distributed nonuniformly over the wafer: their concentration varied from 10^8 up to 10^{10} cm^{-2} in different regions (Fig. 7).

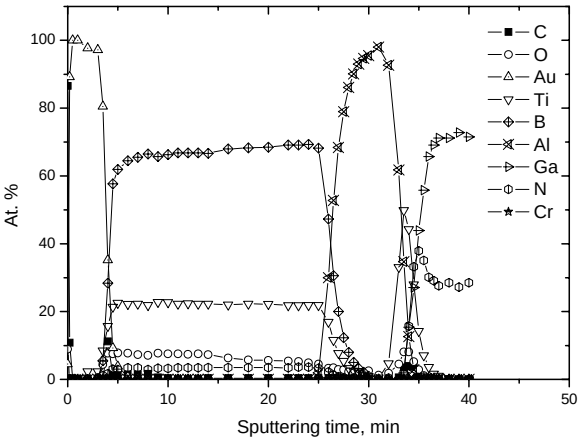


Fig. 5. Auger concentration depth profiles of the Au−TiB_x−Al−Ti−n-GaN contact structure components before (a) and after RTA at T = 700 °C (b).

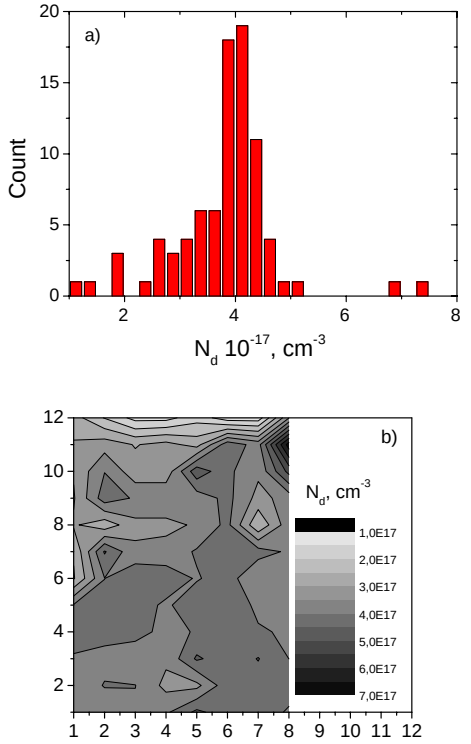


Fig. 6. A histogram (a) and a topogram (b) of the distribution of the dopant concentration N_d over the 8×12-mm wafer section.

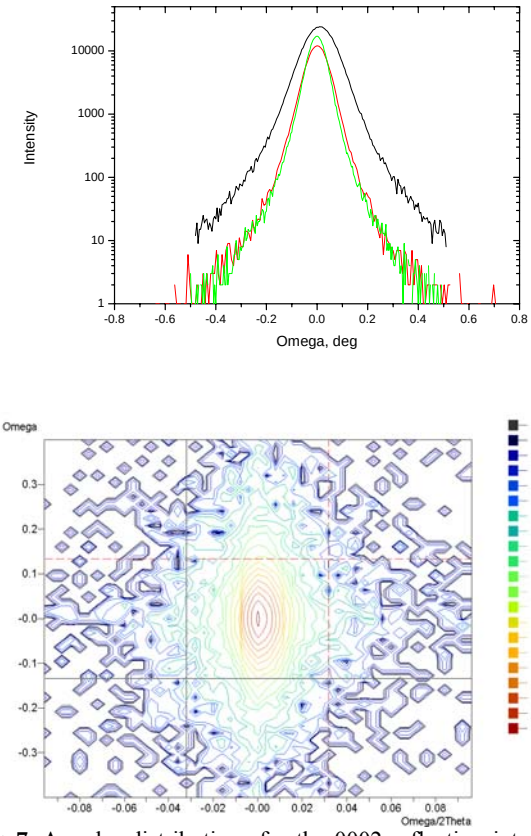


Fig. 7. Angular distributions for the 0002 reflection intensity: (a) ω-scans for three GaN/Al_2O_3 structures; (b) intensity maps around the 0002 reciprocal lattice site.

The main contribution to the broadening of x-ray reflections in the epitaxial system comes from the disorientation of coherent areas. That from the reduction of these areas is much smaller at dislocation densities up to 10^{10} cm^{-2} (in our case, the average dislocation density in the layers is about 2.53×10^{8} cm^{-2}). In addition, the flat configuration of dislocation networks does not lead to considerable coherent size changes along the Q_y direction (normal to the heteroboundary) [4]. All the above considerations enable one to conclude that the predominant effect from dislocation networks is the diffraction pattern broadening at a normal to the reciprocal lattice vector (along Q_x) no matter what measurement geometry. This conclusion refers substantially to the GaN layer.

In Fig. 7(a), we present the rocking curves for three samples taken at a normal to the diffraction vector (ω-scan). The curves are strongly broadened in just that direction, i.e., the broadening results from a block turn relative to the growth axis; the effect of mosaic structure (coherent areas sizes) is smaller. In addition, one can see separate peaks from the areas with different doping levels on the curves obtained for different samples. Lattice misfit for layers is about 0.00083.

Plotting the 2D intensity distribution around the site of symmetric 0002 Bragg reflection as equal intensity contours (Fig. 7(b)) makes it possible to detect directly the location of layer reflection centers in the scattering plane and to determine its coordinates Q_x and Q_y.

The above results indicate an interrelation between the SB parameters, flow current mechanism in SBs, and GaN structure defects whose concentration is over 10^{8} cm^{-2}.

4. Conclusion

Thus, our experimental data evidence that the current flow in the forward-biased Au–TiB$_x$–*n*-GaN SB occurs in the temperature range 80–380 K according to the tunnel mechanism, despite a wide-barrier contact structure $(W >> \lambda)$. The nature of this mechanism is related to the dislocations, which appear at the GaN/Al_2O_3 interface in the course of GaN epitaxial growth and grow into the GaN epitaxial layer.

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