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SEMICONDUCTOR STRUCTURES, LOW-DIMENSIONAL SYSTEMS, AND QUANTUM PHENOMENA

Formation Mechanism of Contact Resistance to III–N Heterostructures with a High Dislocation Density

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Abstract—The temperature dependences of the contact resistance $\rho_c(T)$ of ohmic Pd–Ti–Pd–Au contacts to *n*-GaN and *n*-AlN wide-gap semiconductors with a high dislocation density are studied. The dependences $\rho_c(T)$ for both contacts contain portions of exponential decrease and very weak dependence at higher temperatures. Furthermore, a plateau portion is observed in the low-temperature region for the Au–Pd–Ti–Pd–*n*-GaN contact. This portion appears only after rapid thermal annealing (RTA). In principle, the appearance of the plateau portion can be associated with preliminary heavy doping of the near-contact region with a shallow donor impurity and with doping during contact fabrication as a result of RTA, if the contact-forming layer contains a material that is a shallow donor in III–N. The dependences obtained are not explained by existing charge-transport mechanisms. Probable mechanisms explaining the experimental dependences $\rho_c(T)$ for ohmic contacts to *n*-GaN and *n*-AlN are proposed.

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1. INTRODUCTION

Recently, the materials science of III–N compounds and the technology of devices on their basis, i.e., light-emitting diodes, Schottky diodes, and field-effect transistors, have been actively developed. Hardware components are mostly developed based on GaN and its alloys [1–6]. Promising materials for optoelectronic devices are also InN and alloys in the InN–GaN–AlN system. AlN is used as a substrate material for a number of device structures. Up to now, the problem is the formation of ohmic contacts to III–N wide-gap compounds. For example, to form an ohmic contact to AlN according to classical models, it is necessary for the metal electron work function φ_m to be smaller than the energy of the electron affinity of *n*-AlN [7]. Since AlN is a wide-gap material with a low electron affinity (χ = 0.6 eV) [8], its metal electron work function φ_m exceeds χ_{AlN}. Another feature of AlN is the high concentration of defects with deep levels, which is the reason for its high-resistance *n*-type conductivity due to the compensation of shallow levels [9]. Taking into account these facts, the formation of ohmic contacts to AlN presents certain difficulties.

Since III—N compounds are mostly wide-gap, devices on their basis even today feature operating temperatures higher than silicon- and gallium-arsenide devices by a factor of 1.5–2 [4, 5]. Therefore, ohmic contacts to them are formed at sufficiently high temperatures for firing in contact-forming layers. This promotes the formation of a structurally imperfect metal–semiconductor interface, including those with a high dislocation density in the near-contact region of III–N heterostructures grown mainly on foreign substrates. As the authors of [10–12] note, metal shunts associated with dislocations can be formed in the near-contact region of such structures, which cause a linear increase in the contact resistance ρ_c with temperature. The latter situation is associated with the temperature dependence of the resistivity of the metal and is extremely undesirable for devices operating at elevated temperatures. One of the shunt-formation mechanisms associated with indium mass transfer over dislocations from a contact formed by indium- and tin-oxide alloy in gallium-nitride light-emitting diodes was reported in [13]. In previous studies [14–16], we showed that the temperature dependence of ρ_c in ohmic contacts to semiconductors with a high dislocation density in the near-contact region is more complex than the linear dependence $\rho_c(T)$. In this case, the dependences $\rho_c(T)$ can both increase and decrease with temperature.

As for ohmic contacts to *n*-AlN, there is no detailed information in published works, except for [17] in which an alloyed In–*n*-AlN ohmic contact to

high-resistivity n-AlN with $\rho \approx 10^6\ \Omega$ cm is considered. The authors of [17] noted that the contact possessed high resistance and had a linear current–voltage characteristic and a resistivity close to the bulk one. We know of no published data concerning the temperature dependence of ρ_c of ohmic contacts to n-AlN.

The objective of this work is to comparatively study the features of the temperature dependences of ρ_c of ohmic contacts to n-GaN and n-AlN, grown on foreign substrates.

2. EXPERIMENTAL

Single-crystal n-GaN and n-AlN films were grown at the Ioffe Physical–Technical Institute by chloride vapor-phase epitaxy using a standard setup with a horizontal reactor [18, 19].

GaN layers ~30 μm thick with a donor concentration above 10^{18} cm^{-3} were grown on an AlN "template" on sapphire. AlN layers ~3.5 μm thick with a donor concentration below 10^{17} cm^{-3} were grown on a heavily doped n^+-SiC substrate.

X-ray diffraction curve half-widths measured for the GaN and AlN layers were $\omega_0 \approx 5$ and 30 arcmin, respectively. The average linear dislocation density was $\leq 10^5$ cm^{-1} in both cases. Contact metallization of Au(100 nm)–Pd(70 nm)–Ti(50 nm)–Pd(30 nm)–n-GaN(n-AlN) was formed by sequential vacuum deposition on substrates heated to 350°C; then, test structures with linear and radial template configurations were formed in order to measure the contact resistance by the transmission line method (TLM) [20] in the temperature range of 100–380 K.

On the Au–Pd–Ti–Pd–n-GaN structures, an ohmic contact was formed on the substrate heated to 350°C and the same substrate was then subjected to rapid thermal annealing (RTA) at $T = 900$°C for 30 s. The ohmic contact to the Au–Pd–Ti–Pd–n-AlN structure was formed only after 30-s RTA at $T = 900$°C.

The depth-distribution profiles of components in the metallization layers were studied by the Auger-spectrometry method in combination with ion etching (1-keV Ar^+ ions) using a LAS-2000 Auger spectrometer. A JAMP-9500F Auger microprobe in the scanning-electron-microscopy mode was used to study cleavages of the ohmic contacts and morphological features of the surface of the GaN and AlN films.

Figure 1a shows the depth-distribution profiles of components in the Au–Pd–Ti–Pd–n-GaN contact metallization. We can see that this contact system features a layered metallization structure with a rather sharp interface between the contact-forming metal (palladium) and the gallium nitride, formed during deposition onto the substrate (GaN surface) heated to 350°C. Studying the Au–Pd–Ti–Pd–n-GaN contact cleavage also showed the existence of a rather abrupt metal–GaN interface. In this case, the columnar

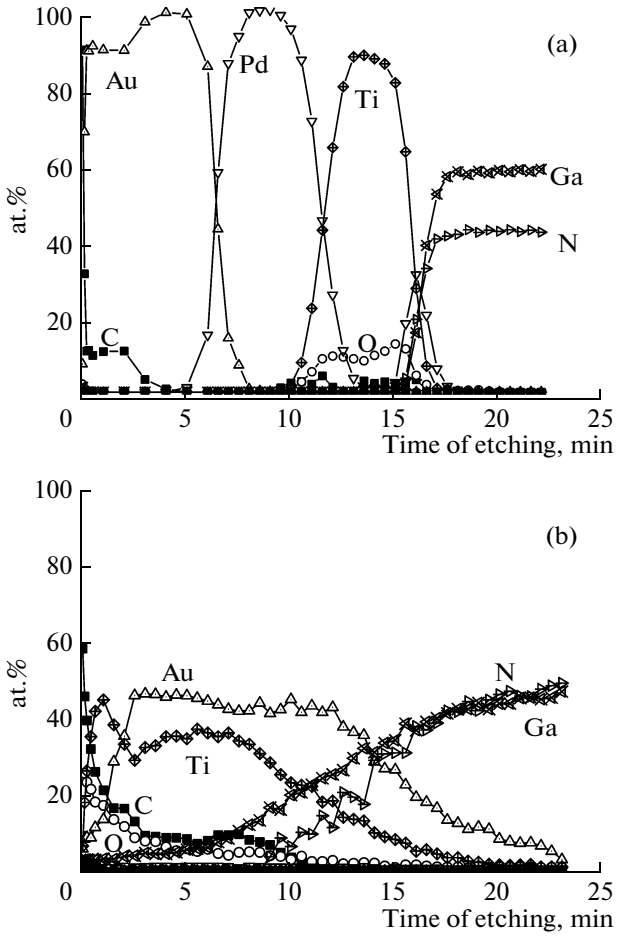

Fig. 1. Distribution profiles of components of the Au–Pd–Ti–Pd–n-GaN contact metallization: (a) initial and (b) after 30-s RTA at 900°C.

structure of the n-GaN film was observed. As for the GaN-film-surface morphology, it exhibited a rather high density of hexagonal defects. Analogous hexagonal defects on similar thick GaN layers (~25 μm thick), grown on GaAs substrates, were observed in [6].

The contact resistance of Au–Pd–Ti–Pd–n-GaN ohmic contacts, measured by the TLM at room temperature was 6.7×10^{-5} and $7.8 \times 10^{-5}\ \Omega$ cm^2 for linear and radial topologies, respectively.

Figure 2 shows the distribution profiles of components in the Au–Pd–Ti–Pd–n-AlN contact metallization formed on the substrate heated to 350°C. We can see that the metal–AlN interface is significantly spread and is the region of AlN, Pd and, Ti component mixing with an oxygen fraction of up to 10 at % in the Ti and Pd layers. The cleavage of the Au–Pd–Ti–Pd–n-AlN contact structure has confirmed the structural heterogeneity of the metal–AlN interface.

The Au–Pd–Ti–Pd–n-AlN contact formed during metal deposition onto the substrate heated to 350°C represented a high-resistance non-ohmic con-

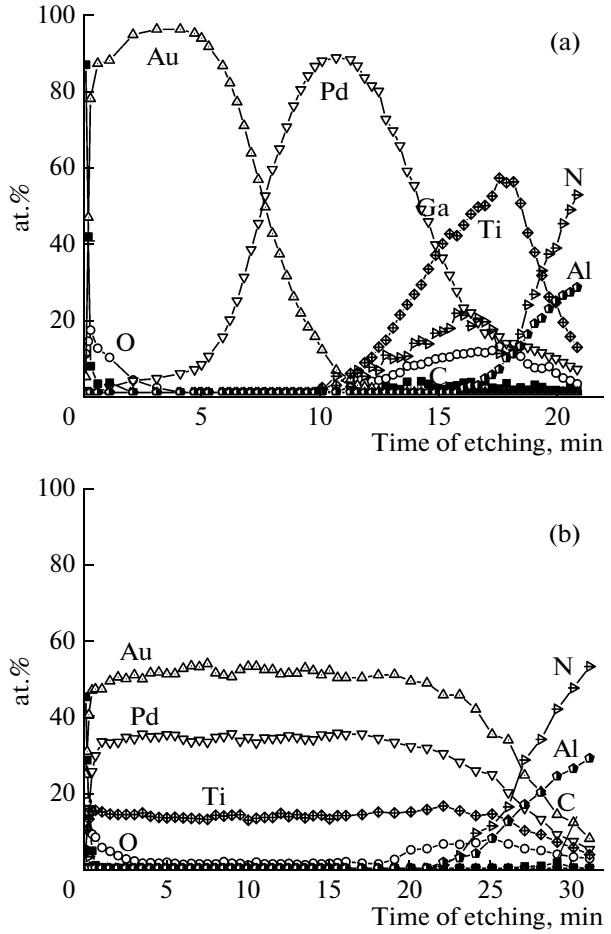

Fig. 2. Distribution profiles of components of the Au–Pd–Ti–Pd–*n*-AlN contact metallization: (a) initial and (b) after 30-s RTA at 900°C.

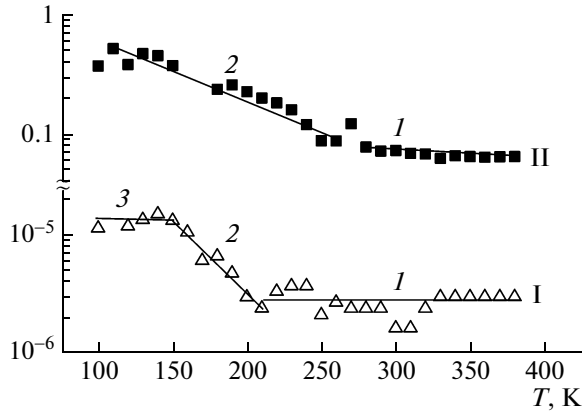

Fig. 3. Temperature dependences $\rho_c(T)$ of the Au–Pd–Ti–Pd–*n*-GaN and Au–Pd–Ti–Pd–*n*-AlN ohmic contacts after 30-s RTA at 900°C (curves I and II, respectively).

tact. Its ohmic properties were implemented only after 30-s high-temperature annealing at $T = 900$°C. The contact resistance of such a contact, measured at room temperature using the radial TLM test structure was 0.05 Ω cm^2. Resistivity ρ_c of the same order at $T =$ 300 K was observed in the In–*n*-GaN alloyed ohmic contact with $n \approx 10^{18}$ and 8×10^{18} cm^{-3} in [17]. We also note that phase transformations of the components occurred in the metallization of the contact structures on *n*-AlN and *n*-GaN after 30-s RTA at 900°C (Figs. 1c and 2b, respectively). These transformations correlate with the X-ray diffraction data. It appeared that RTA results in the interdiffusion of atoms in the contact metallization to *n*-AlN and $Au_x(Pd, Ti)_{1-x}$ alloy formation. In contacts to *n*-GaN, the interdiffusion of metallization atoms and formation of the Pd_3Ti phase and two non-stoichiometric gold-based phases (alloys) with lattice parameters smaller and larger than that of pure Au, presumably, $AuxGa(Pd, Ti)_{1-x}$ and $Au_xPd(Ga, Ti)_{1-x}$, were also observed. These results are in good agreement with the published data on the phase formation in multicomponent metallization layers to device structures, based on GaN and an AlGaN/GaN heterojunction [5, 21, 22].

3. EXPERIMENTAL RESULTS AND DISCUSSION

Figure 3 shows the temperature dependences of ρ_c for the annealed ohmic contacts (curves I and II for the Au–Pd–Ti–Pd–*n*-GaN and Au–Pd–Ti–Pd–*n*-AlN contacts, respectively). Comparison of the behavior of the dependences $\rho_c(T)$ for ohmic contacts to *n*-GaN and *n*-AlN showed that both curves slope in the low-temperature region as the temperature increases from 150 to 200 and 250 K, respectively. As the temperature further increases to 375 K, ρ_c varies very weakly. The significant difference between these dependences is the value of ρ_c for the ohmic contact to *n*-AlN, which is a thousand times higher than the value of ρ_c for *n*-GaN at room temperature. This is associated with the *n*-AlN doping level which is much lower than that of *n*-GaN. Furthermore, as seen in Fig. 3 (curve I), $\rho_c(T)$ is almost independent of temperature in the low-temperature region (100–150 K).

To explain such effects, a new charge-transport concept was proposed in [14, 16], which is valid in the case of high dislocation densities in semiconductors. This concept considered current flow through metal shunts with the limited diffusion supply of electrons. Currents flowing between dislocations were neglected. Depending on the dominant mechanism of electron scattering, ρ_c can increase and decrease with the measurement temperature. However, the dependences $\rho_c(T)$ shown in Fig. 3 do not fit the known charge-transport models in ohmic contacts [7] and the concepts of [14, 16].

We begin to discuss the results obtained with curve *1*, i.e., the temperature dependence of the contact resistance for ohmic contacts to *n*-GaN on the Al_2O_3 substrate. As seen in Fig. 3, this dependence

contains three portions: *1* a very weak dependence $\rho_c(T)$ in the temperature range of 200–380 K; *2* an exponential dependence with an activation energy of ~0.1 eV in the temperature range of 150–200K, and *3* a region of independence at $T < 150$ K. We note that portion *1* can in principle be described by the mechanism of electrical current flow through metal shunts associated with dislocations, taking into account the diffusion limitation of electron supply to the contact [14, 16]. The increase in $\rho_c(T)$ with decreasing temperature in portion *2*, as follows from Fig. 3, is purely exponential. This cannot be explained by the power-law decrease in the electron mobility due to scattering at dislocations and the low-temperature "freezing" of electrons, since silicon is a shallow donor in this case, whose ionization energy does not exceed 20 meV, which should lead to an increase in $\rho_c(T)$ only at temperatures below 50 K. Therefore, to explain portion *2*, we can only assume that it is associated with disordering effects in the metal-shunt conductivity at low temperatures, which cause a change in the metal-conductivity nature to the semiconductor one with the corresponding activation energy. This can be the case, if we take into account that the metal-shunt diameter is close to atomic sizes; in principle, a single defect at low temperatures can lead to the activation character of the conductivity [23].

Since the currents flowing through dislocations associated with metal shunts and the currents flowing between dislocations correspond to the parallel connection of resistances, the plateauing of the dependence $\rho_c(T)$ in portion *3* at $T < 150$ K should be associated with the current flowing between dislocations in the case of a heavily doped near-contact region, hence, strong degeneracy. In this case, as shown in [14, 16], the contact resistance is controlled by the mechanism of thermionic emission and is almost independent of temperature. In principle, the appearance of portion *3* can be associated with both preliminary heavy doping of the near-contact region with a shallow donor impurity and doping during contact formation due to RTA, if the contact-forming layer contains a material that is a shallow donor in III–N, or a thin n^+-type layer enriched with nitrogen vacancies, which are shallow donors in III—N, appears in the near-contact region [8].

The comparatively large value of ρ_c in portion *3* (on the order of $10^{-5}\ \Omega\ \text{cm}^2$) can be explained by potential nonuniformity in the interface plane within Shklovskii–Efros theory [24].

The dependences $\rho_c(T)$ of the ohmic contact to *n*-AlN (curve II in Fig. 3) are explained in the same way as for the contact to *n*-GaN.

The results obtained allow conclusions about the specificity of the physical mechanisms responsible for current flow in ohmic contacts to the wide-gap semiconductors *n*-GaN and *n*-AlN with a high density of structural defects.

4. CONCLUSIONS

Based on a study of the temperature dependence $\rho_c(T)$ of Au–Pd–Ti–Pd–*n*-GaN (*n*-AlN) ohmic contacts, it was revealed that $\rho_c(T)$ in the temperature range of 380–200 K is controlled by the conductivity over metal shunts associated with dislocations, which is limited by the diffusion supply.

The exponential growth of $\rho_c(T)$ with decreasing temperature is observed in the ranges of 250–100 K and 200–150 K for ohmic contacts to *n*-AlN and *n*-GaN, respectively, which is not described by thermionic or field emission. In the temperature range of 150–100 K, ρ_c for the ohmic contact to *n*-GaN is independent of temperature. This is caused by the thermionic mechanism of charge transport for the case of strong degeneracy due to current flow between dislocations.

It was assumed that the exponential dependence $\rho_c(T)$ in the low-temperature region can be explained by taking into account the effects of disordering in the conductivity of metal shunts of atomic sizes, causing, according to [24], the metal-to-semiconductor conductivity transition.

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