Unusual behavior of dislocations freshly-introduced under Schottky contact in GaN

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Abstract. The impact of the dislocations introduced by local plastic deformation on the electric properties of low-ohmic n-GaN was investigated. It was found that the freshly introduced dislocations gave rise to increase of the dc leakage current, to changes in frequency dependence and in the shape of current-voltage, ac conductance and capacitance voltage characteristics of stripe-like Au-Schottky diodes. Besides, a rapid recovery of the dislocation-induced changes of the electric properties to their initial state was observed after several hours at room temperature indicating the impact of the presence of depletion region of Schottky diodes on the dynamic properties of freshly introduced dislocations.

1. Introduction
Gallium nitride is a promising direct-wide-gap semiconductor for high power and optoelectronic applications. Nowadays GaN films are grown mostly heteroepitaxially on diverse substrates with a large lattice mismatch. As a result heteroepitaxial GaN contains a high density of dislocations. The impact of dislocations on the electronic properties of semiconductors may be attributed to a variety of reasons such as the dislocation-induced elastic strains, local electronic states or bands of their own cores, which in turn, can exhibit diverse atomic structure, as well as the point defects attracted to dislocations or introduced/changed during their motion. Recently the observation of a strong cathodoluminescence (CL) band with quantum energies around 3.1-3.2 eV [1,2] due to freshly introduced a-screw dislocation was reported s in low-ohmic resistance GaN samples and 3.3 eV [3] in semi-insulating GaN sample.

Despite the detailed investigation of the optical properties of this type of dislocations, their electric properties remain unknown. In this paper we present the first results of such a study. A new experimental set-up was developed to investigate the impact of the dislocations introduced by scratching the sample surface on the dc current-voltage (I-V), ac conductance and capacitance voltage (G-V and C-V respectively) characteristics of stripe-like Schottky diodes. It was found that the freshly introduced dislocations gave rise to increase of the dc leakage current, to changes in frequency dependence and in the shape of G-V and C-V. Besides, despite of the previously reported stability of the dislocation arrangement created by local plastic deformation – [4], unexpectedly rapid recovery of the dislocation-induced changes of the electric properties to their initial state was observed after several hours at room temperature indicating the impact of the presence of depletion region of Schottky diodes on the dynamic properties of freshly introduced dislocations.
2. Experimental

We investigated 8-10 μm thick intentionally undoped monocrystalline (0001) GaN layer grown by hydride vapor phase epitaxy technique on sapphire with a density of grown dislocations of $10^8-10^9$ cm$^{-2}$ and free electron concentration about $10^{16}$ cm$^{-3}$ measured by capacitance-voltage techniques. According to previous results [1], the extension of the dislocations introduced by scratching does not exceed 50 μm. To avoid possible artefacts appearing by scratching immediately through the metal Schottky contacts, they were formed by thermal deposition of Au on as-grown (0001) surface through a shadow mask of particular shape. The contacts consisted of a square area 500×500 μm$^2$ and stripes of length as long as 5 mm and width 150-200 μm. Fresh dislocations were introduced at room temperature by scratching with a diamond scribe with load 200 mN in the vicinity of and parallel to the stripes. The scheme of contacts and scratches is depicted in figure 1. An ohmic contact was formed by an InGa eutectic on the same surface of the samples.

![Image of GaN/Sapphire structure](image)

**Figure 1.** The scheme of contacts and scratches on GaN/Sapphire structure.

C-V, G-V characteristics were measured with an Agilent Precision Impedance Analyzer 4294A and I-V – with Keithley electrometer 6517B. The dislocation structure after scratching was observed by cathodoluminescent imaging in CZ Supra 40VP scanning electron microscope with Gatan MonoCL3+ system.

3. Results and Discussion

After contact preparation I-V, G-V and C-V measurements were performed on one of the contacts. After that, the scratching in its vicinity was performed and all measurements were repeated. The obtained data before and after scratching will be marked in the following as “Initial” or “Scratched” respectively and were well reproducible on several contacts.

The initial contact possessed well pronounced rectifying behavior with the saturation current of about 1-10 μA at reverse bias voltage of 2-5 V, but rather weak temperature dependence (not shown for brevity) that indicated the presence of significant ratio of tunnel current caused most probably by the presence of grown-in dislocations. The main effect of the introduction of fresh dislocations was a drastic increase of reverse current by more than 3 orders of magnitude as well as the changes of the I-V curve shape at low reverse and forward bias voltages. This is demonstrated on figure 2(a), where sets of I-V dependencies on temperature range from 300 to 50 K are presented for initial and the same contact after the scratching. One can see that in the vicinity of zero voltage scale I-V curve at room temperature is close to linear, i.e. possesses an ohmic behavior, but at T < 150 K transforms into superlinear one in the voltage ranges ±0.25 V that might indicate the presence of a small symmetric barrier for the current flow.

The described peculiarities of dc I-V curves are also apparent on G-V dependencies at different temperatures for scratched contact shown in figure 2(b), when they are compared with G-V curves of initial contact (thin line with square marker). The G-V curve of the initial contact starting from the saturation defined by diode series resistance decreases smoothly with decreasing slope towards the reverse biases. Its shape changed rather weakly with temperature and was similar to the curve presented
in figure 2(b) for 150 K. It is clear to see that in the range of applied voltages from -1.5 to +0.5 V G-value of scratched contact exceeds noticeably the initial one at room temperature. At lower temperatures down to 100 K the dislocation-related excess G-value forms a knob between the voltages ±0.5 V (see G-curve 150 K in figure 2(b)) and at 50 K a dip centered at zero voltage appears.

The presence of dislocations under the contact resulted in the vanishing of G-dependence of testing voltage frequency, ω, in the entire temperature ranges. As an example of G(ω)-dependence at 200 K is presented in figure 2(c). The initial contact shows a strong dispersion of G(ω)-values at reverse biases, and varies by two orders of magnitude when ω changes by a factor of ten, while G(ω) of scratched contact values is practically frequency independent in the voltage region of the knob.

The reason of the difference G(ω) dependence can be explained based on it’s common expression for the Schottky diode:

\[
G_{app} = \frac{1}{R} \frac{1+r/R}{(1+r/R)^2+(\omega r C)^2} + \frac{1}{r} \frac{(\omega r C)^2}{(1+r/R)^2+(\omega r C)^2},
\]  

(1)

Figure 2. (a) I-V dependences of initial contact (lines) and after scratching (symbols) at different temperatures; (b) G-V dependences of initial contact at 150 K and after scratching at different temperatures measured at a testing voltage frequency f = 1 MHz; (c) G-V dependences of initial contact (bold curves) and after the scratching (thin curves) at different f at 200 K; (d) G-V dependences at 1 MHz and 300 K measured after keeping the sample for the time after the scratching shown in legend.

where \( C \) – diode differential capacitance, \( r \) – series resistance of the diode base and is diode leakage resistance \( R \). For the initial contact, the conditions of ideal diode \( \omega r C << 1 \), \( r << R \) are satisfied, and the second term in equation (1) is the main one that has a square dependence on \( \omega \). For a leaky scratched
contact \( \omega rC << 1, R \gg r \) the first term of equation (1) exceeds well the second being inversely proportional to \( R \) and \( G \), accordingly, is simply the first derivative of dc current. Thus, the main impact of freshly introduced dislocations is that they act as a shunt connected in parallel to the diode.

The dislocation shunting action was found to experience temporary change when keeping the unbiased diode at room temperature for few hours and days. This fact is demonstrated in figure 2 (d). One can see that after first 16 hours the ac-conductance at all reverse bias voltages becomes larger than that immediately after the first measurement but after 3 days the enhanced conduction disappears completely.

It is natural to assume that the dislocation diode shunting action is caused by the enhanced conduction along the dislocation lines that go out to the surface and contact immediately the metal or are situated in close to it. According to previous CL and transmission electron microscopy investigations of the dislocation structure produced by scratching and indentation of basal GaN surface, such dislocations could be edge and a-screw ones as components of prismatic half-loops [1]. Such half-loops were reported to persist at room temperature in equilibrium for as long as a few months [4] in the samples with uncovered surfaces. The reason of that is the impossibility of a-screw dislocations to move in the [0001] direction due to the dissociated character of their cores [1].

In the frame of this assumption the complete vanishing of the enhanced dislocation conduction might be due to transformation of the a-screw dislocation core from the dissociated to the perfect one that enables motion of the dislocations to the surface. In turn, such kind of transformation seems to be stimulated by the fact that the dislocations are situated in the depletion region of the Schottky-diode, where there are no free electrons. Possible reasons for the impact of free electrons on the dislocation core structure has been discussed in [5]. One of the mechanisms is the absence of the screening of the dislocation line charge electric field by the free electrons. The two partial dislocations comprising the dissociated a-screw dislocations have different atomic contents along their cores: one contains positively charged Ga atoms, and the other one – negatively charged N atoms. Hence, they experience an electrostatic attraction which is inversely proportional to the lines’ separation. A simple estimation shows that the elastic repulsion given by a well-known expression [6] which is also inversely proportional to the partials’ separation and depends on the Burgers vector and shear module can be completely compensated by the electrostatic attraction, when the partials’ line charge exceeds the value \( 2 \cdot 10^7 \) electron/cm. This value is not in conflict with the theoretically calculated one in [7].

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