Extended core structure and luminescence of a-screw dislocations in GaN

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Abstract. Straight segments of a-screw dislocations introduced by scratching of basal (0001) of intentionally undoped low-ohmic GaN radiate a doublet of narrow luminescent lines in the spectral region at about 3.1-3.2 eV while the dislocation intersection points possess luminescence band at about 3.3 eV. Transmission electron microscopy reveals that the dislocation cores are dissociated into two 30° partials separated by stacking fault (SF) ribbon with the width of 4-6 nm width and that the dislocation nodes contain extended SF of sizes of 25-30 nm. Dislocation-related luminescence (DRL) is ascribed to exciton bound by the states of partial dislocation cores and of SF quantum well. The increase of the SF lateral sizes is assumed to cause the DRL spectral shift between straight dislocations and their nodes due to the system dimensionality transition from 1D to 2D respectively.

1. Introduction

Gallium nitride is a promising direct-wide-gap semiconductor for high power and optical electronic applications. Nowadays GaN films are grown mostly heteroepitaxially on diverse substrates with a large lattice mismatch. As the result heteroepitaxial GaN contains a high density of dislocations. The impact of dislocations on the electronic properties of semiconductors may be defined by a variety of reasons such as the dislocation-induced elastic lattice 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. A few sub-band gap luminescent bands with the maxima at photon energies at 2.9 eV[1], 3.12 eV[2], 3.18 eV[3], 3.35 eV[4] were found in GaN after plastic deformation but the interpretation of their origin is still under discussion.

Recently we reported [3] about the observation of a strong cathodoluminescence (CL) band with quantum energies around 3.1-3.2 eV due to a-screw dislocations in low-ohmic GaN samples. It was found that the dislocation related luminescence (DRL) band exhibited a doublet spectral structure and its intensity exceeded well one of the free exciton band. In this paper we present the results of investigations of the optical and structural properties of locally deformed low-ohmic GaN samples. CL mapping and transmission electron microscopy (TEM) results show that dissociated a-screw dislocations react with each other and formed extended dislocation nodes. Last ones had identical luminescence properties as macroscopic size stacking faults.
2. Experimental

We investigated 500 μm thick GaN (0001) intentionally undoped single crystals grown by hydride vapor phase epitaxy technique with a density of grown-in dislocations of $10^6-10^7$ cm$^{-2}$ and free electron concentration in range from $10^6$ cm$^{-3}$ to $10^{18}$ cm$^{-3}$ measured by Raman spectroscopy and capacitance-voltage techniques. Fresh dislocations were introduced at room temperature either by the indentation with a Vickers indentor of as-grown basal (0001) sample surface under the loads between of 0.1 and 5 N or by its scratching with a diamond scriber.

CL measurements were performed with scanning electron microscope Zeiss Supra 40 equipped with Gatan MonoCL2+ system at accelerating voltages of 3-30 kV with electron beam current in ranges from 0.2 nA to 10 nA in the temperature ranges from 70 K to 420 K. Atomic structure of freshly introduced dislocations was studied TEM Zeiss Libra 200FE with 200 kV accelerating voltage. TEM foils were prepared by mechanical grinding with final Ar+ ions thinning and polishing by Gatan PIPS.

3. Results

Figure 1 (a, b) represent mono CL maps taken at two different energies 3.18 and 3.32 eV near the scratch at 70 K. Energy of photons 3.18 eV corresponds to luminescence of straight a-screw dislocations segments in {12-10} directions, which could be seen on Figure 1 (a). At the same time only bright dots could be recognized on CL map at energy 3.32 eV, represented only in the region with high density of a-screw dislocations, where the probability of a-screw dislocations intersections and interactions which each other is much more higher. Figure 1c represents three distinct types of CL-spectra acquired on: 1) dislocation free region (dash line), 2) a-screw dislocation segments (solid line) and 3) bright dots of a-screw dislocation intersection related luminescence (IRL) (dot line). The spectrum of dislocation free regions consisted of common lines of free exciton (FE, 3.47 eV), line of exciton bound on point defects (3.4 eV) and the second replica of FE (3.27 eV). Spectral measurements on the a-screw dislocation-rich regions revealed the appearance of a set of additional intense narrow lines at around 3.1-3.2 eV, (Figure 1 (c), solid line) with the main doublet denoted as DRL$_{s}$ and DRL$_{s+}$ accompanied with LO-phonon replicas (Huang-Rhys factor S $\approx$ 0.085). Bright dots are presented with a broadened luminescence band at a peak energy of about 3.3 eV with apparent unresolved fine spectral structure accompanied with LO-phonon replica (S $\approx$ 0.17). One of the main feature of both bands associated with freshly introduced screw dislocations and their intersections is their unusual high intensity which exceeds well that of FE. More detailed description of DRL and IRL band properties can be found elsewhere [3,5].

![Figure 1](image_url)

**Figure 1.** Mono CL maps acquired with a photon energy of 3.18 eV (a) and of 3.32 eV (b) near a scratch on basal plane of GaN. Insert in Fig.1b shows secondary electrons image of the scratch; (c) CL-spectra in spot mode measured at the e-beam position: on dislocation free region (dash line), on straight bright segments of a-screw dislocations (solid line) and on bright dots (dot line).

$T = 70$ K, $V_b = 10$ kV, $I_b = 500$ pA
Figure 2(a) shows planar view STEM HAADF (scanning transmission electron microscopy, high angle annular dark-field) image in [0001] zone axis of the sample obtained after multiple indentation of its basal plane. The dark area at the left side of image is a footprint of the indenter with a load of 200 mN. One can see numerous straight dislocation segments propagated in all \{11\-20\} directions from the prick. These dislocations were identified as a-screw dislocations by applying $g \cdot b = 0$ criterion in TEM mode in two-beam conditions. At a higher magnification the straight segments possess a doubled contrast with the separation width of 4 nm to 6 nm (see Fig. 2b). For a-screw dislocations the dissociation take place according to the reaction: $1/3[11\-20] = 1/3[10\-10] + 1/3[01\-10]$, and proceeds into 30° Shockley partial dislocations and I$_2$ stacking fault ribbon. Figure 2 (b) shows also an example of an extended node formed as results of the reaction at screw dislocation intersections. A typical radius of extended node incircle was in the ranges of 10-15 nm. Furthermore on this image it is clear to see two partials of dissociated a-screw dislocation, which were exhibited bright contrast with variable width of stacking fault (SF) along the dislocation line.

![Figure 2](image_url)

**Figure 2.** (a) – STEM HAADF image of GaN basal surface near the prick. Bright straight segments – a-screw dislocations in \{11\-20\} directions. (b) – STEM HAADF image one of extended node in the point of intersection of a-screw dislocations.

### 4. Discussion

Albrecht et al. [7] reported about a single DRL line in semi-insulating GaN with the peak position at 3.35 eV caused by straight individual a-screw dislocations with a perfect core structure according to TEM data. In our low-ohmic GaN samples a-screw dislocations were dissociated into two partials and DRL exhibited the doublet of the CL-lines at 3.15-3.18 eV. These two observations imply that DRL spectral position of the dislocations of the same type depends strongly on their atomic core structure. Recent DFT calculations [4] revealed the conduction band bending due to shear strains which does exists in the analytical model. The sum of the conduction and valence band bending around the perfect screw dislocation could be as high as 0.2 eV that was sufficient to explain the DRL red shift of 0.14 eV in semi-insulating GaN but is still too small to explain the red shift of 0.3-0.34 eV in the low-ohmic material. In this way we came to the conclusion that the additional DRL red shift of about 0.15 eV is due to the presence of SF-ribbon in the extended dislocation cores.

SFs in wurtzite (WZ) GaN can be imagined as a thin layer of sphalerite phase with the band gap of 3.27 eV. They were proposed to be considered as quantum wells (QW) [6]. Luminescence of SFs in GaN was rather extensively investigated and a correlation between the CL energy positions and SF atomic structure was established (see recent review [7]). The only I$_2$ can be obtained by a simple glide in basal plane and, thus, can be a part of gliding dislocation. The energy positions reported for I$_2$ luminescent
line are in the same ranges of 3.32-3.36 eV [7] giving the energy position of the I₂ SF level of about 0.1-0.15 eV below conduction band. That value together with the band bending due to deformation potential at SF bounding partials gives by the order of magnitude just the DRL red-shift in low-ohmic GaN. The doublet of DRL lines has been explained by a model of the optical transitions between the hole states of two partials taking into account spontaneous polarization in GaN wurtzite phase [3].

The energy shift of IRL band relative DRL band could be consider in term of transformation 1D system (dislocation) to 2D system (dislocation node). The dissociation of a-screw dislocations is varied in range 4-6 nm and comparable with the exciton Bohr radius in GaN (3-4 nm). The electron and hole wave functions localized at two partials of a straight dislocation segment overlap enough to form together with SF ribbon a quasi-1D electronic system with the coupled recombination via its joint electronic states. In contrast to that, the extended node formed in point of intersection of a-screw dislocations has I₂ SF with lateral sizes of 25-35 nm well exceeded the exciton Bohr radius. Then, such a system must have the properties of a macro-sized I₂ SF, i.e. of 2D system. Fig. 3 compares the luminescence spectra of IRL (solid line) and of I₂ SF reported in [8,9] (dot and dash lines respectively). Identical energy positions, comparable FWHM and lines form suggest a similar origin of this bands.

Finally one should note that gradual decrease of Huang-Rhys factor in the row IRL-DRL serves as an additional indication of the transition of the system dimensionality from 2D-1D respectively [10].

![Figure 3. CL-spectra of IRL (solid line) and I₂ SF (dot and dash lines) taken from [8,9]](image)

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