Luminescence of a-screw dislocations in low-ohmic GaN

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Abstract. Straight segments of a-screw dislocations introduced by indentation or scratching of the basal (0001) or prismatic (01-10) surfaces of intentionally undoped low-ohmic GaN were found to radiate a doublet of narrow luminescent lines in the spectral region at about 3.1 - 3.2 eV. The components of the doublet were separated by about ~30 meV and accompanied with LO-phonon replicas. The intensity of the dislocation-related luminescence was significantly higher than that of free exciton in dislocation-free regions indicating a giant oscillator strength of dislocation-related luminescence optical transition that was proposed to occur between the electron states of the stacking fault and the hole states of the bounded partials in the core of the dissociated screw dislocation.

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 of about 3.2 eV [1] and 3.4 eV [2] have been attributed to as-grown dislocations while the bands at 2.9 eV [3], 3.12 eV [4], 3.18 eV [5,6], 3.35 eV [7] were found in GaN after plastic deformation but the interpretation of their origin is still under discussion.

Recently we reported [5,6] 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 further investigations of the DRL properties including the dependences of the energy position of DRL on the temperature and internal strains which appeared to be similar to those ones of free exciton. The DRL origin is discussed and is assumed to be exciton bound by the 1D confined states of dissociated screw dislocations.

2. Experimental
We investigated 200 µm thick intentionally undoped GaN (0001) single crystals grown by the hydride vapor phase epitaxy technique with a density of grown-in dislocations of about 10⁶ cm⁻² and free
electron concentration in range from $10^{16}$ cm$^{-3}$ to $10^{18}$ cm$^{-3}$ measured by Raman spectroscopy and capacitance-voltage techniques. Cathodoluminescent (CL) measurements were performed with a scanning electron microscope (SEM) Zeiss Supra 40 equipped with a Gatan MonoCL+ 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 300 K.

Fresh dislocations were introduced at room temperature either by the indentation with a Vickers indenter of as-grown basal (0001) or polished (10-10) prismatic sample surface under the loads between of 0.1 and 5 N or by its scratching with a diamond scriber.

3. Results

Figure 1(a) represents CL spectra taken at two different positions of electron beam. CL spectrum of dislocation-free regions (figure 1 (a), dotted line) of all investigated samples consisted of the line of free exciton (FE) at 3.46 - 3.47 eV, and two low intense bands at 3.27 eV and 3.4 eV that were previously ascribed to the recombination of donor-acceptor pairs or the second phonon replica of FE and exciton bound on point defects, respectively [1]. 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 (a), solid line) with the main doublet denoted as DL$_1$ and DL$_{ii}$ accompanied with LO-phonon replicas. The integrated intensity of DRL lines was at least two times higher than one of FE. The full width at half maximum of both DRL lines was of about 16 meV at 70 K being close to that of FE while the energy separation between DL$_1$ and DL$_{ii}$ components was of about 30 meV.

An examination of the CL image near the scratch on the (0001) surface in figure 1 (b) revealed straight lines stretched in all possible {12-10} directions. According to the crystallography of wurtzite structure and to the data of TEM [3,8], such lines are nothing else than a-screw dislocation with the Burgers vector of $1/3\alpha_{[12\overline{1}0]}$. Under the electron beam excitation these bright lines moved quickly and partly or completely disappeared at both room and liquid nitrogen temperatures. Note that in the CL image in figure 1 (b) the tiny bright dots with dark halos around are caused by optical scattering of outcoming CL near the pits grown-in threading dislocations (TD). The pits were clearly seen on the corresponding secondary electron image (not presented) and will not be discussed further.

![Figure 1](image1.png)

**Figure 1.** (a) – CL spectra obtained in the spot mode from a screw dislocation rich region (solid line) and far away from the scratch (dot line). The Accelerating voltage was 10 kV, the electron beam current was 0.5 nA and the temperature was 70 K; b) – Panchromatic CL images near the indentation prick on the (0001) surface.
An additional information about the origin of DRL was obtained from the spectral behavior of its components on mechanical strains and on temperature. Mechanical strains are inhomogeneous in the vicinity of the indentation prick or of the scratch. The strains are of a complicated character but in any case they decrease with the distance from the impact place that allows one to obtain the dependence of the DRL spectral position with respect to the position of FE. Figure 2 (a) represents the DRL spectra taken at three different distances from a scratch. Note that the intensity of DRL near the scratch is much higher than far from it. This is due to a higher density of dislocations near the scratch. One can see from figure 2 (b) that both components of the DRL doublet exhibit a blue shift when the distance to the scratch decreases, i.e. upon the strain increase. The strain-induced spectral shift of every DRL line coincides quantitatively with the shift of FE (figure 2 (b)). In opposite to that, the energy separation between DL_L and DL_H peaks did not change upon the strain being of about 30 meV in all investigated samples and it was independent on the temperature (figure 2 (d)). The temperature dependence of the DRL spectral position in a range from 70 to 120 K also repeats the behavior of FE (figure 2 (c)) like the strain dependence. The shape of the temperature dependence for FE and DL_H bands can be well fitted with the Varshni approximation (dot lines in the figure 2 (c)).
4. Discussion

The origin of the luminescence localized along the dislocation lines with an emission energy which is significantly less than the semiconductor band gap can be associated either with the local electronic states of dislocations themselves or of point defects in a close vicinity to the dislocation cores.

The point defects localized at dislocations [4] seem unlikely to be an origin of DRL since in this case it is difficult to explain the high dislocation mobility observed in our experiments as well as the other DRL properties. Accordingly, the doublet-line DRL with an energy of about 0.3 eV below the GaN band gap is an intrinsic property of the screw dislocations in low-ohmic GaN. On the other hand, Albrecht et al [7] reported recently about a single line of DRL with the peak position at 3.35 eV also due to straight individual a-screw dislocations in semi-insulating GaN. That line is, thus, red shifted only by 0.14 eV with respect to the GaN band gap energy and vanishes above 100 K. These two observations imply that the DRL spectral position of the dislocations of the same type depends strongly on the sample doping level that, in turn, can be explained by their different core structures.

There are two main core structures of screw dislocations. It can be perfect or dissociated into two 30° partial dislocations bounded the stacking fault (SF) ribbon. The dislocations in semi-insulating GaN [7] were found to be perfect. The deformation potential theory (DFT) based on symmetry considerations [9] predicts that a perfect screw dislocation can produce only shallow bound hole states, confined within a thin cylinder of shear lattice strains around them, which lye less than 0.1 eV above the valance band of GaN. Very recent DFT calculations for a supercell of 400 atoms [7] revealed the conduction band bending due to shear strai ns which does exists in the analytical model [9]. 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 splitting of the dislocation core.

We have no data about the dislocation core structure of the dislocations freshly introduced at room temperature in the low-ohmic samples. However, previously reported TEM investigations of grown-in a-screw dislocations in undoped GaN revealed that they were dissociated with the lateral width of I$_2$ SF of about 5 nm [10].

The energy level of the core states of 30° partials estimated theoretically was of about 1.1 eV [11] above the valence band and, thus, can not be responsible for the observed DRL. SFs in wurtzite (WZ) structure 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) [12,13] with the conduction band offset of 0.27 eV at interface of type II heterostructure [13]. Luminescence of SFs in GaN was rather extensively investigated and a correlation between the CL energy positions and the SF atomic structure was established (see the recent review [14]). The only I$_2$ can be obtained by a simple glide in the basal plane and, thus, can be a part of a gliding dislocation. The energy positions reported for I$_2$ luminescent lines are in the same ranges of 3.32-3.36 eV [14] giving the energy position of the I$_2$SF level of about 0.1-0.15 eV below the conduction band. That value together with the band bending due to the deformation potential at SF bounding partials gives by an order of magnitude just the DRL red-shift in low-ohmic GaN. In addition, the properties of DRL are similar to FE (line width, high intensity, depending on the voltage and temperature) that allows to describe DRL as an exciton bound at the confined states of screw dislocations. The observed energy of the optical transition of DRL is the exciton binding energy, which is of the order of tens of meVs.

The observed SF ribbon width in the dislocation core of 5 nm is comparable with the exciton radius in GaN of about 3 nm, transforming an extended 2D SF into a 1D-like system. As it was shown both theoretically [15] and experimentally [16], the decrease of the QW lateral dimension gave rise to an increase of the exciton binding energy and its oscillator strength that might give an additional small red shift and explain the enhanced DRL yield as well as the doublet line structure as being due to the ground and first excited state of the 1D system.

The reason for the different core structures of screw dislocations in the semi-insulating and low-
ohmic samples might be the impact of the Fermi level on the expansion of SFs as it was originally suggested to explain the “recombination enhanced dislocation glide” (REDG) in SiC [17,18]. It was proposed [18,19] that SF nucleation and expansion in SiC are driven by a reduction in the electronic energy of the system that occurs when conduction electrons become trapped within the SF-induced QWs. In our samples with a net donor density more than $10^{16}$ cm$^{-3}$, the Fermi level at room temperature is situated less than 0.15 eV below the bottom of the conduction band that makes it possible to fill the SF quantum confined states with electrons and, accordingly, stimulate SF nucleation [17]. An indirect confirmation of that assumption is our observation of enhanced dislocation mobility under the electron beam excitation that is known as the recombination enhanced dislocation glide and that was explained in SiC just with the model [17] mentioned above.

Conclusions

A-screw dislocations introduced by room temperature plastic deformation in low-ohmic GaN were shown to be efficient sources of intrinsic dislocation-related luminescence (DRL) with an emission energy of about 0.3 eV less than the band gap, which exhibit the following properties. The brightness of DRL exceeded FE intensity; DRL spectrum consists of doublet of narrow lines separated by 30 meV; the DRL line behavior upon mechanical strains and temperature is very similar to that of FE; the exciton bound at the confined states of a-screw dislocations is assumed to be the mechanism responsible for DRL.

It is suggested that the dislocation core structure in GaN might experience the changes upon the impact of the equilibrium and excess free electron concentration (the Fermi level position being either perfect or dissociated by the mechanism similar to that proposed for SiC [17–19].

Acknowledgments

Yuri Shreter and Vad Voronenkov are greatly acknowledged for providing the samples and helpful discussions.

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