

NEAR-BAND-EDGE RECOMBINATION IN GaN, GaN:Mg AND GaN:Si BETWEEN 12 AND 650 K

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The near-band-edge luminescence in GaN, especially heavily doped with acceptor impurities, such as Mg, is still far from complete understanding, in spite of the big progress achieved recently [1]. However, the knowledge of recombination mechanisms and their adequate description are required in order to establish the structure of the impurity centers involved in recombination. It may be especially useful for obtaining additional information about the defect structure, which is important, for understanding the nature of the processes of conductivity compensation. Since the ionization energies of recombination centers in GaN are relatively high, one may expect that especially PL spectroscopy at higher temperatures may provide useful information related to the recombination mechanisms and to the properties of defects.

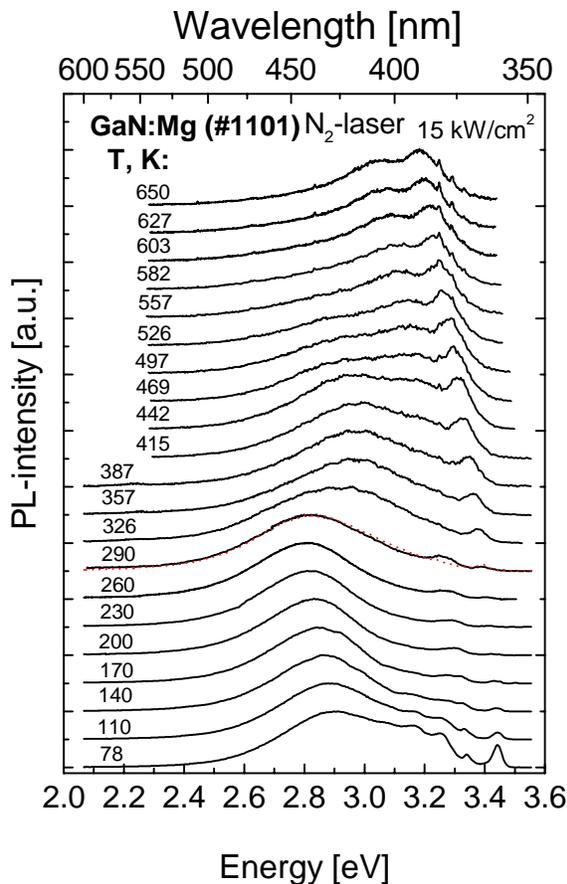


Fig.1. PL spectra of GaN:Mg in the temperature range 78-650 K

In this work, integrated and time-resolved photoluminescence (PL) spectra of GaN, GaN:Mg and GaN:Si in excitonic and near-band-edge region were investigated in a wide range of temperatures (12-650 K) and excitation intensities (from 0.05 W/cm² to several tens of kW/cm²). A special attention was paid to the temperature region above room temperature, since this region is of great interest for high-temperature devices. Excitonic PL and reflection spectra were recorded at low temperatures in order to get an additional information about the impurity levels.

To establish the relationship between the line position of bound excitons and the ionization energies of corresponding impurities, we used the theory [2]. In many semiconductors, this relationship can be written as: $E_A = C_1 E_{B1}$; $E_D = C_2 E_{B2}$, where E_A, E_D are the acceptor and donor ionization energies, respectively, E_{B1} and E_{B2} are the corresponding binding energies of I_1 and I_2 type excitons, $C_{1,2}$ are the coefficients of proportionality. In some semiconductors $C_1 \approx 10$, $C_2 \approx 5$, ($C_1 \approx 2C_2$) which is known as a Haynes's rule. The validity of this rule is still under discussion even in well studied materials, since the values of C depend on many factors, such as the effective mass ratio. For GaN, the theory [2] gives $C_1 = 9.6$, $C_2 = 17$. In undoped GaN samples, several bound excitonic lines were observed with $E_{B2} = 6.44$ meV and $E_{B1} = 12.3, 22.8,$ and 27.6 meV. From these values, $E_D \approx 62$ meV, and $E_A \approx 209, 387$ and 469 meV can be evaluated, which evident of the presence of several deep states with ionization energies different from the values predicted by the simple hydrogen-like model. The near-band-edge spectra of GaN:Mg show several recombination bands. The intensity ratio of these bands

depends on the temperature T , Mg concentration and excitation intensity I_e . The changes of this ratio and the shape of the spectra observed with increasing T , decreasing I_e and increasing Mg concentration are almost equal. Above room temperature, drastic changes in PL spectra of GaN:Mg were observed (fig.1). These changes can be interpreted with the model of the ionization of deep donors with $E_D > 200$ meV. Since the 2.8 eV band in GaN is characterized by the strong electron-phonon coupling, the corresponding theory should be developed in order to describe the interaction with LO phonons for the case of the non-hydrogen-like impurities. For this description, the theory [3] was used. However, it was modified in order to describe more adequately the polaronic nature of bound carriers, as well as the complicated structure of the valence band in GaN having several anisotropic dispersion branches.

The Huang-Rhys factor S being the measure of the electron-LO-phonon coupling and describing the shape of the near-band-edge emission spectra was calculated for the case of DAP and free-to-acceptor recombination. For comparison, the calculation were performed also for the Lukovsky model. However, it gives worse agreement with experiment compared to the quantum defect model. The results of calculation of the dependence of S on the DAP separation for different E_A and E_D are given in fig.2 a,b. The dependencies of S on E_A for the free-to-bound transitions were also calculated. They were applied to the analysis of the near-band-edge luminescence spectra and will be discussed in details. The experimental values of S_{FB} obtained from the luminescence spectra in GaN:Si at $T=78$ K is 0.76-0.81, giving $E_A \approx 0.2$ eV, which is in reasonable agreement with the known literature data.

The time-resolved spectra and PL transients allow to conclude that at least two overlapping bands in the near-band-edge emission of GaN:Mg at $T=78$ K are present. One of these bands shows the exponential decay with characteristic time of 220 ns, the second band has a non-exponential decay. They can be attributed to the free-to-bound and DAP recombination involving deep donors, respectively. The existence of the deep donor centers may be one of the important causes of compensation in the case of the doping of GaN by acceptor impurities.

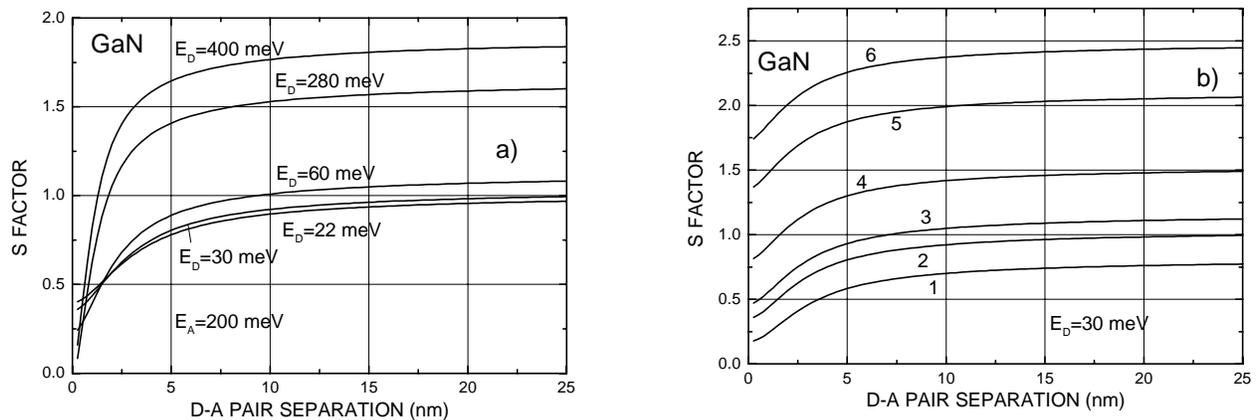


Fig.2. The dependencies of S factor on the DAP separation. a) - E_A is fixed at 200 meV; b) - E_D is fixed at 30 meV; $E_A = 120$ (1), 200 (2), 250 (3), 410 (4), 750 (5) and 1080 meV (6).

The problems connected with the correct estimation of the impurity ionization energies from the excitonic and near-band-edge PL spectra, the validity of Haynes's rule for GaN, the choice of the parameters for calculation from the wide spread of the data reported in the literature, the values of the impurity ionization energies and the possible ways of their estimation from PL spectra using the method described in [4], the calculation procedures for S factor, as well as the value of S for DAP and FB transitions, for E_D ranging from 22 to 430 meV and E_A between 120 and 1080 meV, and their relationship with the near-band-edge PL band shape will be discussed in detail.

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[1] S.C.Jain, M.Willander, J.Narayan, R. van Overstraeten. J. Appl. Phys., 87 (2000) 965.

[2] B.Stebe, G.Munsch. Solid State Commun, 35 (1980) 557.

[3] A.L.Gurskii, S.V.Voitikov. Solid State Commun, 112 (1999) 339.

[4] M.Germain, E.Kartheuser, M.Soltani, O.Pages, M.Cortier, W.Taudt, M.Heuken. Phys. Stat. Sol. (b), 210 (1998) 367.