

Temperature dependence of magnesium related optical transitions in GaN:Mg

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Magnesium is known to be the most successful dopant for the realisation of p-type GaN layers. Despite its common use in nitride-based optoelectronic devices there is a considerable uncertainty about the physical properties of Mg in GaN, e.g. the thermal activation energy which spreads over a large region between 120-200 meV [1]. We investigated the influence of the Mg doping level on the Mg thermal activation energy. For this reason, a series of GaN:Mg layers was deposited by molecular-beam epitaxy at 680^o C on (0001) sapphire substrates after a nitridation step and the growth of a 20 nm nominally undoped GaN layer which was intended to suppress a possible modified nucleation caused by the dopant. The doping was controlled by varying the Mg cell temperature resulting in Mg concentrations of $2 \cdot 10^{19} \text{ cm}^{-3}$ up to $3 \cdot 10^{20} \text{ cm}^{-3}$ as measured by secondary-ion-mass spectroscopy (SIMS). The corresponding free-hole concentration at room temperature increases with the Mg concentration from semiinsulating to about $1 \cdot 10^{18} \text{ cm}^{-3}$ as determined by Hall-effect measurements.

Fig.1 shows exemplarily the temperature dependent photoluminescence (PL) spectra of the Mg-correlated zero-phonon line (ZPL) transition around 3.26 eV for the sample with the lowest doping level. With increasing temperature the ZPL maximum shifts by about 8 meV to higher energies as shown in the inset of Fig. 1. This behaviour is in contradiction to the expected shift to lower energies if one assumes that the recombination mechanism of the ZPL transition is a pure donor-acceptor-pair (DAP) transition. Therefore, we assume that the ZPL is a superposition of the DAP transition which dominates at low temperatures and the corresponding free-to-bound (e, A^0) transition (A^0 neutral acceptor) which dominates beyond about 100K. If one takes into account that the bandgap of GaN is about 17 meV lower at 135 K compared to its position at 5 K [2] one can estimate an energy difference between the DAP and the (e, A^0) transition of about 25 meV. This value is much smaller than the linewidth of the ZPL of about 80 meV, therefore both transitions are not spectrally resolvable (the spectral resolution of the detection system is less than 1 meV). The assumption is in quantitative agreement with the estimated activation energies from the Arrhenius plot of the ZPL maximum (crosses) which is shown in Fig.2. The theoretical curves correspond to a rate equation model with two

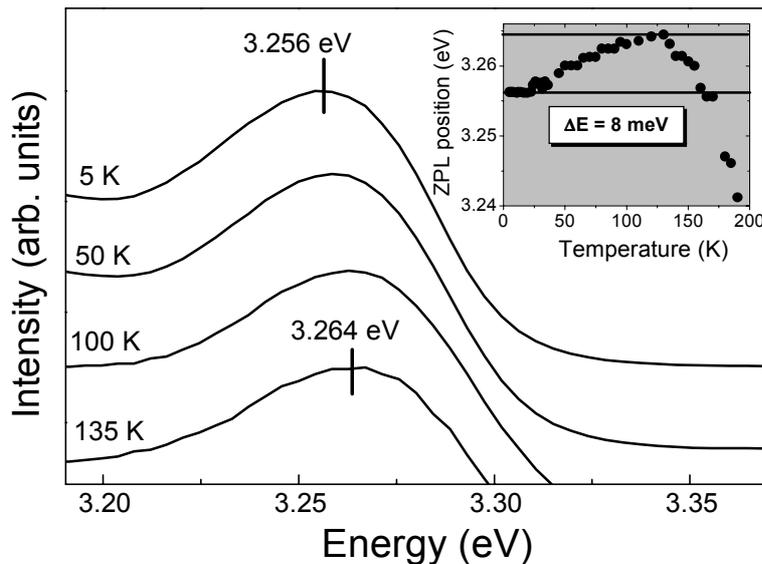


Fig. 1: Luminescence spectra of the Mg-correlated ZPL transition with increasing temperature. All spectra are normalized and shifted vertically for a better representation. **Inset:** Position of ZPL maximum with increasing temperature.

activation energies, $E_{A1} = 17 \pm 5$ meV (dotted line), $E_{A2} = 150 \pm 10$ meV (dashed line), and the combination of both activation energies (solid line). At low temperatures the lineshape of the ZPL is dominated by the DAP recombination. Therefore, E_{A1} is attributed to the activation of residual donor electrons with increasing temperature. However, for temperatures above 100 K the lineshape of the ZPL is dominated by the (e, A^0) transition. Thus, E_{A2} is attributed to the thermalisation of the corresponding acceptor level.

At a fixed doping level (i.e., in the same sample) we found a very slight increase of about 5 meV of the acceptor activation energy with the excitation density increasing from 1 to 100 W/cm^2 . This is

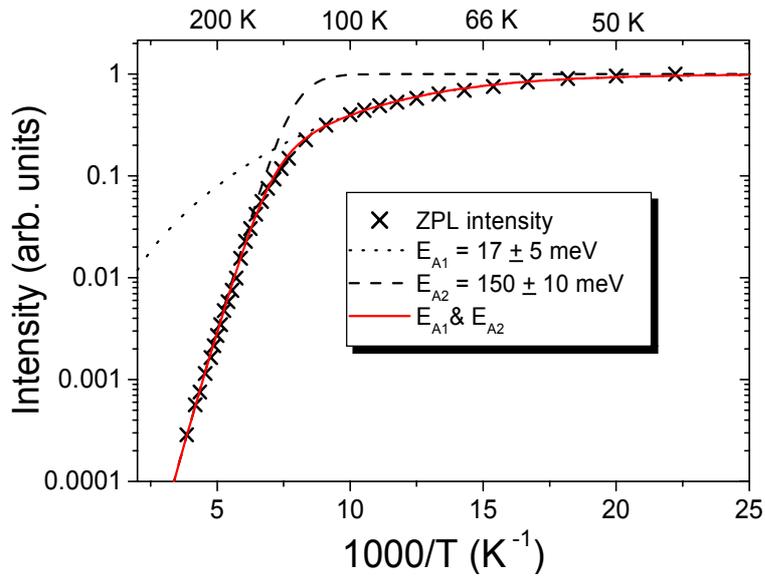


Fig. 2: Arrhenius plot of the ZPL maximum at 3.256 eV (crosses). The theoretical curves correspond to a rate equation model with an activation energy of 17 meV (dotted line) and 150 meV (dashed line) and the combination of both activation energies (solid line), see text.

concentrations of about $5 \cdot 10^{20} \text{ cm}^{-3}$ and therefore close to the highest Mg concentration of $3 \cdot 10^{20} \text{ cm}^{-3}$. However, there is only a weak decrease of the electrically determined activation energies i.e. no indication for a metallic conduction behaviour is observed.

Threading edge dislocations are known to be nonradiative centers in GaN at room temperature, and they are negatively charged, i.e. attractive for holes [3]. Thus, they could be responsible for the thermally activated hole recombination in GaN. We have determined the density of edge dislocations by use of nondestructive high-resolution X-ray diffraction measurements as described in detail in [4] for all investigated samples. With increasing doping level the concentration of screw dislocations decreases slightly from $3.0 \cdot 10^{10}$ to $2.2 \cdot 10^{10} \text{ cm}^{-2}$. If these nonradiative centers are responsible for the PL quenching their concentration should drastically increase for doping levels above $1 \cdot 10^{20} \text{ cm}^{-3}$ which is not observed. It seems to be unlikely that the hole capture at charged screw dislocations is responsible for the drastical drop of the thermal activation energies for doping above $1 \cdot 10^{20} \text{ cm}^{-3}$.

It is known that with increasing Mg doping level the formation of the cubic material phase of GaN is enhanced [5]. Therefore the low activation energy could be attributed to a hole release from the Mg acceptor into the top of the valence band of the cubic phase which maybe energetically favoured in comparison to the release to the top of the hexagonal valence band of GaN. An investigation of the cubic material phase in these samples by use of selective excitation spectroscopy as well as x-ray diffraction measurements is under way to clarify this point.

References:

- [1] e.g. I.P. Smorchkova et al., Appl. Phys. Lett **76**, 718 (2000) and the references cited therein.
- [2] C.F. Li et al. Phys. Rev. B **55**, 9251 (1997)
- [3] e.g. M. Leroux et al. J. Appl. Phys. **86**, 3721 (1999) and the references cited therein.
- [4] H. Heinke et al. phys. stat. sol. (a) **176**, 391 (1999).
- [5] S.C.Y. Tsen et al., J. Appl. Phys. **82**, 6008 (1997).

attributed to local sample heating in the laser spot. However, all measurements were performed under constantly low (1 W/cm^2) excitation density to exclude any thermal change on the determined thermal activation energies.

With increasing doping level the thermal activation energy as determined from the (e, A^0) transition quenching decreases from 150 meV at $2 \cdot 10^{19} \text{ cm}^{-3}$ down to 130 meV at $1 \cdot 10^{20} \text{ cm}^{-3}$. For Mg concentrations above $1 \cdot 10^{20} \text{ cm}^{-3}$ the optically determined activation energy drastically drops to about 40 meV. This decrease is possibly caused by the onset of the Mott transition which has been estimated to occur for acceptor