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Deep-Level Defects in MBE-Grown GaN-Based Laser Structure

T. Tsarova[a], T. Wosiński[a], A. Mąkosa[a], C. Skierbiszewski[b], I. Grzegory[b] and P. Perlin[b]

[a]Institute of Physics, Polish Academy of Sciences
al. Lotników 32/46, 02-668 Warsaw, Poland
[b]Institute of High Pressure Physics "Unipress", Polish Academy of Sciences
Sokołowska 29/37, 01-142 Warsaw, Poland

We present results of deep-level transient spectroscopy investigations of defects in a GaN-based heterostructure of a blue-violet laser diode, grown by plasma-assisted molecular beam epitaxy on a bulk GaN substrate. Three majority-carrier traps, T1 at $E_C - 0.28$ eV, T2 at $E_C - 0.60$ eV, and T3 at $E_V + 0.33$ eV, were revealed in deep-level transient spectra measured under reverse-bias conditions. On the other hand, deep-level transient spectroscopy measurements performed under injection conditions, revealed one minority--carrier trap, T4, with the activation energy of 0.20 eV. The three majority--carrier traps were revealed in the spectra measured under different reverse--bias conditions, suggesting that they are present in various parts of the laser--diode heterostructure. In addition, these traps represent different charge--carrier capture behaviours. The T1 trap, which exhibits logarithmic capture kinetics, is tentatively attributed to electron states of dislocations in the n-type wave-guiding layer of the structure. In contrast, the T2, T3, and T4 traps display exponential capture kinetics and are assigned to point defects.

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1. Introduction

Deep-level transient spectroscopy (DLTS) is a powerful and well-established technique for the investigation of electronic properties of deep-level defects in semiconductor materials and structures. It is based on the variation of the capacitance of a Schottky or p–n junction as a measure of the number of charges trapped within its space charge region during the filling pulse applied to the reverse-biased junction [1]. DLTS allows one to find defect characteristics, such as their activation energy and concentration, and catalogue deep-levels by means of their thermal

capture and emission cross-sections. More information on the structure of deep-level defects can be obtained from the dependence of the DLTS-signal amplitude on the filling-pulse duration. In this case it is possible to distinguish between deep levels associated with isolated point defects or impurities, which exhibit exponential capture kinetics [1], and deep levels associated with extended defects, such as dislocations, which are characterized by logarithmic capture kinetics [2, 3].

III–V nitrides, GaN, InGaN, and AlGaN, are wide direct band-gap semiconductor materials, which have already been used in high-temperature, high-power, and high-frequency electronics. Moreover, they have been applied with a great success in optoelectronics as blue light emitting diodes and lasers and solar-blind ultraviolet detectors [4]. Usually, GaN-based layers are epitaxially grown on sapphire or silicon carbide substrates. However, the mismatch in the lattice constants of the substrates and the GaN-based layers, and also self-compensation tendencies of wide band-gap semiconductors, result in a number of deep-level defects, especially dislocations, which influence the reliability and performance of GaN-based devices. It is very important to identify and understand the defects for improving the device technology.

In this paper we report our recent results of DLTS investigations of deep-level defects in a GaN-based heterostructure of a blue-violet laser diode (LD), grown by plasma-assisted molecular beam epitaxy (PAMBE) on bulk GaN substrate.

2. Laser-diode heterostructure

GaN-based heterostructure of a blue-violet laser diode was grown by PAMBE on n^+-type, dislocation free, bulk GaN substrate synthesized by a high-pressure (2 GPa) high-temperature (1500°C) method [5], which was characterized by a very low dislocation density ($< 100\ \mathrm{cm}^{-2}$). The key parameters for the PAMBE growth were the Ga-rich conditions and relatively low growth temperatures, which resulted in the high quality layers and interfaces. The heterostructure contained multiple InGaN/GaN quantum well as the active region, which was embedded between two, n-type (Si-doped) and p-type (Mg-doped), GaN wave-guiding layers, and two, n- and p-type, AlGaN cladding layers, and was covered with a highly Mg-doped GaN contact layer. In addition, a thin Mg-doped InAlGaN blocking layer was grown on the p-type side of the $p{-}n$ junction. See Ref. [6] for the exact sequence and compositions of the layers. The use of bulk GaN crystal, instead of commonly used sapphire substrates, results in an increase in lifetime and durability of the device owing to a lower number of dislocations in its active region.

3. Results

As we dealt with a complicated heterostructure, it was difficult enough to extract information about a concentration of charge carriers from capacitance–voltage ($C{-}V$) characteristics. Measuring $C{-}V$, the reverse voltage was extended

up to –6 V. However, only two main regions of the reverse voltage were distinguished: first, from 0 V to –2 V and second, from –2 V to –4 V, which corresponded to different carrier concentrations. For the first region the carrier concentration of 3×10^{18} cm^{-3} was found and assigned to the electron concentration in the n-type GaN wave-guiding layer. On the other hand, the second region carried information on the hole concentration of 1.5×10^{18} cm^{-3} in the p-type GaN wave-guiding layer.

Three majority-carrier traps, called T1, T2, and T3, have been revealed in the DLT spectra measured in the temperature range of 80–400 K under typical bias conditions, i.e. under reverse quiescent bias, which was decreased to zero during the filling pulse. On the other hand, DLTS measurements performed under injection conditions, i.e. under zero quiescent voltage and forward-bias filling pulse, revealed one minority-carrier trap, called T4.

The majority-carrier traps have been revealed in the DLT spectra measured under various bias conditions, as demonstrated in Fig. 1. The T1 and T2 traps were observed in the DLT spectrum recorded under the reverse voltage of –2 V, whereas the signal of the T3 trap appeared in the spectrum after increasing the reverse voltage to –4 V, thus suggesting that these traps are present in various parts of the LD heterostructure. We conclude that the T1 and T2 traps are electron traps located in the n-type wave-guiding layer of the structure and the T3 trap is a hole trap present in the p-type wave-guiding layer.

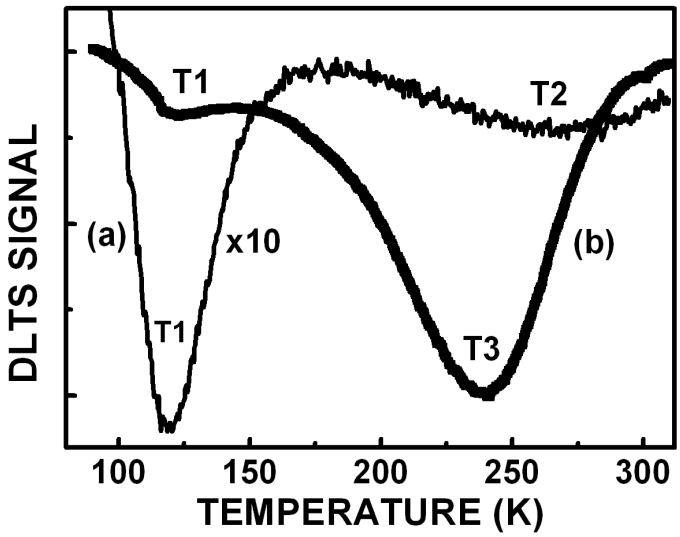

Fig. 1. DLT spectra of the GaN-based laser diode measured under different reverse bias conditions, (a) –2 V and (b) –4 V, at a rate window of 87 s^{-1} and the filling-pulse duration of 0.1 ms. Three majority-carrier traps, called T1, T2, and T3, have been revealed in the spectra. Let us note the scale expansion for the spectrum (a).

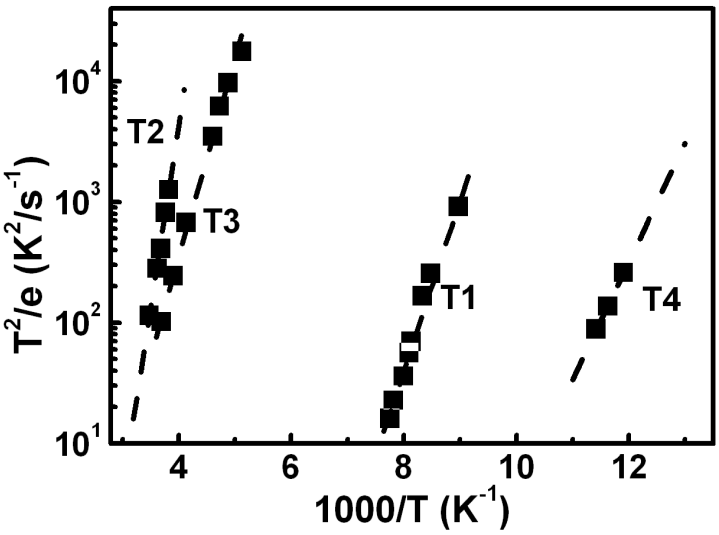

Fig. 2. Temperature dependence of the thermal emission rates (Arrhenius plots) for the T1, T2, T3, and T4 traps revealed with DLTS in the GaN-based laser diode.

The temperature dependences of the thermal emission rates (Arrhenius plots) for the traps are shown in Fig. 2. The activation energies of these traps and the capture cross-sections of the three majority-carrier traps evaluated from these dependences are: $E_{\mathrm{a}} = E_{\mathrm{C}} - 0.28$ eV and $\sigma_n = 7.8 \times 10^{-12}$ cm^2 for T1, $E_{\mathrm{a}} = E_{\mathrm{C}} - 0.60$ eV and $\sigma_n = 4.9 \times 10^{-13}$ cm^2 for T2, $E_{\mathrm{a}} = E_{\mathrm{V}} + 0.33$ eV and $\sigma_p = 4.3 \times 10^{-18}$ cm^2 for T3, and $E_{\mathrm{a}} = 0.20$ eV for T4.

In addition, the traps represent different charge-carrier capture behaviour. Dependences of the DLTS-signal amplitude on the logarithm of the filling-pulse duration for the traps are shown in Fig. 3. The T1 trap, which exhibits the logarithmic capture kinetics, indicated by the dashed line in the figure, shows its relation to electron states of dislocations. In contrast, all the other traps display the exponential capture kinetics and are assigned to point defects.

Additional information on the nature of electronic states of deep levels related to dislocations has been obtained from analysis of the dependence of DLTS--line shape of the T1 trap on the filling-pulse duration. This analysis allowed us to specify the type of electronic states associated with dislocations, which, owing to translational symmetry along dislocation lines, are expected to form one--dimensional energy bands rather than isolated localized electron states. According to the model recently proposed by Schröter et al. [7, 8], which takes into account the rate, at which the states reach their internal electron equilibrium within the band, they can be classified as either so-called *localized* or *band-like* states. The both types of states are characterized by a linear dependence of their DLTS-line amplitude on the logarithm of the filling time. For localized states the DLTS-line

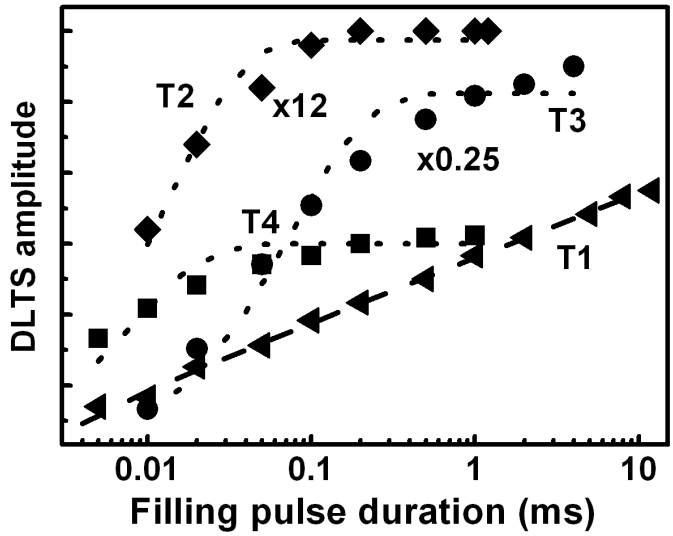

Fig. 3. Dependence of the DLTS-signal amplitude on the logarithm of the filling-pulse duration for the T1, T2, T3, and T4 traps. The dashed and dotted lines represent fittings of the logarithmic [3] and exponential [1] capture kinetics, respectively, to the experimental points.

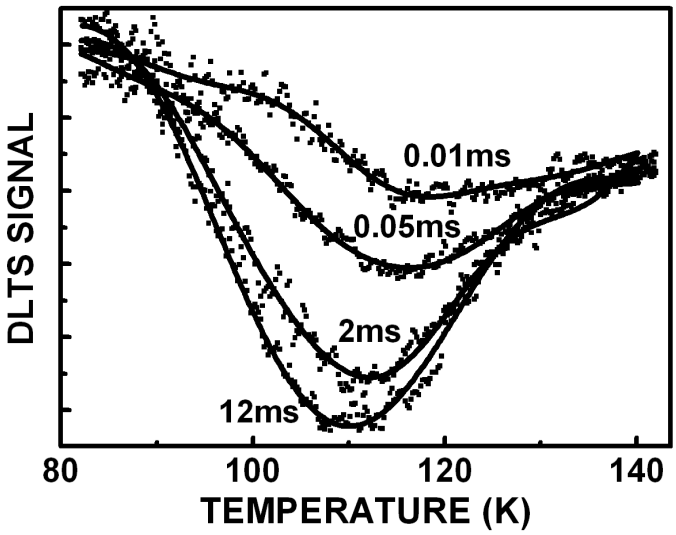

Fig. 4. Dependence of the DLTS-line shape of the T1 trap on the filling-pulse duration, whose values are written in the figure, measured at a rate window of 7.2 s^{-1}.

maximum stays constant on the temperature scale while changing the filling-pulse duration. On the contrary, in the case of band-like states, variation of filling-pulse duration results in broadened DLTS lines, whose maximum shifts towards lower

temperature with increasing pulse duration and whose high-temperature sides coincide. This is the case of the T1 trap in the GaN-based heterostructure, as demonstrated by our experimental results presented in Fig. 4.

4. Discussion and conclusions

The logarithmic capture kinetics observed in our results for the T1 trap, together with its behaviour characteristic of band-like states, strongly suggest its relation to the dislocation core states. The appearance of dislocations in the LD heterostructure grown on the lattice-matched GaN substrate with a very low dislocation density may arise due to the growth of lattice-mismatched AlGaN and InGaN layers, which can give rise to dislocation generation during strain relaxation. Likely the same trap, called E1, was recently revealed in the DLT spectra measured in n-type GaN layers grown by metal-organic vapour-phase epitaxy (MOVPE) on sapphire [9, 10] and in MOVPE-grown LD heterostructure [11], and attributed to the core states of threading dislocations.

The T2, T3, and T4 traps, whose amplitudes of DLTS signals exhibited a distinct saturation for long filling times, were characterized by the exponential capture kinetics indicating that the traps are associated with noninteracting point defects or impurities. Only one of these traps, the T2 trap, has been reported in the literature. This trap, with the activation energy at $E_C - 0.50 \div 0.62$ eV and labelled B2, D2, or E2 in the literature, tends to be the most prominent electron trap revealed by DLTS in n-type GaN [10–15]. Hacke et al. [12] and Haase et al. [13] assigned this trap to the nitrogen antisite point defect, N_{Ga}, on the ground of the results of tight-binding calculations determining the deep donor level of N_{Ga} at $E_C - 0.54$ eV [16]. More recent results by Chung et al. [14] and Cho et al. [10], showing that the concentration of this trap could be effectively suppressed by In doping, support this assignment. Very recently, this trap has been also revealed as the dominant deep-level defect in MOVPE-grown LD heterostructure [11]. However, in our present results the T2 trap concentration is the smallest of all deep-level traps recorded in the DLT spectra. The reasons for it are likely the Ga-rich conditions used for the PAMBE growth of high quality GaN-based layers of the LD heterostructure. This results in a decrease in a number of vacant Ga sites in the crystal lattice necessary for the formation of N_{Ga} antisites during the growth and, as a consequence, very low T2 trap concentration.

Recent extensive theoretical calculations from the first principles of the structure and energetics of native point defects in III–V nitrides [17] show that nitrogen vacancies V_N have the lowest formation energy in p-type GaN and can be produced in a significant concentration during its growth, thus being a good candidate for the assignment to the dominant deep-level trap T3 revealed in our investigations. The theoretically calculated energy level of the positively charged V_N is located between 0.39 eV [18] and 0.59 eV [17] above the valence-band maximum which, taking into account the theoretical uncertainty of a few tens of an eV, accounts fairly well for the energy level of the T3 trap.

In conclusion, basing on the results of charge-carrier capture kinetics at the deep-level traps revealed in GaN-based laser structure and the data reported in the literature we have proposed the assignment of the T1 traps to electron states of dislocations and both the T2 and T3 traps to the native point defects N_{Ga} and V_N, respectively.

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