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Native defect concentration in Czochralski-grown Te-doped GaSb by photoluminescence

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ABSTRACT

Photoluminescence characterization of Czochralaski-grown Te-doped GaSb wafers is presented. Calculations of the photoluminescence line shape of Te-doped GaSb wafers at 77 K have been performed. It has been demonstrated that the photoluminescence line shape analysis can be used for the estimation of native defect concentration. The n-type wafers with the doping level from 2×10^{17} to $2\times10^{18}\,cm^{-3}$ have been studied. The doping level obtained from the photoluminescence data is correlated with the results of the Hall mobility measurements. The native defect concentration has been obtained with the help of the developed analysis. A comparative study of photovoltaic cells manufactured from different wafers is presented. Changes in the recombination-related current flow components, spectral photoresponse curves and fill factor values reveal strong correlation with the obtained native defect concentration values.

1. Introduction

GaSb is known to have a very high concentration of native defects, which depends on the various growth conditions [1]. The origin of these defects is controversial. Based on the assumption of Van der Meulen [2] (who investigated the diffusion coefficients of these recombination centers), the p-type natural conductivity of GaSb was attributed to the high concentration of $V_{Ga}Ga_{Sb}$ complex defects, which act as doubly ionizable native acceptors (NA).

Experimental investigations of Ruhle and Bimberg [3] indicated simpler (non-complex) structure of native defects. Thermodynamical [4] and first-principles [5] calculations suggest that the most probable defect is Ga_{Sb} antisite, which is also doubly ionizable. This result is in agreement with the recent studies [6,7] showing the experimental based evidences of antisite Ga_{Sb} defect dominance in GaSb under Ga-rich conditions and Sb_{Ga} one under Sb-rich conditions. The concentration of these defects is pretty high. The hole concentration at 300 K of the undoped material ranges from $10^{16}\,cm^{-3}$ for MBE [8] or MOCVD [9] grown material to $2\times10^{17}\,cm^{-3}$ and higher for the Czochralaski grown bulk wafers [10]. Presumably, this concentration is ruled by native defects. This difference occurs, most probably, from the growth conditions, which are Sb-rich for the MBE or MOCVD processes and stoichiometric or Ga-rich for Czochralski. It should be noted, that the properties of the Czochralski grown ingots are normally non-uniform. Even the properties of the substrates cut from different ingot parts may scatter significantly [11,12]. Therefore, to choose a proper ingot part for the device fabrication, an effective method for the material characterization is required. The most widespread means for the material characterization is the Hall mobility measurement. According to the calculations presented in [13] the mobility is dependent on the native defect concentration. The aim of the present study is to show a close connection of the PL lineshape with the native defect concentration.

2. Theoretical approach

Photoluminescence of GaSb has been studied intensively during the past few decades [14–20]. However, the quality of the investigated material and its properties due to various dopants and technology differ. Special attention here is paid to the extensive study of Bignazzi et al. [14], who presented a calculation of the photoluminescence lineshape of Te doped GaSb at 77 K. The authors have characterized GaSb layers grown by MBE technique on GaAs substrates. Presented below are the results of similar calculations of PL lineshape, made in accordance with the method elaborated in that manuscript with some specific changes introduced to account for the high native acceptor concentration of Czochrlaski grown GaSb wafers. The aim of the present study was to apply the photoluminescence lineshape analysis to the estimation of the native defect concentration.

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Some short explanations of the calculation details are presented below. The photoluminescence lineshape is given by an integral, which accounts for the electrons' and holes' energies, densities of states (DOS) and occupation probabilities. The following models have been used in the calculation.

For the description of the band tailing due to the high doping concentration, two models have been tested: a semiclassical Kane theory [21,22] of the band tailing and an interacting Fermi liquid model [22]. The second model introduces a more pronounced band tailing effect. It appeared, that, even at high doping concentrations (up to $n \sim 2 \times 10^{18}\ \mathrm{cm}^{-3}$), the Kane theory gives better fit to the experimental spectra. The most heavily doped samples seem to exhibit slightly more pronounced band tails than the Kane model predictions. Band gap narrowing due to the Hartree-Fock exchange interaction was introduced as well.

The acceptor in Te-doped GaSb has a complex nature, which originates from the interaction of a Te atom and a doubly ionizable native defect (NA) resulting in a new singly ionizable complex giving a contribution to the PL spectrum at $\sim$72 meV below the band edge. This level is broadened due to a high concentration of native point defects and Te atoms and is transformed to a band. The DOS in this band is given by the Gauss distribution with the width parameter described as

$$\sigma_a = \sqrt{\frac{4\pi e^4}{\varepsilon^2}\left(N_D z_D^2 + N_A z_A^2\right)\int_{r_0}^{\infty} \exp\left(-\frac{2r}{\chi}\right) dr} \qquad (1)$$

where χ is the effective screening length, N_D and N_A are donor and acceptor concentrations, z is the charge of the donor/acceptor [21,23].

The probability of Te atom interaction with the native defects appears to be proportional to the doping level. Thus, at moderate doping levels ($n \sim 1-5 \times 10^{17}\ \mathrm{cm}^{-3}$), two peaks are present in the PL spectrum: related to the complex Te based acceptor (a so-called T-band) with the activation energy of $\sim$72 meV and to the doubly ionized state of the native defect acceptor with activation energy of $\sim$105 meV (C-band). The singly ionized state of this acceptor (at $\sim$31 meV) is not present in the PL spectra of n-type Te doped GaSb. Its presence in the spectrum clearly indicates that the sample is undercompensated and is p-type. The intensity of the C-band decreases with increasing dopant concentration and entirely disappears at $n \geq 7-8 \times 10^{17}\ \mathrm{cm}^{-3}$.

The position of the Fermi-level is determined according to the free electron concentration. At concentrations of 10^{17}–$10^{18}\ \mathrm{cm}^{-3}$, the Fermi level lies inside the conduction band, thus, controlling the PL energy blue shift. At higher concentrations, the blue shift rate decreases due to filling the L-valley with heavier effective mass. Fig. 1 presents the experimental data obtained from the PL spectra fit. The spectra were taken at the pump power density $\sim$500 W/cm^2.

Increase of the native defect concentration appears as the PL line redshift and FWHM increase due to deeper band-tailing effect and acceptor level broadening. Fig. 2 presents the calculated Fermi-energy shift (this value is proportional to the PL line position shift) caused by different acceptor concentration. It can be seen that increase in the defect concentration leads to decrease in the Fermi energy (note the negative values of the ΔFn), however the effect of Fermi level lowering is minor (few meV at the most), and, thus, cannot be used as an adequate parameter for native acceptor density evaluation, as the accuracy of the Hall measurements is much poorer. On the other hand, the position of the PL line can itself be used for determination of the electron concentration.

The main feature influenced by the defect concentration is, thus, the broadening of the spectrum. Fig. 3 presents examples of

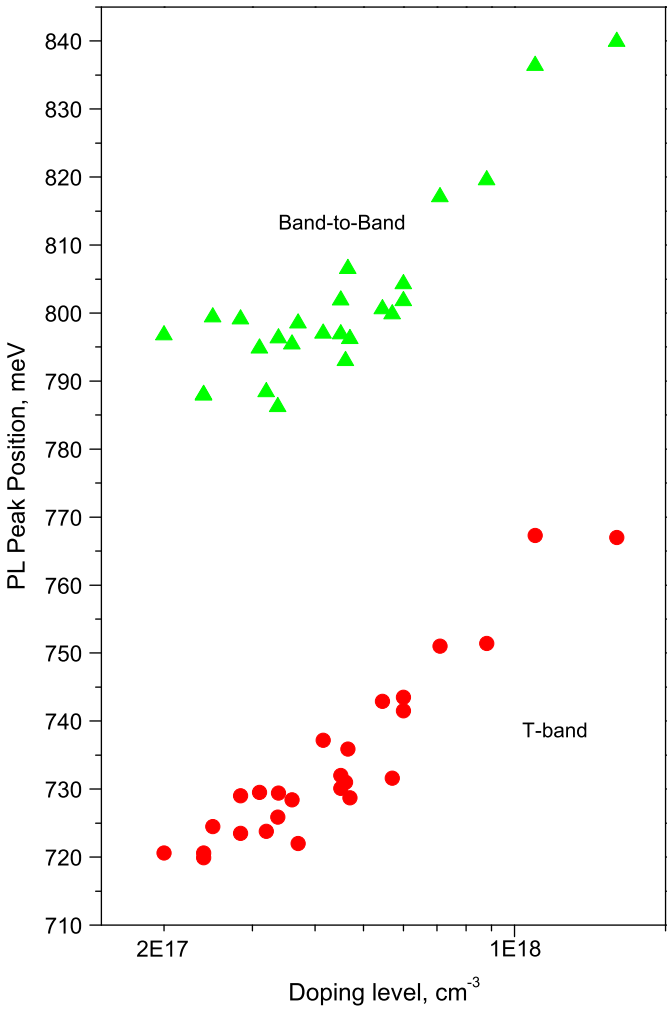

Fig. 1. Experimental dependence of the PL bands (T-band and band-to-band) position on the doping level. The free electron concentration is derived from the Hall mobility measurements at 77 K.

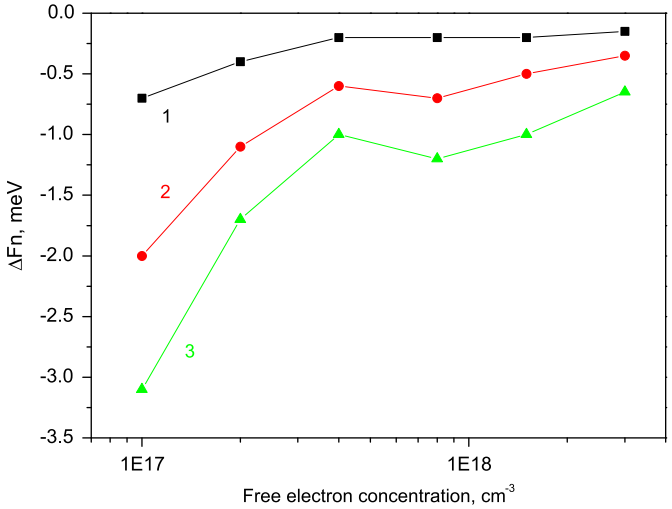

Fig. 2. Fermi-level lowering (in comparison to the non-compensated material value) calculated at different doping levels and native defect concentrations: 1–NA$=1 \times 10^{17}\ \mathrm{cm}^{-3}$, 2–NA$=3 \times 10^{17}\ \mathrm{cm}^{-3}$, 3–NA$=5 \times 10^{17}\ \mathrm{cm}^{-3}$.

4 PL spectra (T-band) calculated with different NA values. The effect of broadening (as well as the Fermi-energy shift) decreases with increasing the doping level, which impairs the calculation