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Influence of surface states and bulk traps on non-equilibrium phenomena at GaAs and GaN surfaces

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The influence of surface state density N_{SS} and bulk non-radiative lifetime τ on room temperature photoluminescence quantum efficiency Y_{PL} and surface photovoltage (SPV) versus the excitation light intensity Φ was studied theoretically for GaAs and wurtzite GaN using self-consistent computer simulations. It was demonstrated that SPV(Φ) dependences are more sensitive than $Y_{PL}(\Phi)$ to a change in magnitude of N_{SS}, especially for high N_{SS} and at low Φ, whereas SPV is practically insensitive to τ contrary to Y_{PL}. The simultaneous measurement of Y_{PL} and SPV versus Φ, combined with rigorous computer analysis, seems to be a very promising method for contactless characterization of the surface and bulk trap parameters.

Keywords: gallium arsenide, gallium nitride, surface states, bulk traps, photoluminescence, surface photovoltage.

1. Introduction

GaAs, GaN, and related compounds due to their electronic, optical, and thermal properties are very promising in the fabrication of high-frequency, high-temperature and high-power transistors [1–7], as well as of light emitting diodes (LEDs) and lasers up to ultraviolet range [8–11]. In such devices, a non-radiative recombination of charge carriers through surface states and bulk traps is very detrimental because it reduces light emission and current amplification, and leads to a device degradation due to heating crystal lattice and forming defects [10–14]. Moreover, the device miniaturization causes that the surfaces and interfaces contribute more and more to the device performance through such undesirable effects as the pinning of surface Fermi level E_{FS}, increasing leakage currents, gate lag *etc.* [14–16]. Therefore, the control and characterization of surface and bulk recombination parameters such as

surface state density N_{SS}, surface recombination velocity S_{eff}, and non-radiative lifetime of charge carriers τ, are very important during the device fabrication process.

It has been already shown that the photoluminescence surface state spectroscopy (PLS^3) which was developed by the group of Hasegawa [17], is a powerful, non-destructive, and contactless method for determination of the energy distribution of the surface state density $N_{SS}(E)$ on both free and covered surfaces, *in situ* and *ex situ*. PLS^3 is based on the measurement of the photoluminescence quantum efficiency Y_{PL} as a function of the excitation light intensity Φ at room temperature and the subsequent fitting of the theoretical dependence to the experimental data allows to determine $N_{SS}(E)$, E_{FS}, and S_{eff}.

However, the surface contribution is often difficult to extract from photoluminescence (PL) due to the complexity of electronic processes in an illuminated semiconductor as well as the lack of precise information about the values of bulk recombination parameters, which is the case of GaN. Therefore, systematic theoretical studies of the influence of both the surface and bulk parameters on measured non-equilibrium phenomena are necessary. Moreover, other techniques complementary to PLS^3 should be developed for more unambiguous and quantitative determination of surface and bulk recombination parameters. A method based on the photoinduced change in the surface potential (surface photovoltage, SPV), whose measurements are widely used in semiconductor science [18], seems to be a promising candidate.

In this work, the authors performed a numerical analysis of the dependences of both Y_{PL} and SPV versus Φ in the wide range of photoexcitation at GaAs and wurtzite GaN surfaces. The $Y_{PL}(\Phi)$ and SPV(Φ) theoretical curves were calculated by a unique computer simulator of non-equilibrium phenomena in semiconductors. In computations, we assumed continuous and discrete distributions of the surface state density, which are typical for surfaces and interfaces of GaAs and GaN used in technology. Using calculation results, the influence of surface parameters $N_{SS}(E)$, and of a bulk parameter τ on the non-equilibrium phenomena in the surface region of the studied semiconductors was investigated.

2. Computation procedure

For numerical calculations of the PL efficiency and surface photovoltage versus excitation intensity Φ, we used a 1D Scharfetter-Gummel-type vector-matrix computer program, developed by SAITOH *et al.* [17] for modelling of photon-induced phenomena in a semiconductor. The program takes account of all possible recombination processes in a bulk, including band-to-band radiative transitions, Shockley–Read–Hall (SRH) recombination through deep levels and Auger recombination, as well as non-radiative recombination via surface states. After the self-consistent solving of the Poisson's equation, current equations and continuity equations in a semi-infinite sample, the simulator rigorously determines the steady-

state electron $n(x)$ and hole $p(x)$ densities, and electric potential $V(x)$ at a distance x from the surface. Then, for different Φ, the simulator calculates Y_{PL}, S_{eff}, SPV, and many other bulk and surface quantities.

In the calculations, a U-shaped continuum of the surface state density distribution $N_{SS}(E)$ was assumed in accordance with the disorder induced gap state (DIGS) model by HASEGAWA and OHNO [19]. The DIGS spectrum origins from the amorphous-like surface structure disorder and thus consists of donor-like states distributed below the so-called charge neutrality level E_{HO}, and acceptor-like ones distributed above E_{HO}. The E_{HO} lies 0.96 eV below the bottom of the conduction band E_C for GaAs surface, and at E_C – 1.2 eV for GaN. The $N_{SS}(E)$ is expressed by the formula:

$$N_{SS}(E) = N_{SS0}\exp\left[\left(\frac{|E - E_{HO}|}{E_{0D,A}}\right)^{n_{D,A}}\right]$$

where N_{SS0} is the minimum surface state density, $E_{0D,A}$ and $n_{D,A}$ are the parameters responsible for the curvature of $N_{SS}(E)$ function for donor-like states (subscript D) and acceptor-like ones (subscript A), respectively. For the GaN surface, we assumed additionally a Gaussian discrete level, frequently attributed to nitrogen vacancy [20], at $E_D = E_C - 0.4$ eV with the full width at half maximum (FWHM) of 0.05 eV.

The GaAs sample was assumed to be excited by the green line (514 nm) of an Ar laser, whereas the GaN one by the 325 nm line of a He-Cd laser. The calculations were carried out for the *n*-type (doping of 10^{17} cm^{-3}) GaAs and GaN, the surface state cross -sections for carrier capturing of 10^{-16} cm^2, the bulk lifetime τ of 10^{-7} s, and at room temperature. Other necessary surface and bulk parameters of GaAs and wurtzite GaN were taken from [21–24].

3. Results and discussion

The dependences of Y_{PL} and SPV versus Φ and N_{SS0} calculated for GaAs and wurtzite GaN are summarized in Figs. 1 and 2, respectively. The surface state density distributions assumed in the computations are shown in the figure insets. From the presented plots, it is evident that the rigorously calculated Y_{PL} and SPV depend strongly on both N_{SS} and Φ. In particular, the changes in Y_{PL} reach 2 orders of magnitude and SPV does not saturate even under very high Φ, contrary to the predictions of simplified models. The former effect is caused by the gradual saturations of surface states as recombination centers and the Φ-induced decreasing of S_{eff}. The latter is due to Dember photovoltage. Both effects have been previously observed for GaAs, AlGaAs, and InP and have been explained in detail elsewhere [25].

The comparison between Y_{PL} and SPV spectra of GaAs and GaN leads to the following statements:

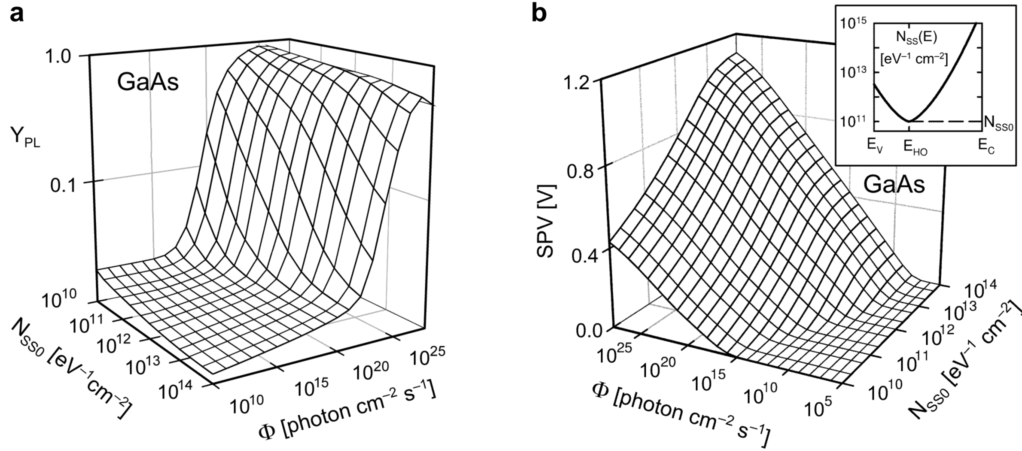

Fig. 1. 3D plots of PL quantum efficiency Y_{PL} (**a**) and surface photovoltage SPV (**b**) *vs.* excitation light intensity Φ and *vs.* the minimum surface state density N_{SS0} for GaAs with $N_{SS}(E)$ shape shown in the inset in Fig. 1**b**.

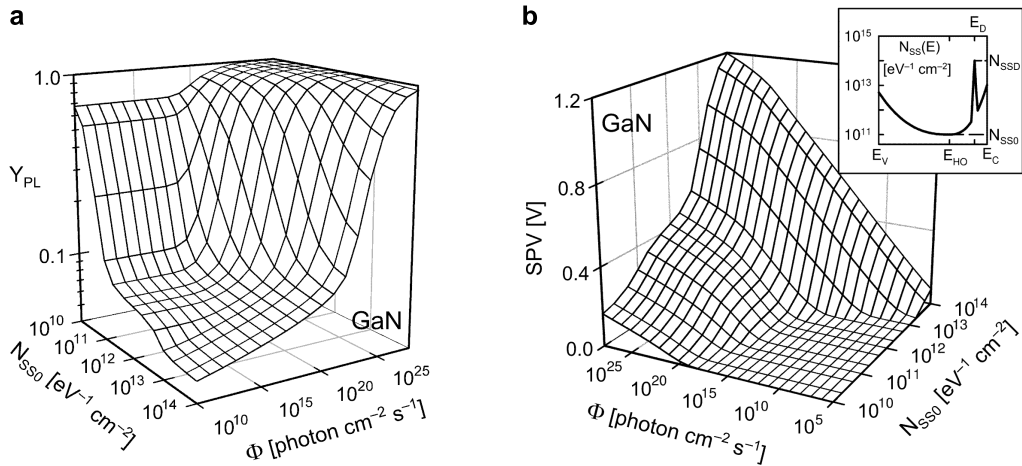

Fig. 2. 3D plots of Y_{PL} (**a**) and SPV (**b**) versus Φ and *vs.* the minimum surface state density N_{SS0} for GaN with $N_{SS}(E)$ shape shown in the inset in Fig. 2**b** (N_{SSD} is fixed at 10^{14} $eV^{-1}cm^{-2}$).

1. The high N_{SS} quenches Y_{PL} due to increasing non-radiative surface recombination but increases SPV because of the sensitisation of the more depleted surface region to photon-generated excess carriers which drastically change the potential profile in the sample.

2. SPV is more sensitive than Y_{PL} to the change in the surface state density in the region of high N_{SS} and at low excitations. The $Y_{PL}(\Phi)$ curves are much less resolved

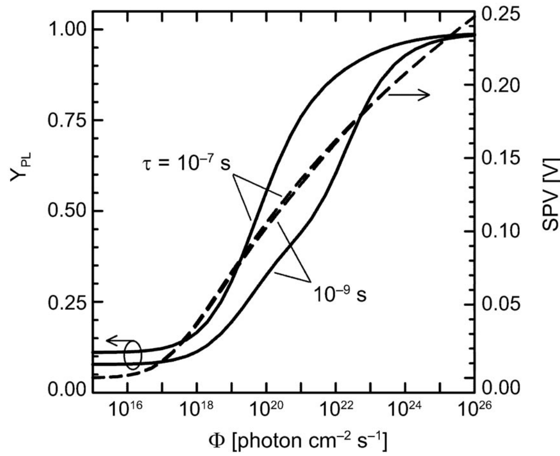

Fig. 3. Y_{PL} (solid lines) and SPV (dashed lines) *vs.* Φ calculated for different values of bulk lifetime τ for GaN with $N_{SS}(E)$ shown in the inset of Fig. 2**b**.

under these surface conditions because of a huge surface recombination. From the measurement point of view, it is a great advantage of SPV to provide electronic information on the highly disordered and defected III-V surfaces because most optical techniques, *e.g.*, PL-based, fail for high N_{SS} due to small signals.

3. Y_{PL} for GaN is generally larger than for GaAs, and $Y_{PL}(\Phi)$ dependences exhibit more dynamical changes versus N_{SS0} probably due to the higher value of the radiative recombination coefficient in GaN.

It should be also underlined that SPV can be measured in absolute units (volts) contrary to Y_{PL}, which is almost always expressed in arbitrary units. Therefore the fitting of theoretical dependences to experimental data and unique quantitative determination of surface parameters, like $N_{SS}(E)$, should be easier for SPV as compared to PLS^3 method.

The influence of the bulk lifetime of carriers τ on Y_{PL} and SPV spectra from GaN is presented in Fig. 3. The values of τ in the range from 10^{-9} to 10^{-7} s were taken from the literature [24, 26–28]. It is clear that the bulk lifetime governs $Y_{PL}(\Phi)$ spectra especially in the low and medium excitation regions (relative change in Y_{PL} up to 50%), whereas the changes in SPV(Φ) curves for different τ are very little. This finding can be explained in terms of recombination mechanism. Namely, the shorter lifetime means the greater non-radiative SRH recombination rate via bulk deep levels and consequently lower Y_{PL}. However, the SRH recombination act is a binary (electron -hole) process and it does not change the net charge of carriers, thus the steady-state potential profile $V(x)$ and, consequently, SPV should be insensitive to τ at least in the first approximation. In this context, the combined use of the PLS^3 and SPV techniques would enlarge markedly contactless characterisation of the surface electronic status.

4. Conclusions

We performed the rigorous numerical analysis of the influence of surface states in terms of their density distribution $N_{SS}(E)$, and bulk traps in terms of lifetime τ on the $Y_{PL}(\Phi)$ and SPV(Φ) dependences. It was shown that SPV is more sensitive to the change in $N_{SS}(E)$ compared to Y_{PL} for the surfaces with high surface state densities and under low excitations. On the other hand, SPV is practically insensitive to the bulk non-radiative lifetime. The combination of power-dependent Y_{PL} and SPV methods seems to be very promising for contactless and non-destructive characterization of wide-bandgap semiconductors like GaAs and GaN.

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References

[1] PEARTON S.J., REN F., ZHANG A.P., LEE K.P., *Fabrication and performance of GaN electronic devices*, Materials Science and Engineering R: Reports **30**(3-6), 2000, pp. 55–212.

[2] HARTNAGEL H.L., *III-V compounds for high-temperature operation*, Materials Science and Engineering B: Solid-State Materials for Advanced Technology **B46**(1-3), 1997, pp. 47–51.

[3] OHNO Y., KUZUHARA M., *Application of GaN-based heterojunction FETs for advanced wireless communication*, IEEE Transactions on Electron Devices **48**(3), 2001, pp. 517–23.

[4] SZWEDA R., *HEMT materials and devices*, III-Vs Review **16**(3), 2003, pp. 36–9.

[5] ZOLPER J.C., *Review of junction field effect transistors for high-temperature and high-power electronics*, Solid-State Electronics: an International Journal **42**(12), 1998, pp. 2153–6.

[6] CHALKER P.R., *Wide bandgap semiconductor materials for high temperature electronics*, Thin Solid Films **343-344**, 1999, pp. 616–22.

[7] SHUR M.S., GASKA R., BYKHOVSKI A., *GaN-based electronic devices*, Solid-State Electronics **43**(8), 1999, pp. 1451–8.

[8] MILLS A., *Compound semiconductors*, III-Vs Review **16**(4), 2003, pp. 32–5.

[9] KOVAC J., PETERNAI L., LENGYEL O., *Advanced light emitting diodes structures for optoelectronic applications*, Thin Solid Films **433**(1-2), 2003, pp. 22–6.

[10] MUKAI T., *Recent progress in group-III nitride light-emitting diodes*, IEEE Journal on Selected Topics in Quantum Electronics **8**(2), 2002, pp. 264–70; MUKAI T., NAGAHAMA S., KOZAKI T., SANO M., MORITA D., YANAMOTO T., YAMAMOTO M., AKASHI K., MASUI S., *Current status and future prospects of GaN-based LEDs and LDs*, Physica Status Solidi A: Applied Research **201**(12), 2004, pp. 2712–6.

[11] TOJYO T., ASANO T., TAKEYA M., HINO T., KIJIMA S., GOTO S., UCHIDA S., IKEDA M., *GaN-based high power blue-violet laser diodes*, Japanese Journal of Applied Physics, Part 1: Regular Papers and Short Notes and Review Papers **40**(5A), 2001, pp. 3206–10.

[12] WEBER E.R., *Understanding defects in semiconductors as key to advancing device technology*, Physica B: Condensed Matter **340-342**, 2003, pp. 1–14.

[13] WILKS S.P., *Engineering and investigating the control of semiconductor surfaces and interfaces*, Journal of Physics D: Applied Physics **35**(9), 2002, pp. R77–90.

[14] BINARI S.C., KLEIN P.B., KAZIOR T.E., *Trapping effects in GaN and SiC microwave FETs*, Proceedings of the IEEE **90**(6), 2002, pp. 1048–58.

[15] Rizzi A., *Surface and interface electronic properties of group III-nitride heterostructures*, Applied Surface Science **190**(1-4), 2002, pp. 311–7.

[16] Hashizume T., Ootomo S., Inagaki T., Hasegawa H., *Surface passivation of GaN and GaN/AlGaN heterostructures by dielectric films and its application to insulated-gate heterostructure transistors*, Journal of Vacuum Science and Technology B: Microelectronics and Nanometer Structures **21**(4), 2003, pp. 1828–38.

[17] Saitoh T., Iwadate H., Hasegawa H., *In situ surface state spectroscopy by photoluminescence and surface current transport for compound semiconductors*, Japanese Journal of Applied Physics, Part 1: Regular Papers and Short Notes and Review Papers **30**(12B), 1991, pp. 3750–4.

[18] Kronik L., Shapira Y., *Surface photovoltage phenomena: theory, experiment, and applications*, Surface Science Report **37**(1-5), 1999, pp. 1–206.

[19] Hasegawa H., Ohno H., *Unified disorder induced gap state model for insulator–semiconductor and metal–semiconductor interfaces*, Journal of Vacuum Science and Technology B: Microelectronics and Nanometer Structures **4**(4), 1986, pp. 1130–8.

[20] Boguslawski P., Briggs E.L., Bernholc J., *Native defects in gallium nitride*, Physical Review B: Condensed Matter **51**(23), 1995, pp. 17255–8.

[21] NSM Archive, Physical Properties of Semiconductors: http://www.ioffe.rssi.ru/SVA/NSM/Semicond/

[22] Matoussi A., Boufaden T., Guermazi S., Eljani B., Mlik Y., Toureille A., *Minority carrier diffusion lengths and optical self-absorption coefficient in undoped GaN*, Physica Status Solidi B: Basic Solid State Physics **240**(1), 2003, pp. 160–8.

[23] Ishikawa F., Hasegawa H., *Cathodoluminescence in-depth spectroscopy study of AlGaN/GaN heterostructures*, Applied Surface Science **212-213**, 2003, pp. 885–9.

[24] Duboz J.Y., Binet F., Dolfi D., Laurent N., Scholz F., Off J., Sohmer A., Briot O., Gil B., *Diffusion length of photoexcited carriers in GaN*, Materials Science and Engineering B: Solid-State Materials for Advanced Technology **B50**(1-3), 1997, pp. 289–95.

[25] Adamowicz B., Hasegawa H., *Computer simulations of the surface photovoltage on Si and GaAs surfaces with U-shaped surface state continuum*, Vacuum **54**(1-4), 1999, pp. 173–7; Adamowicz B., Miczek M., Ikeya K., Mutoh M., Saitoh T., Fujikura H., Hasegawa H., *Electronic properties of $Al_xGa_{1-x}As$ surface passivated by ultrathin silicon interface control layer*, Applied Surface Science, **141**(3-4), 1999, pp. 326–32; Adamowicz M., Miczek M., Brun C., Gruzza B., Hasegawa H., *Rigorous analysis of the electronic properties of InP interfaces for gas sensing*, Thin Solid Films **436**(1), 2003, pp. 101–6; Miczek M., Adamowicz B., Hasegawa H., *Determination of InP surface state density distribution from excitation-power-dependent photoluminescence spectra using genetic algorithm-based fitting procedure*, Surface Science **507-510**, 2002, pp. 240–4.

[26] Bandic Z.Z., Bridger P.M., Piquette E.C., McGill T.C., *Minority carrier diffusion length and lifetime in GaN*, Applied Physics Letters **72**(24), 1998, p. 3166–8; *Values of minority carrier diffusion lengths and lifetimes in GaN and their implications for bipolar devices*, Solid-State Electronics **44**(2), 2000, pp. 221–8.

[27] Pozina G., Bergman J.P., Monemar B., Heying B., Speck J.S., *Radiative and nonradiative exciton lifetimes in GaN grown by molecular beam epitaxy*, Physica Status Solidi B: Basic Solid State Physics **228**(2), 2001, pp. 485–8.

[28] Jursenas S., Miasojedovas S., Kurilcik G., Zukauskas A., Hageman P.R., *Luminescence decay in highly excited GaN grown by hydride vapor-phase epitaxy*, Applied Physics Letters **83**(1), 2003, pp. 66–8.

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