APPLICATION OF THE SAH-NOYCE-SHOCKLEY RECOMBINATION MECHANISM TO THE MODEL OF THE VOLTAGE-CURRENT RELATIONSHIP OF LED STRUCTURES WITH QUANTUM WELLS

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ABSTRACT

The Sah-Noyce-Shockley (SNS) space charge region recombination theory is applied to build the mathematic model of the voltage-current relationships (VCR) of light emitting diodes with quantum wells. Unlike the mathematic model of VCR, for SNS in the proposed model, non-uniformity of recombination centres distribution over the space charge region and dependence of their mean concentration on voltage are assumed as well as the fact that the nonideality factor of forward current dependence on bias voltage may have a continuous series of values from 1 to 5 and is defined by the dependence on bias voltage of both saturation current and exponent of the VCR mathematical model.

Keywords: light emitting diodes with quantum wells, voltage-current relationship, nonideality factor, recombination mechanism

1. INTRODUCTION

Thanks to their remarkable properties, light emitting diodes (LED) based on quantum well (QW) heterostructures have reached the leading positions as light sources and elements of full-colour screens. However, the paradox is that no mathematical model of their voltage-current relationship (VCR) has been created over the 25 years since the start of their serial production. To describe experimentally observed VCRs of QW LEDs, models developed for homogeneous *p-n* junctions are used. This leads to difficulties in interpretation of both behaviour of the dependence of current on bias voltage and quantum efficiency of LED.

The VCR model of a diffusion current mechanism was proposed by Shockley [1]:

$$J_{dif} = q\left(\frac{p_n L_p}{\tau_p} + \frac{n_p L_n}{\tau_n} \right) \cdot \left[\exp\left(\frac{qU}{kT} \right) - 1 \right] = $$
$$= J_0 \left[\exp\left(\frac{qU}{kT} \right) - 1 \right], \quad (1)$$

where J_{dif} is the current density, q is the charge of the electron, p_n and n_p are the concentrations of minor carriers in *n-* and *p-* areas respectively, L_n and L_p are the diffusion lengths, τ_n and τ_p are the electron and hole lifetimes, U is the bias voltage, k is the Boltzmann constant, T is the absolute temperature of *p-n* junction, $J_0 \left[\exp\left(\frac{qU}{kT} \right) - 1 \right]$ is the diffusion current of saturation.

The formula (1) was further amended with the *n* parameter acquired experimentally and called the nonideality factor (NF) (in other works, it is called the ideality factor):

$$J_{dif} = J_0 \left[\exp\left(\frac{qU}{nkT} \right) - 1 \right]. \quad (2)$$

The physical nature of NF for homogeneous *p-n* structures was described in the work by Sah, Noyce and Shockley (SNS) [2]. It presents the VCR model based on the recombination mechanism of charge

carriers (CC) in the space charge region (SCR) of symmetrical *p-n* junction through uniformly distributed defect levels:

$$J_{rec} = q\frac{\sigma_t N_t W}{2} n_t V_T \exp\left(\frac{qU}{2kT}\right) = J_s \exp\left(\frac{qU}{2kT}\right), (3)$$

where W is the width of SCR, σ is the capture cross-section of recombination centres, V_T is the thermal velocity, N_t is the concentration of recombination centres in SCR, n_i is the intrinsic concentration of CC, $J_s = q\frac{\sigma_t N_t W}{2} n_t V_T$ is the saturation current; NF is taken equal to 2 in (3).

Later, this model was developed [3] for asymmetrical *p-n* junctions keeping the assumption on uniform distribution of defect concentration in SCR.

Experimentally observed VCRs with NF varying between 1 and 2 are attributed to competition of particular recombination mechanisms [4], and it is claimed that NF may vary between 1 and 2 due to equality of total forward current to the sum of diffusion and recombination currents.

In 1994–1996, first blue and green QW LEDs were created based on *AlGaN/InGaN/GaN* heterostructures [5, 6] as well as a red LED based on *Al-InGaP* heterostructures. Since that, intensive studies of the properties of these LEDs have been carried out [7–12]. Their electric and physical characteristics, in particular VCR, significantly differ from characteristics of previously developed LEDs. For instance, NF of QW LEDs varies significantly over the entire region of current-voltage relationship [13, 14] and its values may be equal to 1.2 to 5 or even higher. With relatively low values of current density (approx. 1 A/cm²), deviations from the exponential dependence and the trend to saturation of current are observed in semi-logarithmic coordinate VCRs of any and all *GaN* and *AlInGaP* based LEDs. Different models are proposed to explain these facts, with assumptions made on high resistance of contacts and competition between different recombination mechanisms. At the same time, formation of the charge of free CCs in the contact area of wide band gap semiconductors is not taken into account [15, p. 156].

The phenomenological model of the *ABC* recombination rate based on the models of Shockley–Read–Hall (SRH), radiative and Auger recombination mechanisms [16–19] was developed. The *ABC* model rather rationally explains the behaviour of quantum efficiency of QW LEDs with changes

of forward current density but is still not used for building the VCR mathematical model.

Researchers still keep on using the (2) and (3) formulae to describe VCR of QW LEDs, which is not correct given that recombination in the SCR layer of WQ LEDs occurs in narrow local regions, QW layers with width of several nanometres. This fact is taken into account in [20, 21].

Analysis of current formation in QW LEDs is one of the focuses in [13, 22]. These works aspire to explain the fall of efficiency at relatively low values of current density, but no expressions to describe VCR were obtained.

All works analysing experimental VCRs of LEDs, both based on homogeneous junctions and on heterogeneous *p-n* structures with QW, provide a formula that defines NF by differentiating the logarithm of current to voltage:

$$n = \left[kT\left(\frac{d}{dU}\ln(J)\right)\right]^{-1}. \quad (4)$$

It is obviously incorrect since experimental VCRs are not analytical functions but discrete tables of concordance between current and bias voltage. Therefore, the following formula is more appropriate for application

$$n = \left[kT\left(\frac{\Delta\ln(J)}{\Delta U}\right)\right]^{-1}, \quad (5)$$

Here $\Delta\ln(J)$ is the increment of the current density logarithm with bias voltage increment by ΔU. However, no work contains information on the values of these increments for calculations, while the result significantly depends on it.

In the majority of the experimental materials, the NF itself and the pre-exponential factor of the formula of VCR of QW LED distinctly change with changes in bias voltage [14], while the formulae (4) and (5) imply that they are constant.

Given the above, it is necessary to define what parameter is calculated by (5) for the entire range of VCR: kT-fold reciprocal of the ratio of increment of the $\Delta\ln(J)$ function to increment of the argument ΔU or the coefficient characterising non-concordance between the exponential factor exp $[qU/(n^* \cdot kT)]$ and the ideal form exp $[qU/(kT)]$? Obviously, it is the kT-fold reciprocal of the ratio $\Delta\ln(J)/\Delta U$. n^* here is the factor of deviation of the exponential factor from the one given in [1]. The exponent in (2) includes the factor of deviation from the Shockley's ideal VCR model based on the Boltzmann distribu-

tion. Therefore, we will hereinafter identify the NF defined by (5) as n and the factor included in the exponent as n^* (asterisked n).

The review of the works allows us to draw conclusions that:

– When analysing experimental data concerning QW LEDs, they use the Shockley's and SNS mathematical models of VCR, which do not take the distinctions of their technological structure into account;

– The cases of non-uniform distribution of recombination centres [23, 24] common for LED structures are not considered.

These conclusions allowed us to formulate the goal and the objectives of this work:

– The goal is to develop the mathematical model of VCR of *p-n* structures with QW with consideration of their parameters and location in SCR;

– The objectives are to experimentally define VCR properties common for all types of *p-n* LED structures, to substantiate the necessity of development of the mathematical model of VCR of *p-n* structures with non-uniform distribution of recombination centres in SCR, to define the dependence of the n^* factor and NF n on technological parameters of the *p-n* structure [1].

It was initially assumed that *p-n* structures of the LEDs under consideration are uniformly doped both in *p* and *n* regions, have a barrier layer with sharp boundaries, the Boltzmann distribution is true in the barrier region for free CCs, the levels of the recombination centres are located in the vicinity of the middle of the forbidden region and the capture cross-sections of electrons and holes are similar.

2. METHODOLOGY AND THE RESULTS OF THE EXPERIMENT

VCRs of blue and green QW LEDs based on *p-n* structures of *AlGaN/InGaN/GaN* manufactured by *Cree*, blue, green and red LEDs (*AlInGaP*-based) manufactured by *Lumileds* as well as white LEDs manufactured in China were obtained (these LEDs are identified in the experimental results below as A1, A3, CC and CW respectively). Each lot contained at least 10 LEDs and was selected from the same technological group. The experimental results
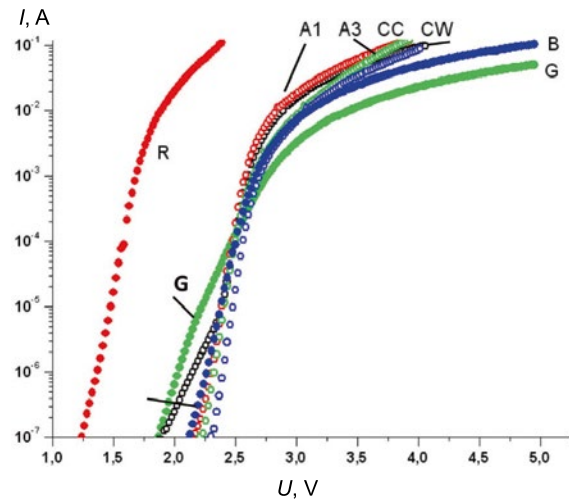

Fig. 1. VCRs of *Lumiled*'s red (*AlInGaP*-based) (*R*), green (*G*) and blue (*B*) LEDs as well as of the white LED with *AlGaN/InGaN/GaN* crystal structure (A1, A3, CC, CW) manufactured in China

presented in the Figs. (1–3) are not for all studied LEDs due to large volume of information, but the main characteristics conform to those presented in the work.

The LEDs used in the experiments had rather long exponential regions of VCRs within the current density range of $(10^{-4}-10^{-2})$ A/cm². Different characteristics if these LEDs, including VCRs, are studied in, for instance, [25, 26]. Measurements at lower values of current density were not conducted since probability of occurrence of creeping currents is high in this case: they would have provided a background addition to the classic generation-recombination mechanism of forward current of the LEDs under consideration.

VCRs of LEDs (Fig. 1) were measured by means of a computerised installation with stabilised bias voltage. Forward current varied within the range of $(10^{-7}-10^{-1})$ A and current density of $(10^{-4}-10^2)$ A/cm². Voltage increment was equal to (20 ± 0.01) mV. With such values of forward current density, the high injection level mode is not generated and a rather long exponential region is observed.

Moreover, in order to define the relationship between the form of VCR and distinctions of doping of *p-n* junction, doping profiles (Fig. 2) were measured for some types of LEDs using the technique and the installation described in [27]. Doping distri-

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[1] The objectives of the work did not include determination of the relation between NF *n* with creeping currents or loss currents through inner bridges of diode structures, consideration of series ohmic resistance of quasi-neutral regions and contacts and analysis of the high injection level mode; the work considered only the forward bias condition mode, the main mode of LED.

Fig. 2. Doping profiles of the lightly doped region of QW structures of *AlInGaP*-based red (*R*), green (*G*) and blue (*B*) LEDs manufactured by *Lumiled* as well as the white LED with *AlGaN/InGaN/GaN* crystal structure (A1, A3, CC, CW) manufactured in China

bution is measured starting from the metallurgical border in a relatively lightly doped region.

All measurements were made at room temperature of (23–25) °C. Thermal potential *kT* was taken equal to 0.0259 eV for measurements and modelling.

Processing of the experimental data and modelling of VCR were conducted using *MathCad-14* and *Origin-8* software.

Fig. 2 shows that the doping profiles in the lightly doped region of *p-n* structures are very variable while VCR forms of similar LEDs have almost no differences. In semi-log coordinates, it is possible to identify the long and almost linear regions of 2–4

Fig. 3. Model VCRs of blue (*B*) and green (*G*) LEDs based on *AlGaN/InGaNGaN* heterostructures with five QWs. The contour shows the regions of VCR corresponding to the experimental VCRs in Fig. 1, the inserts demonstrate corresponding dependences of NF *n* and factors n^* on bias voltage

magnitude orders of current with further significant deviation from exponential dependence at current density values higher than (1–2) A/cm². The formula (5) was used for calculation of *n*.

Increase in NF of the presented VCRs at current values exceeding the ones corresponding to the exponential region occurs due to different causes considered, for instance, in [28] as well as due to special phenomena, e.g. generation of a *p-n* junction of an accelerating electric field within the SCR, but these effects will not be reviewed in this article. The measurements have shown that exponential regions of different VCRs have significant variations of NF *n* and saturation current even within the same groups of LEDs.

3. RESULTS

The energy model of an asymmetrical structure, e.g. *p-n⁺* (with the *n* region heavily doped) may be presented in the form of a potential barrier with infinite length and height of φ_k. The front potential forming the SCR of the *p–n⁺*- junction in the lightly doped *p* layer rises in accordance with a certain law. In the direction of this barrier, a flow of electrons with a broad energy range moves from the quasi-neutral *n⁺*- region with thermal velocity V_T. The electrons with energy exceeding $(\varphi_k - qU)$ cross the SCR and move to the adjacent quasi-neutral *p*-type region. There they form diffusion current of minor CCs with its density at $qU > 3kT$ expressed as

$$J_{dif} = q \frac{L_n}{\tau_n} N_d \exp\left(-\frac{\varphi_k - qU}{kT}\right). \qquad (6)$$

Dividing and multiplying the right part by V_T and identifying $\frac{L_n}{\tau_n V_T}$ as r_d, let us write down the expression of the forward current of the diffusion mechanism in the form

$$J_{dif} = qr_d V_T N_d \exp\left(-\frac{\varphi_k - qU}{kT}\right) =$$

$$= qr_d V_T N_d \exp\left(-\frac{\varphi_k}{kT}\right) \exp\left(\frac{qU}{kT}\right) =$$

$$= J_0 \exp\left(\frac{qU}{kT}\right). \qquad (7)$$

It is Shockley's ideal VCR form with $n = n^* = 1$ over the entire voltage (current) range. With the ide-

$$F(U) = \int_{-x_n}^{x_p} \frac{1}{W(U)} \cdot \frac{f(x,U)\cdot \exp\left(-\dfrac{\varphi_k}{kT}\right)\left(\exp\left(\dfrac{qU}{kT}\right)-1\right)}{b\cdot \exp\left(-\dfrac{(\varphi_k - qU)}{W(U)\cdot kT}(x-x_n)\right) + \exp\left(-\left(\dfrac{(\varphi_k - qU) - \dfrac{(\varphi_k - qU)}{W(U)}(x-x_n)}{kT}\right)\right)+g}\,dx =$$

$$= \exp\left(\frac{-\varphi_k}{n^*\cdot kT}\right)\cdot \exp\left(\frac{qU}{n^*kT}-1\right), \tag{10}$$

al VCR, the multiplier J_o does not depend on bias voltage, therefore $n = n^*$.

The physical meaning of the factor r_d is the ratio of CC diffusion current velocity at the level of $(\varphi_k - qU)$ to thermal velocity; $J_0 = qr_dV_TN_d\exp\left(-\dfrac{\varphi_k}{kT}\right)$ is the density of saturation current. After reaching the front of the barrier,

CCs with energy lower than $(\varphi_k - qU)$ will recombine in accordance with the SNS model via the local recombination centres with holes moved to the SCR from the *p*-region. Total current will be equal to the sum of diffusion and recombination currents.

The SNS theory is applicable also to *p-n* structures with QW if the latter are presented in the form of recombination planes. Such idea was proposed in [20, 21].

In this work, we propose to assume that a thin QW located in any place of SCR serves as a single recombination centre with capture cross-section σ. Positions of QW in VCR and distribution of recombination centres of point defects in the barriers may be described by some function $N(x)$:

$$N(x) = N_t(x) + \sum_i \left|\begin{array}{l}0 \mapsto x < a_i \\ \dfrac{1}{H} \mapsto a_i \geq x \geq (a_i + H) \\ 0 \mapsto x > (a_i + H)\end{array}\right. , \tag{8}$$

where $N_t(x)$ is the concentration distribution of point defects, i is the QW number, H is the QW width, a is the location of the left edge of QW relative to the metallurgical border of the *p-n* structure.

Using the ideas of the SNS model, current density may be expressed by the formulae

$$J_{rec} = qb\sigma N_{tmd}(U)W(U)V_TN_dF(U), \tag{9}$$

where N_{tmd} *(U)* is the mean concentration of recombination centres of point defects and QW of the SCR which depends on bias voltage due to change of the SCR width and the number of QWs and point defects located in it:

$$N_{tmd}(U) = \frac{1}{W(U)}\int_{x_n}^{x_p}[N(x)]dx; \quad f(x,U) = \frac{N(x)}{N_{tmd}(U)};$$

$$x_n = -\frac{W(U)\cdot N_a}{N_d + N_a}, \quad x_p = \frac{W(U)\cdot N_d}{N_d + N_a},$$

$$W(U) = \sqrt{\frac{2\varepsilon\varepsilon_0(N_a + N_d)\cdot\left(\dfrac{\varphi_k}{q}-U\right)}{qN_aN_d}}\ , \text{(for uni-}$$

form doping distribution), N_a and N_d are the concentrations of acceptor and donor dopants, $b = N_d/N_a$, $g = 2n_i/N_a$.

Using the factor $r_r(U) = \sigma N_{tmd}(U)\cdot W(U)$, the formula (9) is written as

$$J_{rec} = qr_r(U)V_TN_d\exp\left(\frac{\varphi_k}{n^*(U)\cdot kT}\right)\times$$

$$\times\left(\exp\left(\frac{qU}{n^*(U)\cdot kT}\right)-1\right) =$$

$$= J_S(U)\left[\exp\left(\frac{qU}{n^*(U)\cdot kT}\right)-1\right]. \tag{11}$$

In the formula (10), there is an assumption that the front of the potential barrier increases linearly, therefore, it is identified as $\varphi(x) = \dfrac{(\varphi_k - qU)}{W(U)}(x_n - x)$,

$J_S(U) = qr_r(U)V_TN_d\exp\left(-\dfrac{\varphi_k}{n^*(U)\cdot kT}\right)$ in it. The

physical meaning of the factor r_r *(U)* is ratio of CC recombinant current at the level of $(\varphi_k - qU)/n^*$ to thermal velocity.

The factor n^* is defined using the formula

$$n^*(U) = -\frac{(\varphi_k - qU)}{kT}\left[\ln(F(U))\right]^{-1}.$$

Obviously, differentiation of (11) will provide the values of NF *n* higher than those of n^*. It is rather difficult to define n^* experimentally.

The function *f(x, U)* in (10) leads to variations of n^* from 1 to 2 and dependence of the pre-exponential factor on voltage leads to high values of NF *n*.

High values of NF, from 3.3 to 5, are common for *p-i-n* structures and with dependence of doping concentration at edges of SCR on variation of bias voltage, i.e. when N_a and N_d in the pre-exponential factor are the functions of bias voltage $N_a(U)$ and $N_d(U)$. This situation is real, since the doping concentration both in n^+ and *p* layers declines towards the metallurgical border virtually exponentially forming the compensated region in the vicinity of it (Fig. 2).

Unlike the cases with homogeneous *p-n* structures and uniform distribution of recombination centres, where recombination rate keeps its value after changes of SCR width, the situation is more difficult in structures with QWs. QWs keep their positions and the edge of SCR moves towards the metallurgical border with rise of voltage. The position of maximum recombination rate changes relative to QWs. This is related to variation of the growth rate of forward current with change in voltage, i.e. variations of NF *n* and n^* factor, as it can be seen from the figures in [13, 14].

In structures with multiple QWs, with $U = 0$, all QWs are located in the SCR. As forward voltage rises, part of QWs located closer to the edge of the SCR of the lightly doped layer leave the SCR and band-to-band recombination occurs in them due to diffusion current flowing in the quasi-neutral region where QWs are located. Therefore total current will be equal to the sum of these currents.

4. CONCLUSION

Based on the obtained mathematical models (9) and (10), using *Mathcad 14* VCR graphs were synthesised for different LEDs. The modelled VCRs of blue (*B*) and green (*G*) LEDs as well as dependences of NF *n* and factors n^* on voltage *U* for them are shown in Fig. 3. The width of QW is 4 nm; during their movement, it is equal to 15 nm and 16 nm for blue and green LEDs respectively. Doping level of the relatively lightly doped region was taken equal

to $7 \cdot 10^{18}$ cm^{-3} and that of the heavily doped region (injector) was taken equal to $2 \cdot 10^{19}$ cm^{-3}. The semiconductor parameters were taken from [29]. For modelling of VCR in the current limitation region within the range exceeding $1 \cdot 10^{-4}$ A, series resistance $R = 10$ Ω.

5. RESULTS

1. The physical and mathematical model of VCR of LED *p-n* structures with QW was developed. It is different from the SNS model in that it includes the function of non-uniform distribution of QWs and point defects in the SCR of the *p-n* structure *f(x, U)*.

2. In LED structures, QWs may be presented as single recombination centres distributed over the SCR, with capture cross-section σ. Recombination rate in QW is defined by the position of maximum distribution of recombination rate as per SNS relative to QW, and quantum efficiency is defined by the relation of rates of radiant and non-radiant components as per the *ABC* model.

3. The factor n^* in the VCR exponent and the derivative of the logarithm of current to voltage *n* (NF) are different terms. The former parameter reflects the difference of the exponential factor from the Shockley model and the latter characterises behaviour of the functional dependence of forward current on voltage.

4. The physical meaning of the factor n^* is ratio of the value of contact potential φ_k to the efficient level of energy of charge carriers flow to the recombination region in the SCR.

5. The NF values exceeding 2 are attributed to dependence of both the exponent and the pre-exponential factor on bias voltage.

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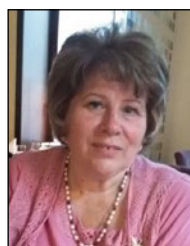
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