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Two-dimensional modeling of surface photovoltage in metal/insulator/*n*-GaN structure with cylindrical symmetry

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The rigorous numerical analysis of the surface photovoltage (SPV) versus excitation UV-light intensity (Φ), from 10^4 to 10^{20} photon/(cm^{2}s) in a metal/insulator/*n*-GaN structure with a negative gate voltage ($V_G = -2$ V) was performed using a finite element method. In the simulations we assumed a continuous U-shape density distribution function $D_{\rm it}(E)$ of the interface states and *n*-type doping concentration $N_D = 10^{16}$ cm^{-3}. The SPV signal was calculated and compared in three different characteristic regions at the interface, namely *i*) under the gate centre, *ii*) near the gate edge and *iii*) between the gate and ohmic contact. We attributed the differences in SPV(Φ) dependences to the influence of the interface states in terms of the initial band bending and interface recombination controlled by the gate bias. The obtained results are useful for the design of GaN-based UV-radiation photodetectors.

Keywords: surface photovoltage, gallium nitride, metal/insulator/semiconductor (MIS) structure, interface states, photodetector.

1. Introduction

Passivated structures of gallium nitride (insulator/GaN) are largely implemented in various optoelectronic and microelectronic devices, like laser diodes, photodetectors and high-power transistors [1] due to GaN unique optical, electrical and thermal properties. However, device efficiency and lifetime is strongly limited by different point defects in GaN layer bulk and high-density electronic states at the insulator–GaN interface. In order to better understand and control the operation of GaN-based optoelectronic elements, the rigorous numerical modeling of light-generated non-equilibrium effects is necessary, including the changes in the surface potential (surface photovoltage, SPV) and the surface recombination, taking into account both bulk structural defects and interface states. It should be pointed out that in the standard approaches the photo-effect calculations are usually limited to the models assuming simplified interface state density distribution (discrete or uniform one) [2, 3].

In this work we performed a rigorous numerical analysis of the surface photovoltage (SPV) versus excitation UV-light intensity in metal/insulator/*n*-GaN (MIS) structures with a cylindrical symmetry using two-dimensional (2D) drift-diffusion model. The considered symmetry is standard for MIS microdiodes implemented as photodetectors. Usually, one-dimensional approach is applied to studies of these structures but more exact calculations are required to understand better the electronic properties of a biased MIS under illumination, in particular the radial distribution of the interface potential. In the performed calculations, we assumed *n*-type doping with a concentration $N_D = 10^{16}$ cm^{-3} and continuous U-shape density distribution function $D_{\text{it}}(E)$ of the interface states. Their density minimum value D_{it0} varied from 1×10^{11} to 5×10^{12} cm^{-2}eV^{-1}. The excitation UV-light intensity (Φ) was changed in a wide range from 10^4 to 10^{20} photon/(cm^{2}s), the negative gate voltage (V_G) was equal to –2 V. The simulations of SPV were carried out for three different characteristic regions at the interface, namely 1 – under the gate centre, 2 – near the gate edge and 3 – between the gate and ohmic contact. We attributed the differences in SPV(Φ) dependences to the influence of the interface states in terms of the non-radiative interface recombination and gate-controlled initial band bending. The calculations were realized by means of a finite element method implemented in an original numerical program. The obtained results of SPV simulations are particularly useful for the design of MIS GaN-based UV-radiation photodetectors.

2. Numerical simulation procedure

The calculations of the SPV(Φ) dependences were performed for an UV-illuminated (λ = 325 nm) and biased (V_G = –2 V) metal–Al_2O_3–GaN structure shown in Fig. 1**a**. The following geometrical parameters of the analyzed cylindrical structure were assumed: the insulator layer thickness of 60 nm, *n*-GaN layer thickness of 10 μm, the ratio of the circular gate diameter to ohmic contact inner diameter of 0.5 (in the micrometer distance range).

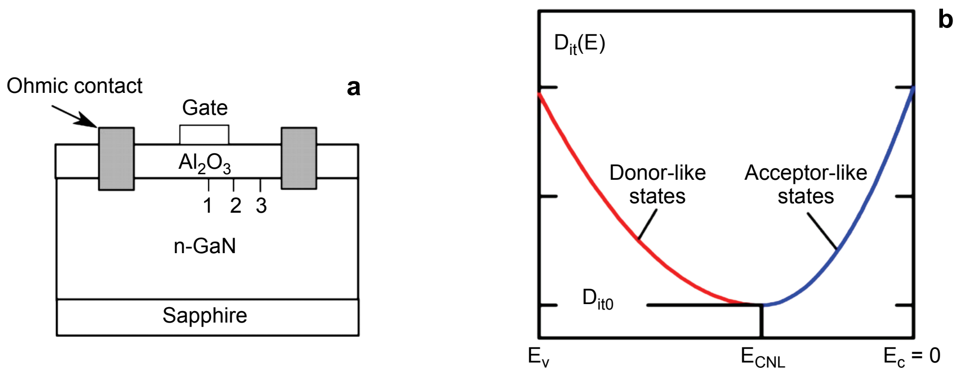

Fig. 1. Scheme of the simulated cylindrical metal–Al_2O_3–GaN structure (**a**) and assumed interface state density distribution $D_{\text{it}}(E)$ (**b**).

For 2D solving of the drift-diffusion equations for electrons and holes in a biased MIS structure under non-equilibrium conditions we used a finite element method and original numerical program implemented through a COMSOL Multiphysics package. We took into account all bulk recombination channels, *i.e.*, band-to-band, Shockley–Read–Hall (SRH) via deep levels, and Auger one as well as SRH interface recombination through the interface state continuum. As a result we obtained the in-depth and spacial distributions of the electric potential and carrier concentrations. The assumed GaN bulk electronic parameters, as summarized in Table 1, were taken from Ref. [1, 4].

T a b l e 1. Electronic parameters assumed in calculations [1, 4].

Bandgap E_g [eV]	3.4
Bimolecular recombination constant B [cm^3/s]	10^8
SRH lifetime τ [s]	10^{-7}
Electron mobility μ_n [$cm^2/(Vs)$]	300
Hole mobility μ_p [$cm^2/(Vs)$]	10
Al_2O_3 dielectric constant ε	8

For the boundary conditions at the insulator–GaN interface in terms of the interfacial electrical field and non-radiative recombination rate we implemented the disorder-induced gap state (DIGS) model [5], which assumes the quasi-amorphous structure of the interfacial region, and thus exponential decay of the interface state density from the bandgap edges towards the midgap. Therefore, the U-shaped $D_{it}(E)$ function (Fig. 1**b**) was expressed by the following formula [5]:

$$D_{it}(E) = D_{it0} \exp\left(\frac{|E - E_{CNL}|}{E_{0d,\,a}}\right)^{n_{d,\,a}} \tag{1}$$

where D_{it0} is the minimum density of interface states, E_{CNL} is the so-called charge neutrality level, located approximately 2.1 eV below the conduction band minimum (E_c), E_{0d}, n_d and E_{0a}, n_a describe the curvature of donor-like and acceptor-like branch of the $D_{it}(E)$ curve below and above E_{CNL}, respectively. The DIGS-related interface recombination rate (U_S) was expressed by the formula taken from the SRH model generalized to the continuous energetic distribution of interface states, $D_{it}(E)$:

$$U_S = \int_{E_v}^{E_c} \frac{\sigma_n \sigma_p v_n v_p \left(n_s p_s - n_i^2\right) D_{it}(E)\, \mathrm{d}E}{\sigma_n v_n \left[n_s + n_1(E)\right] + \sigma_p v_p \left[p_s + p_1(E)\right]} \tag{2}$$

where E_v is the top of the valence band, E_c is the bottom of the conduction band, σ_n and σ_p are the interface state cross-sections for capturing electrons and holes, respectively, v_n and v_p are the thermal velocities of electrons and of holes, respectively,

and n_s and p_s are the interface concentrations of electrons and holes, respectively. The parameters $n_1(E)$ and $p_1(E)$ can be interpreted as densities of electrons and of holes, respectively, in the non-degenerated semiconductor, when the Fermi level equals E.

3. Results and discussion

The results of the SPV simulations versus Φ for various minimum interface state densities D_{it0}, at different interface regions marked 1, 2 and 3 (MIS structure shown in Fig. 1**a**) are summarized in Fig. 2. In the case of regions 1 and 2 (Figs. 2**a** and 2**b**), where the gate field controls the interface, almost all SPV(Φ) dependences are monotonic and logarithmic ones. On the contrary, in the region 3, where the gate field influence is strongly reduced, under weak excitation the SPV(Φ) curves exhibit linear dependence changing into logarithmic one under stronger Φ (Fig. 2**c**). No saturation of the SPV signal is noticeable for higher Φ due to the contribution of the Dember photovoltage [6]. One can also find that SPV reaches the largest values of about 1.2 V

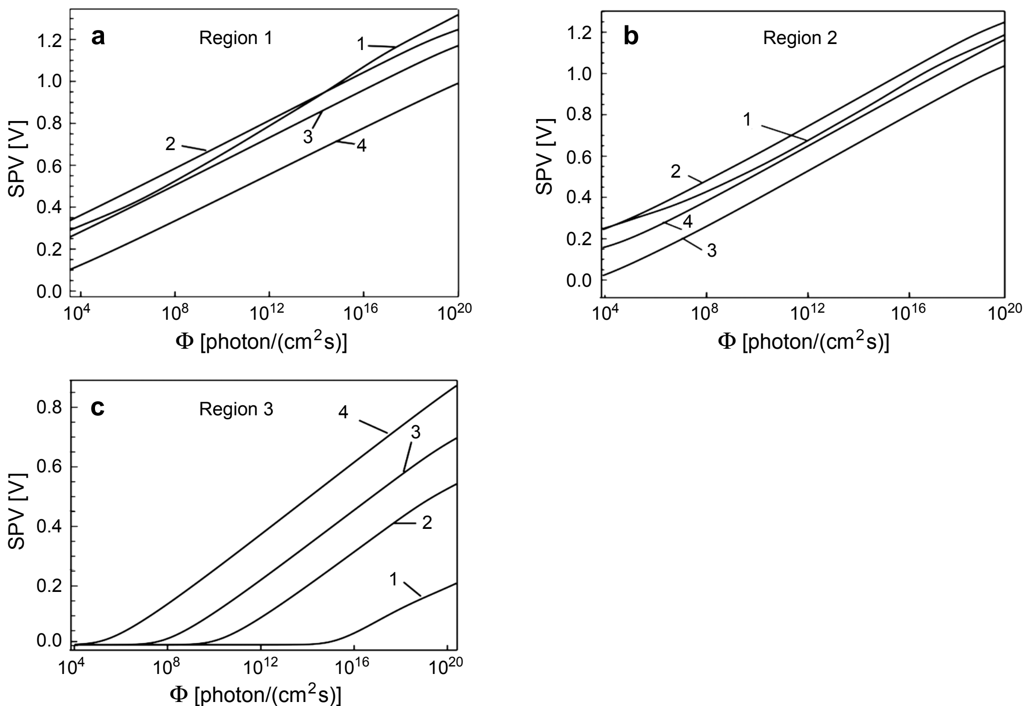

Fig. 2. Surface photovoltage versus excitation light intensity for various minimum interface state densities D_{it0} equal to 1×10^{11} cm^{-2}eV^{-1} (curve 1), 5×10^{11} cm^{-2}eV^{-1} (curve 2), 1×10^{12} cm^{-2}eV^{-1} (curve 3) and 5×10^{12} cm^{-2}eV^{-1} (curve 4), for different three regions of the MIS structure shown in Fig. 1**a**: under the gate centre (**a**), near the gate edge (**b**) and between the gate and ohmic contact (**c**).

near the gate centre (region 1), whereas far from the gate (region 3) only of 0.8 V. This is related to the enhancement of the depletion layer in GaN upon negative MIS structure bias, which results in the larger changes of the interface band bending upon illumination.

Furthermore, an interesting finding is that the bias voltage V_G changes completely the relationship among SPV(Φ) curves corresponding to different D_{it0} values in the region 1 in comparison with the region 3 (region 2 is intermediate between those two ones). Namely, in the region 1 the highest SPV was obtained for the lowest $D_{it0} = 1\times10^{11}$ cm^{-2}eV^{-1}, whereas in the region 3 the same value of D_{it0} corresponds to the smallest SPV because of the lowest dark band bending compared to that induced by $D_{it0} = 5\times10^{12}$ cm^{-2}eV^{-1}. We attribute this opposite behavior of SPV(Φ) dependences against D_{it0} to the dramatic reduction (by 3 orders of magnitude) of the interface recombination rate upon negative bias V_G, which causes the electron depopulation of the acceptor-like interface states and capturing photo-holes by deep donor-like ones. Such condition of non-symmetric concentrations of electrons and holes causes non-effective SRH recombination through the interface states [7]. Therefore, in the gate-controlled region 1 the SPV signal is limited by the interface recombination whereas in the region 3 by the initial band bending induced by ionized acceptors.

4. Conclusions

From the rigorous 2D numerical analysis we proved that the *n*-GaN MIS structure is extremely sensitive to UV illumination in terms of SPV, which can be effectively controlled by the negative gate voltage. The quality of the insulator–GaN interface (in terms of the interface state density D_{it}) and structure bias V_G determine two ranges of different SPV behavior versus excitation intensity. The logarithmic character of SPV(Φ) dependences is advantageous for quantitative Φ-resolved detection of both low and high intensity UV radiation.

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