SIMULATION OF LEAKAGE CURRENT IN AlGaN/GaN HETEROSTRUCTURES WITH A NEW MODEL OF TRAP-ASSISTED TUNNELLING

Juraj Racko[1], Peter Benko[1], Alena Grmanová[1], Ladislav Harmatha[1], Ralf Granzner[2], Mario Kittler[2], Frank Schwierz[2] and Juraj Breza[1]

[1]*Slovak University of Technology, Bratislava, Slovakia*
[2]*Ilmenau University of Technology, Ilmenau, Germany*
E-mail: juraj.racko@stuba.sk

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1. Electro-physical model of the heterostructure

The approach is based on solving the Poisson and continuity equations. The Poisson equation can be written as

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(\kappa(x)\frac{\mathrm{d}\psi(x)}{\mathrm{d}x}-Q_{\mathrm{tot}}(x)\right)=q\left(p(x)-n(x)+N^{\mathrm{D}+}(x)-N^{\mathrm{A}-}(x)+N_{\mathrm{t}}^{\mathrm{D}+}(x)-N_{\mathrm{t}}^{\mathrm{A}-}(x)\right), \quad (1)$$

where κ is the permittivity, ψ is the electric potential, Q_{tot} is the sheet bound interface charge due to spontaneous and piezoelectric polarization at the AlGaN/GaN interface, n and p are concentrations of free charge carriers, $N^{\mathrm{D}+}$ and $N^{\mathrm{A}-}$ are concentrations of shallow ionized donors and acceptors, and $N_{\mathrm{t}}^{\mathrm{D}+}$ and $N_{\mathrm{t}}^{\mathrm{A}-}$ are concentrations of deep ionized donors and acceptors expressed as

$$N_{\mathrm{t}}^{\mathrm{D}+}(x)=\int_{E_{\mathrm{V}}(x)}^{E_{\mathrm{C}}(x)}\left(1-f_{\mathrm{t}}\,(\varepsilon_{\mathrm{t}},x)\right)D_{\mathrm{t}}(\varepsilon_{\mathrm{t}},x)\mathrm{d}\varepsilon_{\mathrm{t}}\,, \qquad N^{\mathrm{i\,A}-}(x)=\int_{E_{\mathrm{V}}(x)}^{E_{\mathrm{C}}(x)}f_{\mathrm{t}}\,(\varepsilon_{\mathrm{t}},x)D_{\mathrm{t}}(\varepsilon_{\mathrm{t}},x)\mathrm{d}\varepsilon_{\mathrm{t}}\,.$$

(2, 3)

Here, E_{t} is the trapping level in the forbidden band of the semiconductor (of either donor or acceptor type), f_{t} is the occupation probability of trapping centres lying at energy levels ε_{t} (see the TAT model below), and the multiphonon distribution functions of trapping centres D_{t} belonging to the trapping level E_{t} is given as [1-3]

$$D_{\mathrm{t}}(\varepsilon_{\mathrm{t}},x)=\frac{1}{S\hbar\omega_0}\frac{N_{\mathrm{t}}}{\sqrt{2\pi}}\frac{(\theta\mp S)^2}{\left(\theta^2+z^2\right)^{\frac{1}{4}}}\exp\left(\sqrt{z^2+\theta^2}-\theta\ln\left(\frac{\theta}{z}+\sqrt{1+\left(\frac{\theta}{z}\right)^2}\right)-S\left(2f_{\mathrm{B}}+1\right)-\frac{\hbar\omega_0\,\theta}{2kT}\right), \quad (4)$$

where S is the Huang-Rhys factor representing the strength of electron-phonon coupling, $\hbar\omega_0$ is the effective phonon energy, $\theta=\frac{|\varepsilon_{\mathrm{t}}-E_{\mathrm{t}}|}{\hbar\omega_0}$, $f_{\mathrm{B}}=\left(\exp\left(\frac{\hbar\omega_0}{kT}\right)-1\right)^{-1}$ is the Bose distribution function, and $z=2S\sqrt{f_{\mathrm{B}}(1+f_{\mathrm{B}})}$. The sign inside the bracket in the nominator is negative for $\varepsilon_{\mathrm{t}}>E_{\mathrm{C}}(x)-E_{\mathrm{t}}$ and positive for $\varepsilon_{\mathrm{t}}<E_{\mathrm{C}}(x)-E_{\mathrm{t}}$.

The continuity equation for electrons (the hole component is neglected) is expressed as

$$-\frac{\mathrm{d}}{\mathrm{d}x}\mu^{\mathrm{e}}(x)\left(n(x)\frac{\mathrm{d}\psi^{\mathrm{e}}(x)}{\mathrm{d}x}-\frac{kT}{q}\frac{\mathrm{d}n(x)}{\mathrm{d}x}\right)=\frac{\mathrm{d}}{\mathrm{d}x}\int_{E_{c\min}}^{E_{c\max}}\int_{x_0}^{x}\left(\frac{1-f_{\mathrm{t}}\,(\varepsilon_{\mathrm{t}},x)}{\tau_{\mathrm{e\,R_{right}}}^{\mathrm{TUN}}}-\frac{f_{\mathrm{t}}\,(\varepsilon_{\mathrm{t}},x)}{\tau_{\mathrm{e\,G_{right}}}^{\mathrm{TUN}}}\right)D_{\mathrm{t}}\,\mathrm{d}x_{\mathrm{t}}\mathrm{d}\varepsilon_{\mathrm{t}}\,, \quad (5)$$

where $\tau_{\mathrm{e\,R_{right}}}^{\mathrm{TUN}}$ and $\tau_{\mathrm{e\,G_{right}}}^{\mathrm{TUN}}$ are the tunnelling exchange times (see TAT model). The electron effective electric potentials ψ^{e} is

$$\psi^{\mathrm{e}}(x)=\psi(x)+\frac{\Delta E_{\mathrm{c}}(x)}{q}+\frac{kT}{q}\ln\left(\frac{\mathrm{N_c}(x)}{\mathrm{N_c}\left(\mathrm{x_{GaN}}\right)}\gamma^{\mathrm{e}}(x)\right). \quad (6)$$

In these expressions ΔE_c is the electron band offset.

2. Model of trap assisted tunnelling

The currents of free charge carriers flowing into and out of the traps are defined in terms of respective 12 exchange times. The reciprocal value of the exchange time represents the repetition frequency with which a particular process contributes to the occupation of the trap by electrons. The advantage of this concept is in simply calculating the occupation probability of trapping centres. The exchange times are defined as

$$1/\tau_{\mathrm{e\,R}}^{\mathrm{TH}}(x_t) = v_e^{\mathrm{th}}\sigma_e n(x_t), \qquad 1/\tau_{\mathrm{e\,G}}^{\mathrm{TH}}(\varepsilon_t, x_t) = v_e^{\mathrm{th}}\sigma_e N_C \exp\left((\varepsilon_t - E_c(x_t))/kT\right), \qquad (7, 8)$$

$$1/\tau_{\mathrm{h\,R}}^{\mathrm{TH}}(x_t) = v_h^{\mathrm{th}}\sigma_h p(x_t), \qquad 1/\tau_{\mathrm{h\,G}}^{\mathrm{TH}}(\varepsilon_t, x_t) = v_h^{\mathrm{th}}\sigma_h N_V \exp\left((E_v(x_t) - \varepsilon_t)/kT\right), \qquad (9, 10)$$

$$1/\tau_{\mathrm{e,h\,R\ right/left}}^{\mathrm{TUN}}(\varepsilon_t, x_t, x_{\mathrm{e,h\ right/left}}) = f_{\mathrm{e,h}}^{\mathrm{FD}}(x_{\mathrm{e,h\ right/left}})\frac{m_{\mathrm{e,h}}^{\mathrm{R}}\sigma_{\mathrm{e,h}}}{2\pi^2\hbar^3}(\Delta E_x)^2\sum_{j=0}^{N}(j+1)\Gamma_{\mathrm{e,h\ right/left}}^{j}, \qquad (11)$$

$$1/\tau_{\mathrm{e,h\,G\ right/left}}^{\mathrm{TUN}}(\varepsilon_t, x_t, x_{\mathrm{e,h\ right/left}}) = \left(1 - f_{\mathrm{e,h}}^{\mathrm{FD}}(x_{\mathrm{e,h\ right/left}})\right)\frac{m_{\mathrm{e,h}}^{\mathrm{R}}\sigma_{\mathrm{e,h}}}{2\pi^2\hbar^3}(\Delta E_x)^2\sum_{j=0}^{N}(j+1)\Gamma_{\mathrm{e,h\ right/left}}^{j}, \qquad (12)$$

where $f_{\mathrm{e,h}}^{\mathrm{FD}}$ are the Fermi-Dirac distribution functions for electrons and holes, $m_{\mathrm{e,h}}^{\mathrm{R}}$ are the effective electron and hole masses for calculating the Richardson constant in the semiconductor, ΔE_x is an energy increment chosen by a reasonable compromise between the time of computation and calculation accuracy. Summation of the series terminates, when the ratio of the exponential term $\Gamma_{\mathrm{e,h\ right/left}}^{j}$ for $j=N$ to that for $j=0$ is smaller than a chosen accuracy, e.g., $\Gamma_{\mathrm{e,h\ right/left}}^{j=N}/\Gamma_{\mathrm{e,h\ right/left}}^{j=0} < 10^{-6}$ The electron and hole tunnelling probability is calculated from the WKB approximation as

$$\Gamma_{\mathrm{e,h\ right/left}}^{j}(x_t, \varepsilon_t) = \exp\left(-\frac{\sqrt{8m_{\mathrm{e,h}}^{\mathrm{TUN}}}}{\hbar}\int_{x_t}^{x_{\mathrm{right/left}}}\sqrt{\left|E_{\mathrm{c,v}}(x) - \varepsilon_t + j\Delta E_x\right|}\,\mathrm{d}x\right), \qquad (13)$$

where $m_{\mathrm{e.h}}^{\mathrm{TUN}}$ are the effective tunnelling masses of electrons and holes. The occupation probability of trapping centres is then calculated as

$$f_t = \frac{\frac{1}{\tau_{\mathrm{e\,R}}^{\mathrm{TH}}} + \frac{1}{\tau_{\mathrm{e\,R_{right}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{e\,R_{left}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{h\,G}}^{\mathrm{TH}}} + \frac{1}{\tau_{\mathrm{h\,G_{right}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{h\,G_{left}}}^{\mathrm{TUN}}}}{\frac{1}{\tau_{\mathrm{e\,R}}^{\mathrm{TH}}} + \frac{1}{\tau_{\mathrm{e\,R_{right}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{e\,R_{left}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{h\,G}}^{\mathrm{TH}}} + \frac{1}{\tau_{\mathrm{h\,G_{right}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{h\,G_{left}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{e\,G}}^{\mathrm{TH}}} + \frac{1}{\tau_{\mathrm{e\,G_{right}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{e\,G_{left}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{e\,G}}^{\mathrm{TH}}} + \frac{1}{\tau_{\mathrm{e\,G_{right}}}^{\mathrm{TUN}}} + \frac{1}{\tau_{\mathrm{e\,G_{left}}}^{\mathrm{TUN}}}}$$

3. Simulations

The model was employed to simulate metal/GaN/$\mathrm{Al}_x\mathrm{GaN}_{1-x}$/GaN Schottky hetero-structures. The vertical geometry of the structure along with the concentration profile of ionized shallow donors $N^{\mathrm{D+}}(x)$ is given in Tab. 1.

Tab. 1. *Vertical geometry of the simulated structure.*

	Cover GaN	Doped AlGaN	Undoped GaN	Doped GaN
Thickness (nm)	10	10	30	10
$N^{\mathrm{D+}}$ (cm^{-3})	-	10^{18}	-	10^{17}

The concentration of traps was assumed to be $N_t=5\times10^{17}\ \mathrm{cm}^{-3}$ at energy level E_t placed 0.5 eV below the conduction band, and a Schottky barrier height $\phi_b = 0.86$ eV. We considered

the Huang-Rhys factor S=4.2 and effective phonon energy $\hbar\omega_0$=0.032 eV. The effective cross section of the traps was set constant σ_t=1.5×10^{-13} cm^2.

The molar concentrations of aluminium in the GaN cover and in the doped AlGaN layer were simulated by error functions, see Fig. 1. The assumed Al distribution determines all other parameters. Non-linear dependences of Q_{tot}, ΔE_c and ΔE_g on the concentration of Al were simulated in accordance with [4-6]. The shape of the band gap strongly affects the interface charge Q_{tot} as shown in Fig. 1. The dependences of ΔE_c and ΔE_g on the concentration of Al are shown in Fig. 2. Other parameters, such as relative dielectric constant κ, effective electron density of states N_c, longitudinal effective electron mass in the central (Gamma) valley m_e^T depend on Al concentration only weakly. For calculating the tunnelling exchange times effective masses $m_e^R = m_e^T = 0.2\ m_0$ were used.

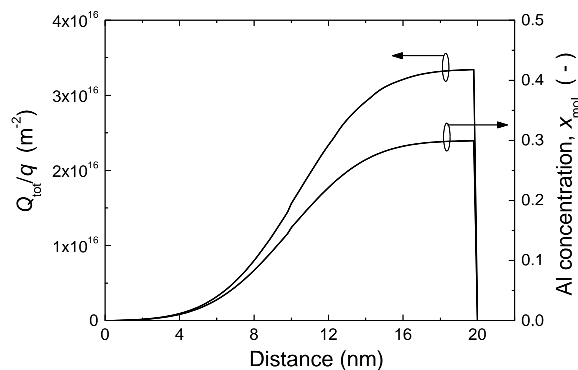

Fig. 1. *Molar concentration of aluminium and the sheet bound interface charge* Q_{tot} *in the* GaN *cover and in the doped* AlGaN *layer.*

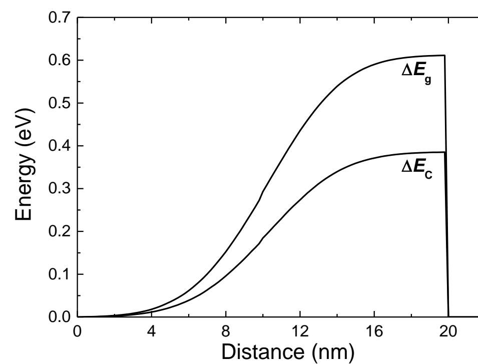

Fig. 2. *Band offset* ΔE_c *and band gap* ΔE_g *in the* GaN *cover and in the doped* AlGaN *layer.*

Figure 3 shows the band diagram of the structure in thermodynamic equilibrium taking into account the distribution of Al in the structure. Corresponding distributions of free electrons and ionized deep traps are shown in Fig. 4.

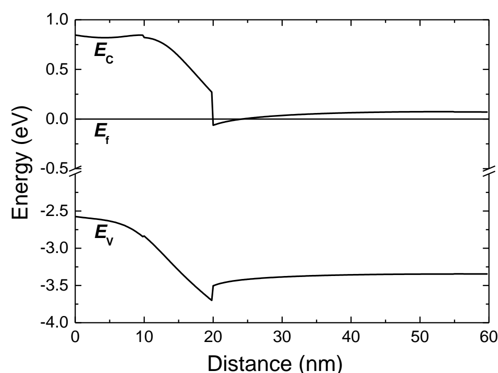

Fig. 3. *The band gap diagram of the structure in thermodynamic equilibrium.*

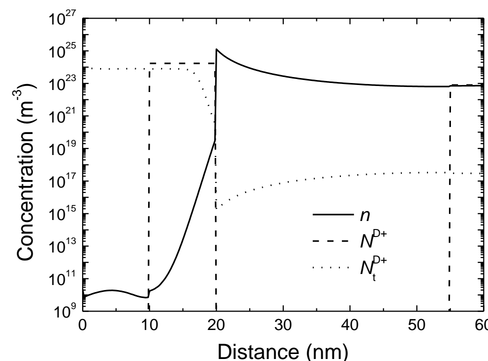

Fig. 4. *Distribution of free electrons, n, ionized donors,* N^{D+}*, and deep traps,* N_t^{D+}.

On applying a reverse voltage on the structure we have simulated the current density, see Fig. 5. The total current consists of two components: the trap-assisted current, TAT, and the drift-diffusion current at the metal/GaN interface. The graph shows very good agreement between the measured and simulated currents. Finally, Fig. 6 shows the simulated tunnelling and drift-diffusion currents in the structure at reverse voltage V_a=1.2 V.

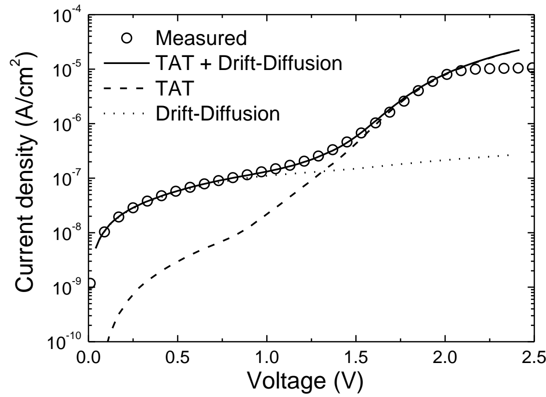

Fig. 5. *Comparison of measured and simulated I-V curves.*

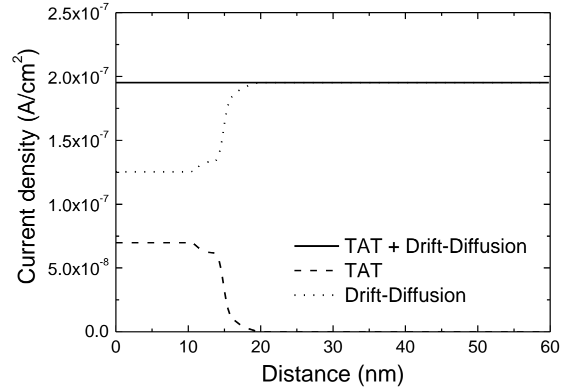

Fig. 6. *Tunnelling and drift-diffusion currents in the structure at applied reverse voltage* V_a=1.2 V.

4. Discussion

Simulation of the currents flowing through the heterostructure has confirmed that they are strongly affected by the distribution of Al in the structure. The step-wise interface between the cover GaN layer and the doped AlGaN layer brings about a roof-shaped of the band diagram in thermodynamic equilibrium, which in turn yields considerably smaller values of currents than those observed experimentally. Therefore it will be useful to analyse the distribution of Al at the heterojunctions by means of analytical techniques, such as SIMS or AES.

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