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A model of trap-assisted tunneling in GaN/AlGaN/GaN heterostructure based on exchange times

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ABSTRACT

The work presents a physical model of trap-assisted tunneling that can quantitatively determine the effect of traps upon the total current through a GaN/AlGaN/GaN heterostructure. The model is based on expressing the occupation probability of the trapping centers by electrons in terms of thermal and tunneling exchange times. The occupation probabilities calculated in this way are then used to work out the generation–recombination rates occurring in the continuity equations. This allowed us to simulate *I–V* curves of the structure with disabled and enabled trap-assisted tunneling and to verify the sensitivity of the model to the effective phonon energy. Although the model is proposed and tested for a particular structure, it is more general and can be applied to other structures as well.

1. Introduction

The efforts to explain the charge transport in thin MOS and MIM structures led to the development of various models of trap-assisted tunneling (TAT) [1–6]. Many of them had been implemented in simulators of semiconductor structures and devices [7,8]. Among the numerous models, specific position belongs to those of TAT in semiconductor heterostructures [9–12]. In the present work we describe a novel model of TAT based on the idea of exchange times characterizing the kinetics of thermal and tunneling exchange processes.

AlGaN/GaN heterostructures contain numerous deep trapping levels in the forbidden band of the semiconductor. Each of these levels has its specific density and effective cross-section the trapping centers. These centers may capture and emit free charge carriers from/to the conduction and valence bands not only due to thermal exchange processes but also due to tunneling.

Trap-assisted tunneling of free charge carriers has a higher probability in the case of multiphonon excitation of the deep traps. Due to the interaction of phonons with electrons localized at the trap the single deep level splits into a set of discrete levels. Their density is described by the multiphonon distribution function.

The high density of traps created during the growth of GaN/AlGaN/GaN layers enables the transport of free charge carriers through the structure. On applying an external voltage this leads to a high leakage current.

The presented model of TAT is based on expressing the occupation probability of the trapping centers by electrons in terms of thermal and tunneling exchange times. The occupation probabilities calculated in this way are then used to obtain the generation–recombination rates occurring in the continuity and Poisson equations. The model takes into account the changes in the band diagrams caused by charges at the heterointerfaces depending on the aluminum content in the ternary compound. The outcome are simulated *I–V* curves with both disabled and enabled tunneling exchange processes. Finally, we present the sensitivity of the designed TAT model to the chosen effective phonon energy $\hbar\omega_0$, which is the only fitting parameter of our model. Although the model is proposed for the GaN/AlGaN/GaN structure, it is more general and can be applied to other structures as well.

2. Theory of trap-assisted tunneling

The studied structure and considered electron and hole, thermal and tunneling exchange processes are shown in Fig. 1.

Tunneling of free charge carriers between the trap and the conduction or valence band becomes more pronounced due to the assistance of phonons causing that instead of a single deep trapping level E_t with trap density N_t in the forbidden band of the

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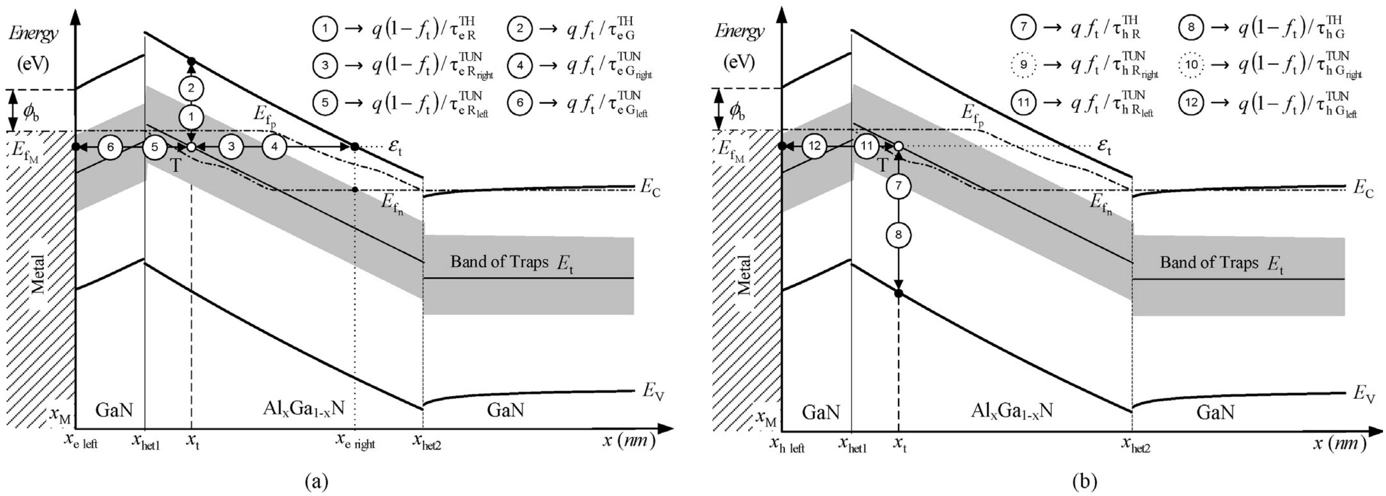

Fig. 1. Electron (a) and hole (b) capture and emission currents considered in the model of trap-assisted tunneling in a reverse biased metal/GaN/$Al_xGa_{1-x}N$/GaN heterostructure.

semiconductor one has to consider a set of trapping levels ε_t described by distribution function D_t. Calculation of the multiphonon distribution function is based on the multiphonon transition probability [8]

$$M(\varepsilon_t, x_t) = \frac{1}{\sqrt{2\pi S}} \frac{\left(\theta \mp S\right)^2}{\left(\theta^2 + z^2\right)^{\frac{1}{4}}}$$

$$\exp\left(\sqrt{z^2+\theta^2} - \theta \ln\left(\frac{\theta}{z} + \sqrt{1+\left(\frac{\theta}{z}\right)^2}\right) - S(2f_B+1) - \theta\frac{\hbar\omega_0}{2kT}\right), \qquad (1)$$

where S is the Huang–Rhys factor representing the strength of electron–phonon coupling, $\hbar\omega_0$ is the effective phonon energy and $S\hbar\omega_0$ is the Franck–Condon shift (the lattice relaxation energy), and $f_B = (\exp(\hbar\omega_0/kT) - 1)^{-1}$ is the Bose distribution function. Further, these abbreviations have been used in Eq. (1): $z = 2S\sqrt{f_B(1+f_B)}$ and $\theta = |\varepsilon_t - E_t(x_t)|/(\hbar\omega_0)$. The sign inside the bracket in the nominator in Eq. (1) is negative for energies ε_t lying below the basic level E_t and positive for energies ε_t lying above the basic level. The Huang–Rhys factor S and the effective phonon energy $\hbar\omega_0$ are material parameters. The effective phonon energy $\hbar\omega_0$ is responsible for broadening of the distribution function. The lower the effective phonon energy $\hbar\omega_0$, the broader the multiphonon function and the phenomenon of TAT is stronger. The distribution function is described as

$$D_t(\varepsilon_t, x_t) = \frac{N_t}{\hbar\omega_0} M(\varepsilon_t, x_t). \qquad (2)$$

The model of TAT takes into account exchanges of free charge carriers (electrons and holes) between the trapping centers lying in the forbidden band of the semiconductor and their surroundings. Under the surroundings one should understand the conduction band from the top, the valence band from the bottom and the metal from the sides as shown in Fig. 1. The exchange processes create the currents of electrons and holes flowing from the traps into the surroundings and vice versa. The currents of free charge carriers flowing into and out of the trap are defined in terms of respective 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. Naturally, the sum of currents of free charge carriers flowing into the trap is equal to the sum of currents flowing out of the trap. From this condition we can calculate the probability of electron occupation of the trap f_t.

The sums of three electron currents flowing into and out of the trap are expressed in terms of aggregate exchange times (see Fig. 1a) denoted by abbreviations τ_e^{ESCAPE} and $\tau_e^{CAPTURE}$:

$$\frac{q(1-f_t)}{\tau_e^{CAPTURE}} \equiv q(1-f_t)\left(\frac{1}{\tau_{e\,R}^{TH}} + \frac{1}{\tau_{e\,R_{right}}^{TUN}} + \frac{1}{\tau_{e\,R_{left}}^{TUN}}\right) \qquad (3)$$

and

$$\frac{qf_t}{\tau_e^{ESCAPE}} \equiv qf_t\left(\frac{1}{\tau_{e\,G}^{TH}} + \frac{1}{\tau_{e\,G_{right}}^{TUN}} + \frac{1}{\tau_{e\,G_{left}}^{TUN}}\right). \qquad (4)$$

Similarly, the sums of three hole currents flowing into and out of the trap are written in terms of aggregate exchange times (see Fig. 1b) τ_h^{ESCAPE} and $\tau_h^{CAPTURE}$:

$$\frac{qf_t}{\tau_h^{CAPTURE}} \equiv qf_t\left(\frac{1}{\tau_{h\,R}^{TH}} + \frac{1}{\tau_{h\,R_{right}}^{TUN}} + \frac{1}{\tau_{h\,R_{left}}^{TUN}}\right) \qquad (5)$$

and

$$\frac{q(1-f_t)}{\tau_h^{ESCAPE}} \equiv q(1-f_t)\left(\frac{1}{\tau_{h\,G}^{TH}} + \frac{1}{\tau_{h\,G_{right}}^{TUN}} + \frac{1}{\tau_{h\,G_{left}}^{TUN}}\right). \qquad (6)$$

In Eqs. (3)–(6), the four electron and hole thermal capture (subscript R) and emission (subscript G) exchange times are defined as

$$\frac{1}{\tau_{e\,R}^{TH}(x_t)} = \nu_e^{th}\sigma_e n(x_t), \qquad (7)$$

$$\frac{1}{\tau_{e\,G}^{TH}(\varepsilon_t, x_t)} = \nu_e^{th}\sigma_e N_C \exp\left(\frac{\varepsilon_t - E_c(x_t)}{kT}\right), \qquad (8)$$

$$\frac{1}{\tau_{h\,R}^{TH}(x_t)} = \nu_h^{th}\sigma_h p(x_t), \qquad (9)$$

$$\frac{1}{\tau_{h\,G}^{TH}(\varepsilon_t, x_t)} = \nu_h^{th}\sigma_h N_V \exp\left(\frac{E_v(x_t) - \varepsilon_t}{kT}\right), \qquad (10)$$

where $\sigma_{e,h}$ are the effective trap cross-sections for electrons and holes, and $\nu_{e,h}^{th}$ are thermal velocities of charge carriers [13–15].

Besides thermal exchange processes, the trapping center may exchange electrons and holes with the surrounding structures also by quantum-mechanical tunneling. The energy level ε_t passing through the trapping center defines two points in the band diagram, left and right from the trap x_t, $x_{e,h\,left}$ and $x_{e,h\,right}$, see Fig. 1.