DERIVATION OF THE TUNNELLING EXCHANGE TIME FOR THE MODEL OF TRAP-ASSISTED TUNNELLING

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Received 07 May 2014; accepted 25 May 2014

1. Introduction

We present derivation of the tunnelling exchange times that play the key role in the model of trap assisted tunnelling (TAT) considering the electron and hole exchange processes between the trapping centre lying in the forbidden band of the semiconductor and the conduction band, valence band or a metal (Fig. 1). All exchange processes are quantitatively described by respective exchange times. The reciprocal values of these exchange times represent the frequency with which the exchange processes contribute to the probability of occupation of the trap by free charge carriers. The crucial problem in any model of TAT is the calculation of the occupation probability. In our approach this probability is expressed in terms of only thermal and tunnelling exchange times. Our model has been published in [1, 2], however, without presenting in detail how the exchange times had been derived.

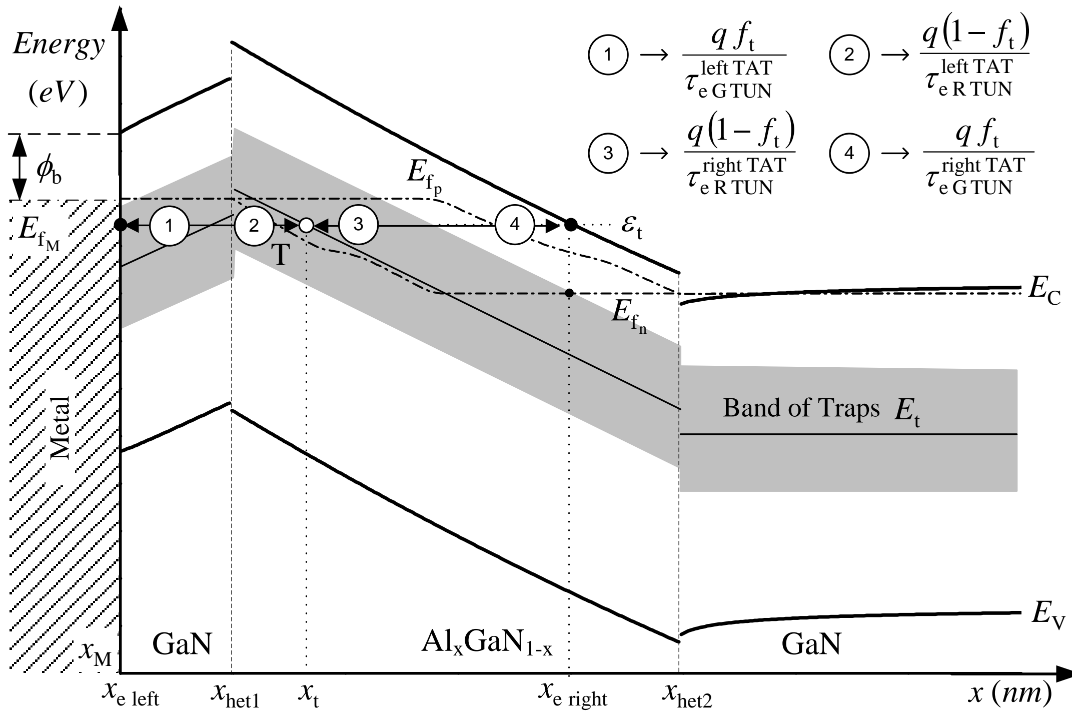

Fig. 1:*Electron exchange tunnelling currents flowing out of the trap to the left ① or right side and flowing into the trap from the left ② or right side ③ of a reverse biased* $GaN/Al_xGaN_{1-x}/GaN$ *heterostructure.*

2. Model calculations

Let us choose point T defined by coordinates $(\varepsilon_\mathrm{t}, x_\mathrm{t})$ which lies in the forbidden band of the semiconductor and define an infinitesimally small ”volume” $\mathrm{d}\varepsilon_\mathrm{t}\mathrm{d}x_\mathrm{t}$ around the chosen point T. In this volume, the density of trapping centres with cross-section $\sigma_\mathrm{t}^\mathrm{e}$ is given by the distribution function $D_\mathrm{t}(\varepsilon_\mathrm{t}, x_\mathrm{t})$ [3]. Then, the product $\sigma_\mathrm{t}^\mathrm{e} D_\mathrm{t}\,\mathrm{d}\varepsilon_\mathrm{t}\mathrm{d}x_\mathrm{t}$ is a dimensionless quantity and we canbe seen asthe trapping ability of point T.

Let us consider tunnelling of electrons from point T in the forbidden band into the conduction band at place, see Fig. 1. The tunnelling current density of electrons ④ between point T and the conduction band at places $x \equiv x_\mathrm{eright}$ is general expressed as a triple integral in ***k***- space [4]

$$\frac{q}{(2\pi)^3}\iiint 2\, v_x\, \Gamma_\mathrm{e}(k_x)\, f_\mathrm{t}(\varepsilon_\mathrm{t}, x_\mathrm{t})\left(1 - f_\mathrm{e}^\mathrm{FD}(x_\mathrm{right}^\mathrm{e})\right)\mathrm{d}k_x \mathrm{d}k_y \mathrm{d}k_z$$

However, the tunnelling current density between trapping centres in point T defined by coordinates $(\varepsilon_\mathrm{t}, x_\mathrm{t})$ and the conduction band CB defined by coordinates $(\varepsilon_\mathrm{t}, x_\mathrm{eright})$, taking into account the trapping ability of point T, is expressed as

$$d^2 J_\mathrm{Gright}^\mathrm{eTUN} = \frac{q\sigma_\mathrm{t}^\mathrm{e} D_\mathrm{t}(\varepsilon_\mathrm{t}, x_\mathrm{t})}{4\pi^3}\mathrm{d}\varepsilon_\mathrm{t}\mathrm{d}x_\mathrm{t}\iiint v_x\, \Gamma_\mathrm{e}(k_x)\, f_\mathrm{t}(\varepsilon_\mathrm{t}, x_\mathrm{t})\left(1 - f_\mathrm{e}^\mathrm{FD}(x_\mathrm{right}^\mathrm{e})\right)\mathrm{d}k_x \mathrm{d}k_y \mathrm{d}k_z \quad (1)$$

where $v_x = \hbar k_x / m_\mathrm{T}^\mathrm{e}$ is the carrier velocity of tunnelling electron in the direction of transport, $\Gamma_\mathrm{e}(k_x)$ is the transmission coefficient of tunnelling electrons between point $\mathrm{T}(\varepsilon_\mathrm{t}, x_\mathrm{t})$ and the conduction band $(\varepsilon_\mathrm{t}, x_\mathrm{right}^\mathrm{e})$, $f_\mathrm{t}(\varepsilon_\mathrm{t}, x_\mathrm{t})$ is the electron occupation probability of trapping centres lying at deep energy levels ε_t at place x_t, $f_\mathrm{e}^\mathrm{FD}(x_\mathrm{right}^\mathrm{e})$ is the Fermi-Dirac distribution function in the semiconductor at place $x_\mathrm{right}^\mathrm{e}$, and $k_{x,y,z}$ are the Cartesian wave numbers of tunnelling electrons. Index G indicates that electrons are generated at place $x_\mathrm{right}^\mathrm{e}$ by tunnelling from the trap placed at x_t.

Equation (1) will be simplified by transforming it from the Cartesian wave number space into energy space in a cylindrical coordination system. This is facilitated by the fact that the energy of tunnelling electrons assumes polar symmetry in the movement direction of electrons. For this purpose, transformation relations are used between the energy and wave numbers of electrons: $k_x = \sqrt{2m_\mathrm{T}^\mathrm{e} E_x / \hbar^2}$, $k_y = \sqrt{2m_\mathrm{R}^\mathrm{e} E_\perp / \hbar^2}\cos\varphi$,
$k_z = \sqrt{2m_\mathrm{R}^\mathrm{e} E_\perp / \hbar^2}\sin\varphi$, $\rho = k_y^2 + k_z^2 = \sqrt{2m_\mathrm{R}^\mathrm{e} E_\perp / \hbar^2}$

The energy of the tunnelling electron consists of two components: $E_x = \hbar^2 k_x^2 /(2m_\mathrm{T}^\mathrm{e})$ is the electron energy in the direction of tunnelling transport and $E_\perp = \hbar^2 (k_y + k_z)^2 /(2m_\mathrm{R}^\mathrm{e})$ is the electron energy in the direction perpendicular to the tunnelling transport.

For electrons tunnelling between point T and the conduction band it must hold that their total energy $\varepsilon_\mathrm{t} = E_x + E_\perp$ does not change, remains constant, in contrary to its two components. If one component increases, the other component decreases by the same amount. Utilizing the transformation formula between Cartesian and cylindrical coordinates $\mathrm{d}k_x \mathrm{d}k_y \mathrm{d}k_z = \rho\,\mathrm{d}\rho\,\mathrm{d}\varphi\,\mathrm{d}k_x$ we rewrite Eqn. (1) into the following energy form:

$$d^2 J_\mathrm{Gright}^\mathrm{eTUN} = q\frac{m_\mathrm{R}^\mathrm{e}\sigma_\mathrm{t}^\mathrm{e} D_\mathrm{t}(\varepsilon_\mathrm{t}, x_\mathrm{t})}{4\pi^3\hbar^3}\left(\iint\int_0^{2\pi} \Gamma_\mathrm{e}(E_x)\, f_\mathrm{t}(\varepsilon_\mathrm{t}, x_\mathrm{t})\left(1 - f_\mathrm{e}^\mathrm{FD}(x_\mathrm{right}^\mathrm{e})\right)\mathrm{d}E_\perp \mathrm{d}E_x\, \mathrm{d}\varphi\right)\mathrm{d}x_\mathrm{t}\, \mathrm{d}\varepsilon_\mathrm{t} \quad (2)$$

This expression can be further simplified. The inner integral over angle φ around axis x simply gives the result 2π. Probability $f_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})$ is a function of the total energy rather than of its components, therefore it can be withdrawn in front of the integrals. Finally, tunnelling probability $\Gamma_{\mathrm{e}}(E_x)$ depends only on component E_x. Therefore, the integral over variable $\mathrm{d}E_{\perp}$ will be $E_{\perp} = \varepsilon_{\mathrm{t}} - E_x$. The maximum value of E_x is equal to ε_{t}, when the whole kinetic energy of the electron belongs to the direction of tunnelling and $E_{\perp} = 0$. The lower value of E_x goes down to the bottom of the forbidden band. For this value of E_x the tunnelling probability can be considered as zero. Then Eqn. (2) can be rewritten into the form

$$d^2 J_{\mathrm{Gright}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}}, x_{\mathrm{right}}^{\mathrm{e}}) = q \frac{f_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}}) D_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})}{\tau_{\mathrm{Gright}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}}, x_{\mathrm{right}}^{\mathrm{e}})} \mathrm{d}x_{\mathrm{t}}\, \mathrm{d}\varepsilon_{\mathrm{t}} \tag{3}$$

where we defined the tunnelling exchange time $\tau_{\mathrm{Gright}}^{\mathrm{e\,TUN}}$ as

$$\frac{1}{\tau_{\mathrm{Gright}}^{\mathrm{e\,TUN}}} = \left(1 - f_{\mathrm{e}}^{\mathrm{FD}}(x_{\mathrm{right}}^{\mathrm{e}})\right) \frac{m_{\mathrm{R}}^{\mathrm{e}} \sigma_{\mathrm{t}}^{\mathrm{e}}}{2\pi^2 \hbar^3} \int_{E_{\mathrm{v}}(x_{\mathrm{t}})}^{\varepsilon_{\mathrm{t}}} \Gamma_{\mathrm{e}}(E_x)(\varepsilon_{\mathrm{t}} - E_x) \mathrm{d}E_x \tag{4}$$

The term on the rightside of Eqn. (4)has a dimension of s^{-1} and its reciprocal value will be called the tunnelling exchange time $\tau_{\mathrm{Gright}}^{\mathrm{e\,TUN}}$. The right side of Eqn. (3) represents the contribution of one trap lying in the forbidden band at place $(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})$ to the current density of electrons tunnelling into the conduction band at place $x_{\mathrm{right}}^{\mathrm{e}}$ (see Fig. 1). The total current density of electrons tunnelling from all traps lying in the forbidden band on energy level ε_{t} along x axis with trap density distribution $D_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})$ [2] flowing into the conduction band at place x_{eright} is obtained by integrating Eqn. (3) with respect to variable x_{t}:

$$\mathrm{d}\, J_{\mathrm{Gright}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{eright}}) = q \left(\int_{x_{\mathrm{eleft}}}^{x_{\mathrm{eright}}} \frac{f_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}}) D_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})}{\tau_{\mathrm{Gright}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}}, x_{\mathrm{right}}^{\mathrm{e}})} \mathrm{d}x_{\mathrm{t}} \right) \mathrm{d}\varepsilon_{\mathrm{t}} \tag{5}$$

The lower integration limit $x_{\mathrm{left}}^{\mathrm{e}}$ is the second intersection of energy level ε_{t} withthe conduction band on the opposite side, where $E_{\mathrm{c}}(x_{\mathrm{left}}^{\mathrm{e}}) \equiv \varepsilon_{\mathrm{t}}$ (see Fig. 1) or if $\varepsilon_{\mathrm{t}} < E_c(x_{\mathrm{M}})$, then $x_{\mathrm{left}}^{\mathrm{e}} = x_{\mathrm{M}}$. Finally, the total current density (5) is differentiated with respect to spatial coordinate, whereby one obtains the generation rate of tunnelling electrons $G_{\mathrm{TAT}}^{\mathrm{e\,TUN}}$ at $x_{\mathrm{right}}^{\mathrm{e}}$ occurring on the right side of the continuity equation. Hereby, the TAT model is incorporated into the fundamental semiconductor equations.

$$G_{\mathrm{TAT}}^{\mathrm{e\,TUN}}(x \equiv x_{\mathrm{right}}^{\mathrm{e}}) = \frac{1}{q} \frac{\mathrm{d}\, \mathrm{J}_{\mathrm{Gright}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{right}}^{\mathrm{e}})}{\mathrm{d}x_{\mathrm{right}}^{\mathrm{e}}} \tag{6}$$

For practical reasons the integral in this definition (4) will be replaced by summation, thus $dE_{\mathrm{x}} \Rightarrow \Delta E_{\mathrm{x}}$, and the electron energy component in the direction of tunnelling E_x will be decremented from the value ε_{t} in every summation step "j" by value ΔE_{x} until the tunnelling probability assumes a negligible, zero value $\varepsilon_{\mathrm{t}} - E_{\mathrm{x}} \Rightarrow j\Delta E_{\mathrm{x}}$. Then

$$\int_{E_{\mathrm{v}}(x_{\mathrm{t}})}^{\varepsilon_{\mathrm{t}}} \Gamma_{\mathrm{e}}(E_{\mathrm{x}})(\varepsilon_{\mathrm{t}} - E_{\mathrm{x}}) \mathrm{d}E_{\mathrm{x}} \Rightarrow (\Delta E_{\mathrm{x}})^2 \sum_{j=0}^{N} (j+1) \Gamma_{\mathrm{e}}^{j}$$

and the tunnelling exchange time $\tau_{\mathrm{Gright}}^{\mathrm{e\,TUN}}$ is expressed as

$$\frac{1}{\tau_{\mathrm{G\,right}}^{\mathrm{e\,TUN}}} = \left(1 - f_{\mathrm{e}}^{\mathrm{FD}}(x_{\mathrm{right}}^{\mathrm{e}})\right) \frac{m_{\mathrm{R}}^{\mathrm{e}} \sigma_{\mathrm{t}}^{\mathrm{e}}}{2\pi^2 \hbar^3} (\Delta E_{\mathrm{x}})^2 \sum_{j=0}^{N} (j+1) \Gamma_{\mathrm{e}}^{j} \tag{7}$$

where Γ_{e}^{j} are transmission coefficients for electron tunnelling. In WKB approximation is one has

$$\Gamma_{\mathrm{e}}^{j} = \exp\left(-\frac{2}{\hbar} \int_{x_{\mathrm{t}}}^{x_{\mathrm{right}}^{\mathrm{e}}} \sqrt{2 m_{\mathrm{T}}^{\mathrm{e}} (E_{\mathrm{c}}(x) - \varepsilon_{\mathrm{t}} + j \Delta E_{\mathrm{x}})}\, \mathrm{d}x \right). \tag{8}$$

For tunnelling in the opposite direction (from the conduction band to the traps) it holds

$$d^2 J_{\mathrm{R\,right}}^{\mathrm{e\,TUN}}(x_{\mathrm{right}}^{\mathrm{e}}) = q \frac{\left(1 - f_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})\right) D_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})}{\tau_{\mathrm{R\,right}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}}, x_{\mathrm{right}}^{\mathrm{e}})} \mathrm{d}\varepsilon_{\mathrm{t}} \mathrm{d}x_{\mathrm{t}}, \tag{9}$$

where the electron tunnelling exchange time is

$$\frac{1}{\tau_{\mathrm{R\,right}}^{\mathrm{e\,TUN}}} = f_{\mathrm{e}}^{\mathrm{FD}}(x_{\mathrm{right}}^{\mathrm{e}}) \frac{m_{\mathrm{R}}^{\mathrm{e}} \sigma_{\mathrm{t}}^{\mathrm{e}}}{2\pi^2 \hbar^3} (\Delta E_{\mathrm{x}})^2 \sum_{\mathrm{j}=0}^{N} (j+1) \Gamma_{\mathrm{e}}^{j}. \tag{10}$$

Here, index R indicates, that electrons flow out of the conduction band, by tunnelling, at place $x_{\mathrm{right}}^{\mathrm{e}}$ an flow into the trap at place x_{t}. Similarly one obtains the total current density flowing from place $x_{\mathrm{right}}^{\mathrm{e}}$ into the trapping centres lying on energy level ε_{t} by integrating Eqn. (9) with respect to variable x_{t}:

$$\mathrm{d} J_{\mathrm{R\,right}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{right}}^{\mathrm{e}}) = q \left(\int_{x_{\mathrm{left}}^{\mathrm{e}}}^{x_{\mathrm{right}}^{\mathrm{e}}} \frac{\left(1 - f_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})\right) D_{\mathrm{t}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}})}{\tau_{\mathrm{R\,right}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{t}}, x_{\mathrm{right}}^{\mathrm{e}})} \mathrm{d}x_{\mathrm{t}} \right) \mathrm{d}\varepsilon_{\mathrm{t}} \tag{11}$$

And by differentiating this expression one obtains the recombination rate of tunnelling electrons $R_{\mathrm{TAT}}^{\mathrm{e\,TUN}}$ at place $x_{\mathrm{right}}^{\mathrm{e}}$:

$$R_{\mathrm{TAT}}^{\mathrm{e\,TUN}}(x_{\mathrm{e\,right}}) = \frac{1}{q} \frac{\mathrm{d}\,\mathrm{J}_{\mathrm{R\,right}}^{\mathrm{e\,TUN}}(\varepsilon_{\mathrm{t}}, x_{\mathrm{right}}^{\mathrm{e}})}{\mathrm{d}x_{\mathrm{right}}^{\mathrm{e}}} \tag{12}$$

Then, on the right side of the continuity equation with implemented TAT model there is a difference of the recombination and generation rates. $U_{\mathrm{TAT}}^{\mathrm{e\,TUN}} = R_{\mathrm{TAT}}^{\mathrm{e\,TUN}} - G_{\mathrm{TAT}}^{\mathrm{e\,TUN}}$. In a similar way we can derive also the tunnelling exchange times $\tau_{\mathrm{G\,left}}^{\mathrm{e\,TUN}}$ and $\tau_{\mathrm{R\,left}}^{\mathrm{e\,TUN}}$.

3. Conclusion

The concept of tunnelling exchange times presents a dominant contribution to our model of TAT. The new approach allows to simply calculate the probability of occupation of the trapping centre by a free charge carrier and subsequently to get the thermal and tunnelling generation-recombination rates occurring in the continuity equations. This is why the TAT model based on thermal and tunnelling exchange times is suitable for simulating the electrical properties of semiconductor nanostructures in which quantum mechanical phenomena play a key role. We have successfully applied the new TAT model to simulate the charge transport in thin MIM structures [5] and in the AlGaN/GaN heterostructure [6] which are part of power HEMT transistors.

Acknowledgments

The work has been supported by the Scientific Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and of the Slovak Academy of Sciences (projects VEGA 1/0712/12 and 1/0377/13).

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