Validation of the model for predicting VAC RTD photonics

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Abstract. This paper discusses the processes of current transfer in resonant tunneling diodes during the transition from the region of positive differential conductivity to the region of negative differential conductivity. The behavior features of the self-consistent potential and tunnel transparency coefficient in the region of peak stresses are demonstrated.

1. Introduction

A resonant tunneling diode (RTD) is a nanoelectronic device with wide potential for use in optoelectronics, for example, as electro-absorption modulator (RTD-EAM), photodetector (RTD-PD), laser diode (RTD-LD), optoelectronic oscillator (RTD-OEO) [1,2], and development of high-frequency signal mixers [3], as well as high-frequency frequency generators [4,5] and logic and memory devices [6,7]. Many of these RTD applications are based on the feature of their current-voltage characteristics (CVC), called negative differential resistance (ODR) [8-10].

One of the important simulation issues of RTD’s CVC is the behavior of CVC during the transition from the section of positive differential resistance (PDR) to the section of the ODR, that is, at the peak of the CVC. In this paper, we consider the behavior of a self-consistent potential at the peak of RTD’s CVC based on GaAs/AlAs heterojunctions.

2. Simulation

The transition from PDR to ODR is associated with the departure of metastable states to the forbidden zone level at the source. An important role in simulation of this VAC region is played by taking into account the Coulomb interaction of electrons using the self-consistent field method [11,12]. Firstly, this affects the peak voltage and peak current, and secondly, the sharpness of the peak. When calculating the RTD’s CVC without taking into account the self-consistent field, in some cases the peak is smoothed due to the fact that metastable levels are characterized by “natural broadening”, although the peak is “sharp” in the experimental CVCs.

CVC peak is always “sharp” when self-consistent potential are took into account due to a sharp drop in the current density, which is explained by a jump in the self-consistent potential (Figure 1), which explains the difference in current density and is caused by the departure of the first resonance level to the band gap of the source reservoir. Movement of metastable levels with increasing voltage is linear without taking into account the self-consistent potential. In self-consistent simulation the nature of the dynamics of metastable levels becomes non-linear and gap appears on the trajectory of their movement.
Figure 1 Self-consistent potential and tunnel transparency of AlAs/GaAs resonant-tunneling structure. The gap is observed at a voltage of 0.67 V. Barrier width – 3 nm, well width – 5 nm.

The tunnel transparency coefficient depends on the profile of the potential energy of the electron in the structure, which, in turn, depends on the electron concentration. Therefore, to analyze the behavior of the tunnel transparency coefficient at near-peak voltages, an analysis was made of the electron concentration in this section of the CVC. The concentration of electrons was considered in the approximation that the wave function of electrons in a quantum well is proportional to the Cauchy distribution (formula 1). It was also assumed that the electron concentration is due to energy states in a small neighborhood of the first resonance level.

$$|\psi(z,E)|^2 \sim \frac{\Gamma^2}{(E - \varepsilon)^2 + \Gamma^2} = \rho C(\varepsilon, \Gamma)$$  \hspace{1cm} (1)

where $\varepsilon$ – first resonance level energy, $\Gamma$ – resonance level half width, $C(\varepsilon, \Gamma)$ – probability density of the Cauchy distribution.

The electron concentration in the framework of the wave function formalism [13] is described by the following formula

$$n = \int_{k_c}^{\infty} |\psi(z,E)|^2 g(z,E) dE$$  \hspace{1cm} (2)
where $\psi(z, E)$ – wave function of electrons with energy $E$ at point $z$, $g(z, E)$ – energy distribution function of electrons at point $z$, $E_c$ – conduction band bottom at point $z$.

Within the framework of the accepted approximations, the electron concentration is proportional to the Cauchy distribution function

$$n \sim \pi \Gamma \int_{E_c}^{\infty} C(\varepsilon, \Gamma) = \pi \left[ \frac{\pi}{2} - \arctan \left( \frac{E - \varepsilon}{\Gamma} \right) \right]$$

(3)

At near-peak voltages, the resonance level is close to the bottom of the conduction band, that is $\varepsilon \approx E_c$, and a change in voltage leads to a shift in the resonance level by a certain amount $\Delta E$. Thus, it follows from formula (3) that the electron concentration at the post-peak and d-peak voltage obeys the relation

$$\frac{n'}{n} \sim 1 - \frac{2}{\pi} \arctan \left( \frac{\Delta E}{\Gamma} \right) \rightarrow \begin{cases} 1 & \Delta E << \Gamma \\ \frac{1}{\pi} & \Delta E = E \\ 0 & \Delta E >> \Gamma \end{cases}$$

(4)

If $\Delta E >> \Gamma$, then $n'$ is the concentration of electrons at the post-peak voltage, and it is incomparably less than the concentration of electrons at the peak voltage. Then, in accordance with the Gauss theorem, a sharp drop in the concentration of electrons in a quantum well leads to a jump in the self-consistent potential. The rapid decrease in concentration is explained by the small half-width of the first resonance level, as was obtained in numerical experiments, of the order of $10^{-3}$ eV and less. In turn, a sharp change in the self-consistent potential leads to a jump in the tunnel transparency coefficient.

In another case, when the shift of the resonance levels does not exceed the half-width of the level, the concentration ratio tends to 1. This situation is possible for structures with a wide well (of the order of ten nanometers), when the first resonance level is located close to the bottom of the conduction band, and the voltage shift leads to a smaller shift of resonance levels than for structures with a narrow well (of the order of several nanometers). It should also be considered that $\Delta E << \Gamma$ in the case of a large influence of dissipative processes, which make an additional contribution to the width of the broadening of resonance levels. It follows that for accurate simulation of current transport at near-peak voltages, in addition to the Coulomb interaction of electrons, dissipative processes should be taken into account.

Various types of electron scattering were introduced into the developed model, in particular, inelastic scattering by phonons using the optical potential method [14, 15], which allows one to obtain more accurate estimates of the current-voltage characteristic of the CVC in the PDR region. However, an excessively large selected optical potential value “smooths” the peak due to wider estimates of the width of metastable states. Therefore, for the successful validation of the model for predicting the negative differential conductivity of resonant tunneling diodes, an adequate estimate of the constants determining the scattering intensity is important. The developed algorithm for the effective estimation of these model parameters allowed us to establish that, for example, for structures whose CVCs are shown in Fig. 2, the optical potential in a quantum well of 0.02 eV is optimal. As can be seen from the graphs, satisfactory agreement was obtained between the calculation and the experiment on the PDR section, as well as in the assessment of peak and valley currents and voltages.
3. Conclusion

An analysis of the behavior of the CVC during the transition from the PDS to the ODS section was made, which made it possible to establish that a sharp drop in current density is associated with the nature of the change in the self-consistent potential in the region of peak voltages and the movement of metastable levels with increasing voltage. A methodology has been developed for estimating parameters that determine the intensity of dissipative processes in the region of negative differential conductivity, which made it possible to obtain adequate estimates of the peak current and voltage. Minimization of the error of the entire section of the ODR in the attention of the experimentally observed region of the "plateau" which has the ability to study the energy dependence of the parameters of the models in the area of the ODR.

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