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Modelling of high-temperature dark current in multi-quantum well structures from MWIR to VLWIR

Diogo de Moura Pedroso[a], Gustavo Soares Vieira[a,b], Angelo Passaro[a,b,*]

[a] Aeronautics Institute of Technology, ITA, Praça Mal. Eduardo Gomes, 50, 12228-900 São José dos Campos, SP, Brazil
[b] Division of Applied Physics – Institute for Advanced Studies, IEAv, Trevo Cel. Av. José A. A. do Amarante, 1, 12228-001 São José dos Campos, SP, Brazil

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ABSTRACT

In this paper, a model to calculate the dark current of quantum well infrared photodetectors at high-temperature regime is presented. The model is derived from a positive-definite quantum probability-flux and considers thermionic emission and thermally-assisted tunnelling as mechanisms of dark current generation. Its main input data are the wave functions obtained by time-independent Schrodinger equation and it does not require empirical parameters related to the transport of carriers. By means of this model, the dark current of quantum well infrared photodetectors at high-temperature regime is investigated with respect to the temperature, the barrier width, the applied electric field and the position of the first excited state. The theoretical results are compared with experimental data obtained from lattice-matched InAlAs/InGaAs, InGaAsP/InP on InP substrate and AlGaAs/GaAs structures with rectangular wells and symmetric barriers, whose absorption peak wavelengths range from MWIR to VLWIR. The corresponding results are in a good agreement with experimental data at different temperatures and at a wide range of applied electric field.

1. Introduction

The infrared detection using QWIPs (Quantum Well Infrared Photodetectors) is based on intersubband transitions induced by photon absorption. As the temperature increases, this detection mechanism competes increasingly with the dark current generated by charge-phonon interactions. This competition is enhanced by the fact that the levels in QWIPs are quantized only in the growth direction, resulting in a continuum in the two other directions, what increases the likelihood of phonon activation [1]. As a result, dark current is one of the main limitations of the device performance at a high temperature regime [2,3], mainly for structures with very long absorption peak wavelength [4]. The reduction of dark current plays an essential role on the optimization of photodetectors, demanding generalized models that are able to reproduce, with a good agreement, experimental data for structures with different band-edge potentials.

Phenomenological models can provide a good qualitative understanding of the experimental data of dark current of QWIPs. Additionally, after the experimental characterization of the sample, they can also obtain good quantitative agreements by fitting a set of parameters [3,5]. However, due to the variability of the corresponding parameters and the consequent impact on the theoretical results, phenomenological models present limitations when used as predictive tools of dark current [6,7].

As an alternative for the calculation of dark current in the low-temperature regime, the model discussed in [8] separates the current in low and high electric field regions, which are described respectively by miniband and Wannier-Stark pictures with no fitting parameters. In the high-temperature regime, an alternative with no adjusting parameters might be the model recently presented in literature derived from a semi-classical interpretation of the carriers' motion based on the Ehrenfest Theorem [7]. This model accounts for the drift of thermally excited carriers above the barrier level, but do not includes the component of dark current caused by thermally assisted tunnelling.

In this paper, theoretical results of dark current at high-temperature regime for QWIPs encompassing a broad range of absorption peak wavelengths are obtained from a model based on a positive-definite quantum probability-flux operator and quantum density operator. Such model also does not require empirical parameters related to the transport of carriers. Moreover, it includes the thermally-assisted tunnelling in addition to the thermionic emission as mechanisms of dark current generation. The model can be used to estimate the dark current for QWIPs with different potential profiles, including structures with more than one bound state.

The theoretical results of dark current are compared with experimental data obtained from lattice-matched InAlAs/InGaAs, InGaAsP/

* Corresponding author at: Division of Applied Physics – Institute for Advanced Studies, IEAv, Trevo Cel. Av. José A. A. do Amarante, 1, 12228-001 São José dos Campos, SP, Brazil.
E-mail addresses: diogo.mourapedroso@gmail.com (D. de Moura Pedroso), gvieira@ieav.cta.br (G.S. Vieira), angelo.passaro@pq.cnpq.br (A. Passaro).

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InP and AlGaAs/GaAs structures, whose absorption peak wavelengths range from mid- to far infrared. The contributions of the two main mechanisms of dark current generation at high-temperature regime are numerically investigated as a function of the temperature, the applied electric field, the barrier width and the position of the first excited state.

2. Theory

The high-temperature regime refers to the range of temperature at which the main contribution to the dark current of QWIPs comes from the drift of excited carriers above the barrier level [3]. These carriers can be generated by thermionic emission or even by thermally-assisted tunnelling. The temperature at which this regime is observed depends on the activation energy of the structure. At zero Kelvin, the activation energy corresponds to the minimum energy required by a confined carrier in order to contribute to the current. Its value is identical to the average energy carried by the carrier during the transport along the structure [9]. For the case of conventional QWIPs with no applied bias, it can be determined by the difference between the barrier top and the Fermi level [2].

At the high-temperature regime, the dark current flowing above the barrier level in multiple quantum well structures (MQW) can be computed considering the average contribution of the probability-flux weighted by the number of carriers occupying each sub-band, as expressed by:

$$J = q\sum_n \int \langle n|\rho j^{(+)}(z)|n\rangle dz \tag{1}$$

where q is the fundamental charge, z is the position along the growth direction of the MQW and $\rho = \sum_n c_n |n\rangle\langle n|$ is the density operator. The one-dimensional n-states are normalized. The argument of the integral in (1) represents the probability-flux for each point of the domain of study for each n^{th} state with the corresponding occupation probability given by the density operator. The positive-definite quantum probability-flux operator, $j^{(+)}(z)$, can be given by [10,11]:

$$j^{(+)}(z) = \sqrt{\frac{|\hat{p}|}{m}}\delta(\hat{z} - z)\sqrt{\frac{|\hat{p}|}{m}} \tag{2}$$

where z is the position, m is the effective mass, and the operator $\sqrt{|\hat{p}|} \equiv \int_{-\infty}^{\infty} dp\sqrt{|p|}|p\rangle\langle p|$, at which p is the linear momentum.

The coefficients c_n of the density operator are associated with the number of carriers occupying the nth state. Considering a given electric field applied in the growth direction, the respective occupation probability will depend on the position, z. This dependence is outcome of the positional variation of the quasi-Fermi energy. Thus, the normalization of the coefficients c_n is performed as follows:

$$\sum_n \int c_n(z)\ dz = N_T \tag{3}$$

where N_T is the free carriers concentration in the system. In this context, these terms represent the variation of the carrier concentration along the growth direction for a determined state:

$$c_n(z) = \frac{\partial N_n}{\partial z} \tag{4}$$

where N_n is the effective free carrier concentration in the nth state, at which the possibility of confinement by potential barriers must be considered, since only free carriers can contribute to the dark current. Thus:

$$N_n(z) = \int T(E)D_n(E)f(E, z)dE \tag{5}$$

where $D(E)$ is the density of states, $f(E, z)$ is the thermal distribution function and $T(E)$ is the transmission coefficient, which aims to weigh the decreasing of free electron concentration due to a possible confinement by potential barriers.

A widely used method to model the states above the barrier level is to consider highly energetic barriers at the limits of the domain of study, which results in a discrete spectrum of one-dimensional states above the barrier level [6,12,13]. These one-dimensional states are associated with the z-component of wave vector of the sub-band. Thus, the density of states can be modelled as a two-dimensional electron gas for each sub-band above the barrier level. Consequently, $N_n(z)$ can be written as:

$$N_n(z) = \frac{4\pi\ m}{h^2 N}\int_{E_n}^{\infty} T(E)f(E, z)dE \tag{6}$$

where E_n is the minimum energy of the nth sub-band and h is the Planck constant. The number of periods in the domain of study, N, is included in order to consider the degeneracy originated by non-coupled periods. Notice that, instead of a constant density of states, other approaches could also be employed [14–17].

Substituting (2), (4) and (6) in (1) allow us to obtain the following approximate expression for the dark current:

$$J = \frac{-2\ q^2 F}{h\ N\ k_B T}\sum_n \int_{z0}^{zf}\int_{E_n}^{\infty} |\psi_n|\sqrt{\frac{\partial \psi_n^*}{\partial z}\frac{\partial \psi_n}{\partial z}}\, T(E)\exp\left[\frac{-(E - E_F - eFz)}{k_B T}\right] dEdz \tag{7}$$

where z_0 and z_f represent the initial and final positions of the domain of study, F is the applied electric field, ψ_n are the wave functions associated with the nth sub-band and E_F is the Fermi energy. The transmission coefficient, $T(E)$, is obtained by WKB approximation. Notice that, if $T(E)$ is disregarded, the contribution of carriers under the barrier level is neglected. Additionally, it is worth to mention that the use of the standard quantum probability flux operator [10], $j(z) = 1/2m(\hat{p}|z\rangle\langle z| + |z\rangle\langle z|\hat{p})$, results in the expression:

$$J = \frac{-2\ q^2 F}{h\ N\ k_B T}\mathrm{Re}\left\{i\sum_n \int_{z0}^{zf}\int_{E_n}^{\infty} \psi_n^*\frac{\partial \psi_n}{\partial z}T(E)\exp\left[\frac{-(E - E_F - eFz)}{k_B T}\right] dEdz\right\}. \tag{8}$$

However, since that the standard quantum flux operator is not positive-definite, its use to obtain the current assumes that the backward quantum flux is negligible [10,11,18]. At the limit of a sufficiently well-defined momentum, for instance at high applied bias, the results obtained from $j^{(+)}(z)$ and $j(z)$ are coincident [11].

It is reinforced that the model does not require empirical or fitting parameters, such as mobility and saturation velocity, but it relies on an adequate selection of the band parameters in order to obtain the wave functions of the system. Among these parameters, the dark current is more sensitive to the band-offset, ΔE_c, once it has a direct effect upon the activation energy of the structure and upon the position of the first excited state.

Expression (7) deals with the drift of carriers generated by the mechanisms of thermionic emission and thermally-assisted tunnelling. The thermionic emission, TE, refers to carriers which are thermally excited from bound states directly to extended states above the barrier level. The thermally-assisted tunnelling, TAT, refers to carriers with energy below the barrier level which escape from the well by tunnelling. The corresponding transmission coefficient depends on the total energy of the carriers [19,20]. The drift velocity is determined based on the perpendicular component of the momentum of each considered sub-band. Thus, any sub-band below or above the barrier top with non-zero perpendicular moment can contribute. Other transport mechanisms besides drift of carriers are neglected, such as sequential tunnelling and hopping transport [21].

In (7), it is considered a Boltzmann-like distribution and a linear distribution of the quasi-Fermi energy, which is a consequence of uniform distribution of electric field along the structure. Therefore, it does not take into account the effects due to unbalanced injection of