

The numerical method for solving the transport equations in HgCdTe heterostructures using the non-equilibrium distribution functions

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Abstract This paper presents a numerical method for solving the set of transport equations in semiconductor heterostructures by using the non-equilibrium distribution function for electrons and holes. This method enables the calculation of carrier concentration, carrier mobility and entropy by integrations in the space of wave vector. In this same way the electrical current density and density of entropy currents are determined. The influence of quasi-Fermi energy gradients and the gradient of temperature on the physical parameters of the heterostructure is taken into account.

I. INTRODUCTION

Usually semiconductor devices work in non-equilibrium conditions caused by an electrical biasing and optical excitations. The flows of electric carriers and energy are caused by gradients of electrochemical potentials $\nabla\Phi_n(\vec{r})$ and $\nabla\Phi_p(\vec{r})$ and the gradient of temperature ∇T . These gradients have a significant impact on the non-equilibrium distribution functions determining the statistical probability that the electrical carrier has position \vec{r} and wave vector \vec{k} . Typically, non-equilibrium distribution functions for electrons and holes are derived by solving the kinetic Boltzmann equation, as it was done for example in the classic work by van Vleit and Marshak [1]. We have shown in [2] that such derived distribution functions are only an approximation of the more general terms. We derived them by applying the variational principles of non-equilibrium thermodynamics [2]. This function for electrons is shown below:

$$f_e^C = \frac{1}{1 + \exp\left(\frac{-\chi(\vec{r}) - e\Psi(\vec{r}) + \varepsilon_C^k(\vec{k}) - \Phi_n(\vec{r}) - \tau_e(k) \frac{\hbar\vec{k}}{m_e^*(\vec{r})} \nabla\Phi_n(\vec{r}) + \frac{1}{6(m_e^*)^2 k_B} \tau_e^2(k) \hbar^2 k^2 \frac{(\nabla\Phi_n)^2}{T}}{k_B \left[T(\vec{r}) + \tau_e(k) \frac{\hbar\vec{k}}{m_e^*(\vec{r})} \nabla T(\vec{r}) - \frac{1}{6(m_e^*)^2 k_B} \tau_e^2(k) \hbar^2 k^2 \left(\frac{\nabla\Phi_n \nabla T}{T} + \frac{s_e(\vec{r}) (\nabla T)^2}{n(\vec{r}) T} \right) \right]}\right)} \quad (1)$$

A similar figure is -equilibrium distribution function for holes, while for ionized impurities distribution functions are expressed in a standardized form (see for example [3]). In relation (1) $\chi(\vec{r})$ denotes electron affinity, m_e^* it's effective mass, $\tau_e(k)$ relaxation time, $\varepsilon_C^k(\vec{k})$ kinetic energy, e elementary charge, Ψ electrical potential, T_e electron temperature, s_e density of electron entropy, \hbar Planck's constant, k_B Boltzmann's constant, n electron concentration, Φ_n quasi-Fermi energy. The function expressed by equation (1) is the asymmetric function of wave vector \vec{k} , so integrating it into

vector \vec{k} enables the calculation of important physical parameters of devices.

II. NUMERICAL METHOD

By integration in the space of the wave vector k , we can determine the concentration and density of the carrier entropy carrier mobility, it's current density and current density of its entropy. For example, for electrons, these values are expressed as follows:

$$n = \frac{1}{2\pi^2} \int_0^\infty dk \int_{-\pi}^\pi k^2 \sin\Theta f_e(k) d\Theta \quad (2)$$

$$\mu_e = \frac{1}{n} \frac{e}{m_e^*} \frac{1}{2\pi^2} \int_{-\pi}^{+\pi} \int_0^\infty k^2 \sin\Theta \tau_e(k) f(k) d\Theta dk \quad (3)$$

$$j_e = \frac{1}{2\pi^2} \int_0^\infty \frac{\hbar k}{m_e^*} dk \int_{-\pi}^\pi k^2 \sin\Theta f_e(k) d\Theta \quad (4)$$

$$s_e = \frac{k_B}{2\pi^2} \int_0^\infty dk \int_{-\pi}^\pi \sin\Theta \{ f_e(k) \ln f_e(k) + [1 - f_e(k)] \ln [1 - f_e(k)] \} k^2 d\Theta \quad (5)$$

$$j_{s_e} = \frac{k_B}{2\pi^2} \int_0^\infty \frac{\hbar k}{m_e^*} dk \int_{-\pi}^\pi \sin\Theta \{ f_e(k) \ln f_e(k) + [1 - f_e(k)] \ln [1 - f_e(k)] \} k^2 d\Theta \quad (6)$$

Modeling semiconductor devices, we know the spatial distributions of molar composition, electron affinity, and doping and the use of local electrical equilibrium condition, enables us to determine the initial value of the electric potential $\Psi_0(\vec{r})$. We solve then Poisson equation using iterative methods in order to determine the electric potential in thermal equilibrium. It enables the calculation of n, μ_e, s_e in

thermal equilibrium by using relations (2), (3) and (5). In biased heterostructures the gradients of intensive parameters occurs and the electron distribution function should be expressed by relation (1). To determine the intensive parameters $\Psi(\vec{r}), \Phi_n(\vec{r}), \Phi_p(\vec{r}), T(\vec{r})$, which change with the change of the voltage, we have to solve the set of 4 nonlinear transport equations; the Poisson's equation, the continuity equation for electrons, the continuity equation for holes and the energy balance equation. These equations allow us to determine the iterative corrections $\delta\Psi(\vec{r}), \delta\Phi_n(\vec{r}), \delta\Phi_p(\vec{r})$

and $\delta T(\vec{r})$. Next the corrected parameters $\Psi(\vec{r}) = \Psi(\vec{r}) + \delta\Psi(\vec{r})$, $\Phi_n(\vec{r}) = \Phi_n(\vec{r}) + \delta\Phi_n(\vec{r})$, $\Phi_p(\vec{r}) = \Phi_p(\vec{r}) + \delta\Phi_p(\vec{r})$, $T(\vec{r}) = T(\vec{r}) + \delta T(\vec{r})$ are inserted into Eqs. (1)-(6) to calculate the corrected values of $f_e^C, n, \mu_e, j_e, s_e$ and j_{s_e} . A similar procedure is applied for holes. We have derived the energy balance equation in the following form: (7)

$$\frac{\partial u}{\partial t} = -\nabla(T_e j_{s_e}) - \nabla(T_h j_{s_h}) - \nabla(T_L j_{s_L}) - \nabla(\Phi_n j_e) + \nabla(\Phi_p j_h) + G^{opt} E_g + G^{opt} \bar{\epsilon}_{e,opt}^k + G^{opt} \bar{\epsilon}_{h,opt}^k$$

where u is the density of internal energy, index h refers to holes, E_g is the energy gap, G^{opt} is the optical generation rate, $\bar{\epsilon}_{e,opt}^k$ and $\bar{\epsilon}_{h,opt}^k$ is the average kinetic energy generated optically of electrons and holes, respectively. L denotes the crystal lattice.

III. SOME NUMERICAL RESULTS

From the following update these selected results of calculations of physical parameters of the cylindrical $Hg_{1-x}Cd_xTe$ nBn MESA detector with a diameter of 60 micrometers. Spatial distributions of physical parameters are shown along the axis of symmetry of the structure.

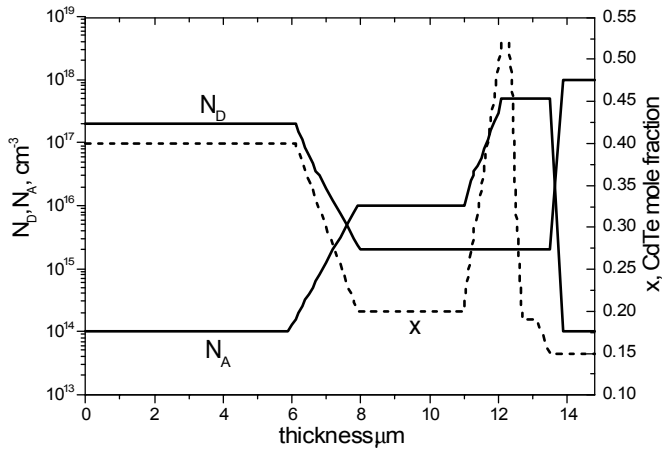


Fig. 1. Spatial distribution of mole fraction x donor concentration N_D and acceptor concentration N_A

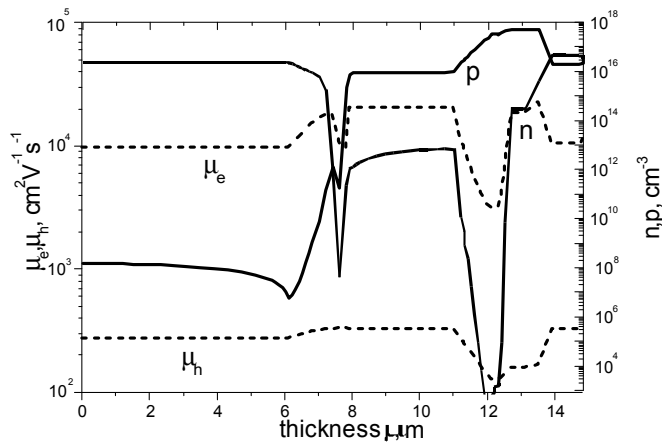


Fig. 2. Spatial distribution of calculated electron concentration n , hole concentration p , electron mobility μ_e and hole mobility μ_h .

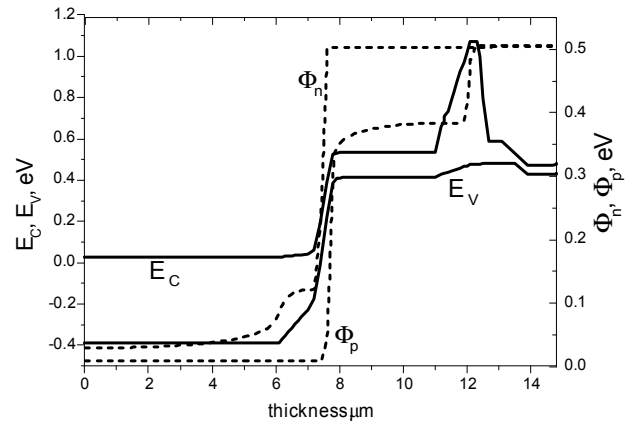


Fig.3. Spatial distribution of calculated energy band diagram and quasi Fermi energy for electron Φ_n and holes Φ_p , after biasing with 550 mV.

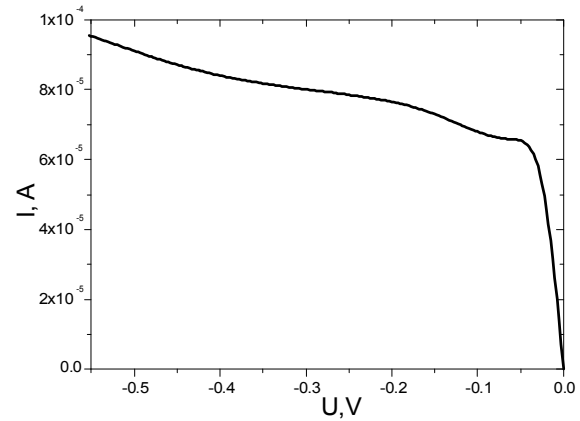


Fig. 4. Calculated $I(V)$ characteristic for presented nBn detector.

III SUMMARY

We have applied, derived earlier by ourselves, the non-equilibrium distribution function for electrons and hole in the numerical modelling of nBn MESA infrared detectors. The proposed numerical method enables the calculation of physical parameters by the numerical integration of distribution function in the space of wave vector k . The influence of gradients of quasi Fermi energies and the gradient of temperature on distribution functions was taken into account.

REFERENCES

- [1] K. Jóźwikowski, A. Jóźwikowska and M. Nietopiel, „ The non-equilibrium distribution function for electrons and holes in semiconductor heterostructures in steady state conditions”Entropy,17, pp4110-4133,2015
- [2] A.H. Marshak and K.M. van Vliet” Electrical current and carrier density in degenerate material with non-uniform band structure” Proc. IEEE,72,pp 148-162, 1984
- [3] J. S. Blakemore, ”Semiconductor Statistics”,chap.3, Pergamon Press, 1962