Nonstationary effects of the space charge in semiconductor structures

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A study of nonstationary effects of space charge in semiconductor structures, such as nonlinear wave interactions in active media operating in the microwave and millimeter wave range, is presented in this paper. Also, an exhaustive analysis of different models describing the propagation of space charge waves is carried out. Furthermore, we have concluded that the most appropriate nonlocal model to describe the space charge wave propagation in thin films possessing negative differential conductivity is the detailed balance model.
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I. INTRODUCTION

The millimeter and submillimeter microwave range is very important for applications in communications, radar, and spectroscopy. However, the structure of semiconductor devices (transistors, diodes, etc.), required for such a short wavelength, becomes very complex, which makes its fabrication difficult and expensive. One potential alternative in exploring the use of such a part of the electromagnetic spectrum resides in the use of nonlinear wave interaction in active media. For example, the space charge waves in thin semiconductor films, possessing negative differential conductivity (GaAs at 300 K and strained Si/SiGe heterostructures at 77 K), propagate at frequencies that are higher than the frequencies of acoustic and spin waves in solids. This means, for example, that an elastic wave resonator operating at a given frequency is typically 100 000 times smaller than an electromagnetic wave resonator at the same frequency. Thus attractively small elastic wave transmission components such as resonators, filters, and delay lines can be fabricated.

Space charge waves have been researched a long time ago, which can be traced back to the 1950s.[1,2] However, the early experimental work on the amplification of space charge waves with a perturbation field started in the 1970s,[1,3–8] which continues today. The first monolithic device using space charge waves was a two-port amplifier developed at the beginning of 1970s in the United States. This device contained a n-GaAs film on the dielectric substrate and a couple of source and drain Ohmic contacts (OCs). A microwave signal applied to the input electrode modulates the electron density under this electrode. These modulations are drifted to the drain and amplified due to the negative resistance effect. The amplified signal is taken from the output electrode placed near the drain, see Fig. 1. Obviously, the output signal is maximal when all the waves reach the output electrodes with the same phase.[9–12]

Devices based on space charge waves use an attractive property of GaAs. An electric field in excess of 3 kV/cm applied to a n-GaAs sample causes the differential electron mobility to become negative. To analyze the wave phenomena in thin films of two-valley semiconductors,[13–15] a set of equations to describe the charge transport is commonly used. In this theory, with small initial perturbations, continuity, momentum, and energy equations and Poisson's equation are solved. The solutions show that the modulations of electron density travel along the beam in the form of waves called space charge waves. The scope of space charge wave's applications is very large because it can be useful in implementing monolithic phase shifters, delay lines, and analog circuits for microwave signals.

The study of nonstationary effects of the space charge in semiconductor structures, applied to solid-state microwave devices using the negative differential conductivity phenomenon, will be one of the most relevant topics in microelectronics and communications in the coming years due to the potential it represents in terms of amplification of micro- and millimeter waves. However, in order to understand the behavior of nonstationary effects, a special attention must be paid to the transverse inhomogeneity, carrier-density fluctua-

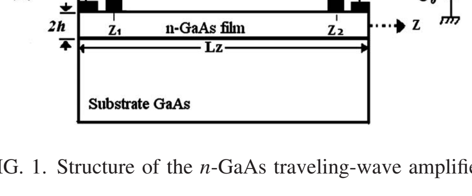

FIG. 1. Structure of the n-GaAs traveling-wave amplifier.

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tions in the plane of the film, because it may affect, in a negative way, the nonlinear wave interaction. Thus, a creation of effective algorithms and computer programs for simulations of nonlinear interaction of space charge waves in semiconductor films, where the effects of nonlocality and transverse inhomogeneity should be taken into account, becomes of high importance. Also, an exhaustive analysis of different models to describe the propagation of space charge waves is presented at the end of the work.

II. ELECTRON TRANSPORT MODELS

In this section, we study different models that describe the effect of an external electric field on free carriers in a semiconductor and compare with semiclassical carrier transport models. The response of these carriers to an electric field depends on the field intensity. There are two cases: the first case is when the electric field is low, so the behavior of carriers can be described by Ohm's law, and the second case is when the electric field is high, so that the average kinetic energy of the carriers becomes higher than the lattice energy. Since energetic electrons, also know as hot electrons, have sufficient energy to populate upper valleys of the conduction band.

Semiconductor device simulation has played an important role for the industrial development of integrated circuits in the last two decades. The semiclassical or quasiclassical carrier transport models are the most applicable for device simulation. The formulations used for calculating semiclassical carrier transport properties are based essentially on classical mechanics in the sense that one considers the electrons and holes as particles with well defined positions and crystal momentum, with the only exception for the duration of a collision, which is assumed negligible compared to the time between collisions; this system is completely analogous to an ideal classical gas.[16] The physical conditions for a semiclassical treatment in semiconductors for a very wide range of temperatures and fields are given in Refs. 16 and 17 so we can apply the classical treatment to the electron and hole gases in semiconductors. The most popular one is the drift-diffusion (DD) model; however, the DD model is not good enough in describing the nonlocal transport of carriers especially when feature sizes of devices are scaled down to the nanoscale region. Therefore, the transport models have been continuously refined and extended to more accurately capture transport phenomena occurring in this kind of devices. The DD model is the simplest current transport model which can be derived by integrating the Boltzmann's transport equation (BTE) in the momentum space. The hydrodynamic of the energy-balance equations for carrier density, momentum density, and energy density are obtained by the same method, assuming parabolic energy bands.[18,19,21] In the DD approach, the electron gas is assumed to be in thermal equilibrium with the lattice temperature. This section gives details about the semi-classical carrier transport treatment by DD model and balance-equation models.

A. Drift-diffusion model

The DD transport model for electrons reads:

$$J_n = ne\mu_n\mathbf{E} - e\,\nabla\,(D_n n), \tag{1}$$

where D_n is the diffusion coefficient, e is the magnitude of electronic charge, n is the electron density, and μ_n is the electron mobility, where μ_n is assumed as a function of the electric field $\boldsymbol{E}$. The term DD comes because the current density, J_n, is made up of two contributions: one due to the drift of electrons under the action of the electric field (first term), and the other due to the diffusion of electrons caused by gradients of electron density (second term).

B. Balance-equation models

Recently, the balance equations for carrier density, momentum density and energy density for semiconductors have received a significant attention in the the simulation of new devices. We empolyed two different balance-equation models: the first model is the detailed balance model by Kazutaka[15] and the second is the averaged balance model by Rodrigues Paulo[18] and Shur,[22] where the main difference is when the model incorporates the collision terms.

The first model considered is the detailed model where the balance equations are written for each valley.[15] It consists of balance equations for carrier density, momentum balance equation to describe the electron velocity, and energy balance equation for GaAs.

In GaAs an electron gas exists, defined as a large number of electrons N in a volume V, with different distribution function for each of its conduction band valleys. Therefore the balance equations are separately valid for each of the conduction band valleys in GaAs. The electrons in GaAs at a low electric field reside primarily in the Γ-valley, but at a high electric field the electron transfer to higher valleys takes place. It is a two-valley model in which only the Γ-valley and L-valleys are taken into account. Therefore, this model needs two sets of balance equations, namely, for the Γ-valley and the L-valleys. The following are the balance equations:

$$\frac{\partial n_i}{\partial t} = -\nabla\cdot(n_i v_i) + \left(\frac{\partial n_i}{\partial t}\right)_C, \tag{2}$$

$$\frac{\partial v_i}{\partial t} = -(v_i\nabla)v_i + \frac{eE_i}{m_i^*} - \frac{1}{n_i m_i^*}\nabla\,(n_i T_i) + \left(\frac{\partial v_i}{\partial t}\right)_C, \tag{3}$$

$$\frac{\partial w_i}{\partial t} = -v_i\cdot\nabla w_i + eE_i\cdot v_i - \frac{1}{n_i}\nabla\cdot\left[\left(n_i v_i - \frac{\kappa}{k_B}\nabla\right)T_i\right] + \left(\frac{\partial w_i}{\partial t}\right)_C, \tag{4}$$

where the subscript i is the valley index (i=1 for the Γ-valley and i=2 for the equivalent L-valleys). Therefore n_i, v_i, and w_i are, respectively, the carrier density, the average drift velocity, and the average energy in the valley i and $T_i=(2/3)\times(w_i - m_i v_i^2/2)$ is the electron temperature (energy units). $\boldsymbol{E}$ is the electric field and the index c represents the collision terms, in which the intervalley transfer between the Γ-valley and L-valleys is accounted for. The collision terms employed are as follows and can be found in Refs. 15 and 23:

$$\left(\frac{\partial n_i}{\partial t}\right)_C = -n_i\gamma_{nij}(w_i) + n_j\gamma_{nij}(w_j), \tag{5}$$

$$\left(\frac{\partial v_{di}}{\partial t}\right)_C = -v_{di}[\gamma_{pi}(w_i) + \gamma_{nij}(w_i)], \tag{6}$$

$$\left(\frac{\partial w_1}{\partial t}\right)_C = -(w_1 - w_0)\gamma_{w1}(w_1) + \frac{w_{12}(w_1)}{n_1}\left(\frac{\partial n_1}{\partial t}\right)_C, \tag{7}$$

$$\left(\frac{\partial w_2}{\partial t}\right)_C = -(w_2 - w_0)\gamma_{w2}(w_2). \tag{8}$$

Equations (5) and (6) are for both Γ- and L-valleys, while Eq. (7) is for the Γ-valley and Eq. (8) is for the L-valleys. γ_{nij} and γ_{nji} are the relaxation rates related to the variation in electron density due to the intervalley transfer and n_i and n_j are the electron concentrations in the ith and jth valleys. γ_{pi} is the momentum relaxation rate. γ_{w1} and γ_{w2} are the energy relaxation rates due to scattering within the valley. The second term on the right-hand side of Eq. (6) represents the momentum transfer due to the intervalley scattering from valley i to the valley j, and the second term on the right-hand side of Eq. (7) represents the energy transfer between valleys i and j associated with intervalley scattering. Therefore, w_{12} is the average transfer energy per electron. The value of w_{12} is also evaluated by Monte Carlo method by sampling and averaging the electron energies just before the intervalley transfer takes place.

The momentum relaxation $\gamma_p(w)$ and energy relaxation $\gamma_w(w)$ rates are defined for these equations based on the definition[15]

$$\gamma_p(w) = \frac{e|E(w)|}{m^*|v_d(w)|}, \tag{9}$$

$$\gamma_w(w) = \frac{e|E(w)|\cdot|v_d(w)|}{w - w_0}, \tag{10}$$

where e is the electronic charge, $\boldsymbol{E}$ is a uniform electric field applied along the material, $m^*|v_d(w)|$ is the average momentum of electrons in the ith valley, which is a function of the average electron energy w, and w_0 is the background electron energy density associated with the lattice temperature.

The relaxation rates γ_{nij}, γ_{nji}, γ_{pi}, and γ_{w1} are calculated with the Monte Carlo method, as described in Refs. 15 and 24.

The averaged balance models[18,22] are similar to the detailed balance model,[15] except that these models do not take into account the intervalley transfer terms directly; besides n, v, w, and m^* are averaged over the available conduction band valleys:

$$n = n_\Gamma + n_L,$$

$$v = (n_\Gamma v_\Gamma + n_L v_L)/n,$$

$$w = (n_\Gamma w_\Gamma + n_L w_L)/n,$$

$$m^* = (n_\Gamma m_\Gamma + n_L m_L)/n. \tag{11}$$

The average electron energy consists of a drift component and a thermal one associated with the random motion for averaged balance model,[22] Eq. (12). However, in the case of the averaged balance model[22] an additional term is added, $F\Delta_{LU}$, such as Eq. (13).

$$w = \tfrac{1}{2}m^* v^2 + \tfrac{3}{2}T_e, \tag{12}$$

$$w = \tfrac{1}{2}m^* v^2 + \tfrac{3}{2}T_e + F\Delta_{LU}, \tag{13}$$

where T_e is the electron temperature in energy units. The difference appears in the specified form $F\Delta_{LU}$, where $F(w)$ is the probability of occupancy of states in the upper valleys, which is also assumed to be a function of w only, and $F\Delta_{LU}$ is a constant. Furthermore, F has an absolute value in the low and high energy limits, where F equals to 0 and 1, respectively (the electrons are situated either in the lower valley or in the upper ones). The constant $F\Delta_{LU}$ expresses a difference between the bottoms of the Γ- and L-valleys. In our simulations we take $F\Delta_{LU}$=0.36 eV. Thus, the model[18] coincides with Ref. 22 when F=0.

These averaged balance models use the single-electron-gas approximation and accounts for all the intervalley transfer effects using effective values for carrier velocity, energy, effective mass, and relaxation rates. It is assumed that the energy, the momentum relaxation rates, and the averaged effective electron mass depend on the averaged electron energy w. In general, these averaged balance models do not take into account the thermoconductivity term; however, an expression is necessary for the thermoconductivity of the electron gas. The inclusion of thermoconductivity may explain the fact that the model of Rodrigues Paulo[18] gave acceptable results for simulations of short (<0.5 μm) transistor structures, which seems from theoretical considerations to be

$$\kappa = \left(\frac{5}{2} + r\right)n\frac{k_B{}^2\mu(T_e)}{e}T_e. \tag{14}$$

where k_B is the Boltzmann constant. Several different choices for r can be found in the literature, while many other authors[25,26] neglect heat conduction in their models.

III. NONSTATIONARY CARRIER TRANSPORT IN *n*-GaAs THIN FILMS

To describe the nonstationary carrier transport in GaAs devices, it is necessary to use Monte Carlo methods or hydrodynamic (or energy transport) models which incorporate the population transfer between different valleys. To describe the propagation of space charge waves in n-GaAs thin films, the hydrodynamic models have been widely studied.[13–27] We consider three different two-valley quasihydrodynamic models for space charge wave propagation, intended for electron transport, in GaAs. They are simple DD model, detailed balance model,[15] and averaged balance model.[18,22] These models use balance equations where carrier transport can be analyzed by following spatial and temporal variations in particle, momentum, and energy densities. The detailed balance model is described in Ref. 15; it incorporates the colli-

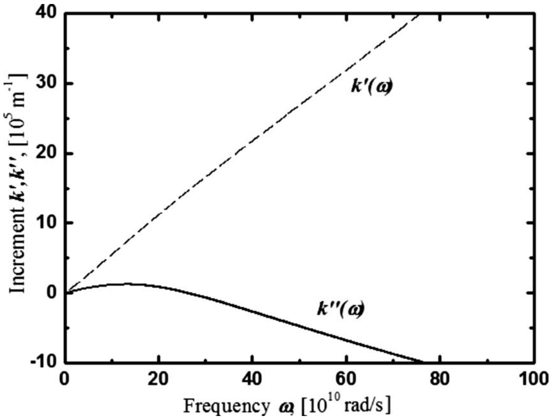

FIG. 2. Simulation results obtained with the detailed balance model (Ref. 15).

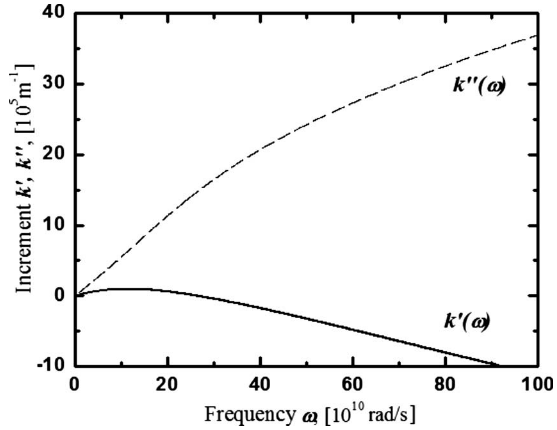

FIG. 3. Simulation results obtained with DD transport model.

sion terms for two valleys. The averaged balance models[18,22] do not take into account the collision terms directly; also n, v, w, and m^* are averaged over the available conduction band valleys, described in Eq. (11). There is no variation in averaged electron energy term between averaged models, like what was described in Sec. II too.

In this section, a comparative study of three two-valley quasihydrodynamic models for space charge wave propagation in n-GaAs semiconductor thin films with respect to the spatial increment is presented. In particular, the results show that the detailed model is appropriate in describing the space charge waves. The averaged balance model may lead to incorrect results in the case of long structures, whereas in the short structures the thermoconductivity becomes dominating and such model yields correct results.

The space charge wave propagation in thin n-GaAs films has been considered within a framework of different quasihydrodynamic balance models. A comparative study of the dependencies $k(\omega)$ of a complex longitudinal wave number on frequency, which is obtained from different balance-equation models, is presented and discussed by using the dispersion relation $|D(\omega,k)|=0$. The dispersion relations $k(\omega)$ have been calculated numerically within the framework of different balance models with a program in FORTRAN. The unperturbed (stationary) values of E_0 and v_0 have been chosen in the regime of negative differential conductivity ($dv/dE<0$). The results of direct simulations of $k(\omega)$ of linearized equations are shown in Figs. 2–4. In general, we consider the cases where ω is real and $k=k'+ik''$ has real and imaginary parts. The case $k''>0$ corresponds to the spatial increment (amplification), whereas the case $k''<0$ corresponds to the decrement (damping). In Fig. 2, the spatial increment for detailed balance model[15] is shown. This model seems to be the most correct one because $k''(\omega)$ has positive values only for the frequencies below 30×10^{10} rad/s. This is correct because in this frequency range we can obtain the amplification of space charge waves in a thin film of GaAs. In Fig. 3, the spatial increment for the simple DD model is shown and it seems to be correct too. In Fig. 4 one can see the real and imaginary parts of the longitudinal wave number $k(\omega)$ for the averaged balance model.[18,22] This model has some problems when it does not consider the thermoconductivity term because $k''(\omega)$ gets positive values for frequencies $\omega>50\times10^{10}$ rad/s, which is not realistic and means that one always has an active medium for any value of frequency. Note that the decrease in k'' with the increase in ω ($\omega>90\times10^{10}$ rad/s) can be obtained when the thermal conductivity is taken into account. The influence of thermal conductivity may explain the fact that the model by Rodrigues Paulo[18] gave acceptable results under a simulation of short (<0.5 μm) transistor structures. The Shur model gives qualitatively the same behavior of the spatial increment $k''(\omega)$. Note that the inclusion of thermoconductivity gets better results and has physical meaning.

The frequency dependence of $k(\omega)$ was obtained from different balance-equation models presented and discussed here. The most appropriate model in describing the space charge wave propagation in thin films possessing negative differential conductivity is the detailed balance model.[15] It has been demonstrated that the balance models with averaging over the different values may give incorrect results under simulations of space charge waves in semiconductors possessing negative differential conductivity. A qualitative explanation of this is neglecting the jumplike intervalley transitions in the balance models with averaging. However, when taking into account the thermoconductivity, the averaged balance model[18,22] can lead to reasonable physical results.

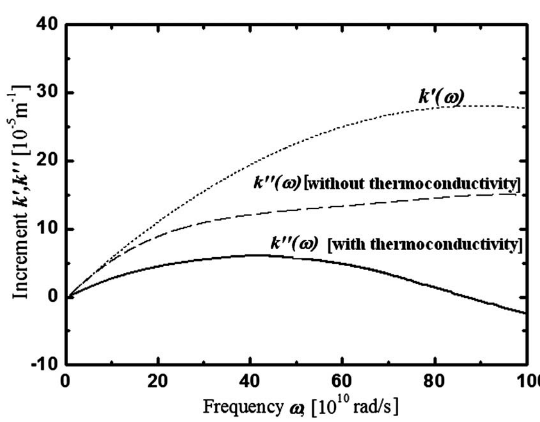

FIG. 4. Simulation results obtained with the averaged balance energy balance model (Refs. 18 and 22) with and without thermoconductivity term.

IV. PROPAGATION AND AMPLIFICATION OF SPACE CHARGE WAVES IN *n*-GaAs THIN FILMS

The propagation and amplification of space charge waves in *n*-GaAs thin films with negative differential conductivity have been widely studied[7–11] in the past few decades; however, an exhaustive study about the best model to describe the amplification and a two-dimensional (2D) analysis has not been fully addressed. The numerical simulations are performed with the device shown in Fig. 1. The coordinate system is chosen as follows: *X*-axis is oriented perpendicular to the film, the drift field E_0 is applied along the *Z* direction, and exciting and receiving antennas [coupling elements (CEs)] are parallel to the *Y*-axis. A 2D model of electron gas in the thin *n*-GaAs epitaxial film is used. Thus, the 2D electron concentration is present only in the *Y*-*Z* plane at $x=0$. The space charge waves possessing phase velocity equal to drift velocity of electrons $V_0=V(E)$ and $E_0=U_0/L_z$ are considered, where U_0 is the bias voltage, L_z is the length of the film, and the length of the active region is the distance between the CEs. This length must also be greater than several space charge wave wavelengths. Generally, a nonlocal dependence of the drift velocity v of electrons on the electric field takes place.

Figure 1 shows the layout (transversal view) of a thin-film structure with a planar design implementing the structure. A *n*-GaAs epitaxial film with a thickness of 0.1–1 μm is put on an *i*-GaAs semi-insulating substrate. The 2D electron density in the film is chosen to be $n_0=10^{15}$ m^{-2}. On the film surface are the cathode and anode OCs, together with the input and output CEs. Designed as a Schottky-barrier strip contacts, the CEs connect the sample structure to microwave sources. A dc bias voltage (above the Gunn threshold of 3 kV/cm) was applied between the cathode and anode OCs, causing negative differential conductivity in the film. The CEs perform the conversion between electromagnetic waves and space charge waves, where the excitation of space charge waves in the 2D electron gas takes place. In the simulations an approximation of 2D electron gas is used. The set of balance equations for concentration, drift velocity, and averaged energy in describing the dynamics of space charge waves within the thin GaAs film takes the following detailed model.[15]

A small microwave electric signal $E_{\text{ext}}=E_m\times\sin(\omega t)\times\exp\{-[(t-t_1)/t_0]^2\}\times\exp\{-[(z-z_1)/z_0]^2\}$ is fed in the input antenna. Here z_1 is the position of the input antenna and z_0 is its half-width. Therefore, the parameter $2t_0$ determines the duration of the input electric pulse. In our simulations, this parameter is $2t_0=2.5$ ns. The carrier frequency ω is in the microwave range $\omega=3\times10^{10}-3\times10^{11}$ rad/s.

When a small microwave signal is applied to the input antenna, the excitation of space charge waves in the 2D electron gas takes place. The space charge waves are subject to amplification due to the negative differential conductivity.

The set of equations of detailed model has been solved numerically. The stable implicit difference scheme has been used. A transverse inhomogeneity of the structure in the plane of the film along the y axis has been taken into account. The following parameters have been chosen: 2D electron concentration in the film is $n_0\approx10^{11}$ cm^{-2}, the initial uniform drift velocity of electrons is $V_0\approx1.7\times10^7$ cm/s ($E_0=4.5-4.7$ kV/cm), the length of the film is $L_z=50-100$ μm, and the thickness of the film is $2h=0.1-1$ μm.

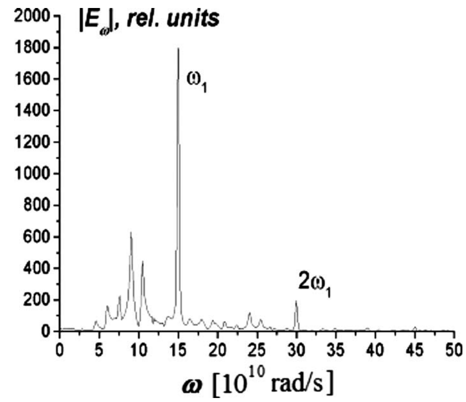

FIG. 5. Spectral components of the electric field of space charge wave at the output antenna (its position is $z_2=95$ μm and $y_2=500$ μm). The length of the film is 100 μm. The transverse width of the film along the *Y* axis is 1000 μm. A visible effective excitation of the second harmonic ($2\omega_1=30\times10^{10}$ rad/s).

The typical output spectrum of the electromagnetic signal is given in Fig. 5. The input carrier frequency is $\omega=15\times10^{10}$ rad/s. The amplitude of the input electric microwave signal is $E_m=25$ V/cm. Although the growth rate decreases as the rf increases, in our case an amplification of 20 dB is obtained. The duration of the input pulse is $2t_0=2.5$ ns. The maximum of the input pulse occurs at $t_1=2.5$ ns. One can see both the amplified signal at the first harmonic of the input signal and the second harmonic of the input signal, which is generated due to the nonlinearity of space charge waves. The spatial distributions of the alternate component of the electric field $E^{\sim}_z$ are shown in Fig. 6. The length of the film is 100 μm. The transverse width of the film along the *Y* axis is 1000 μm. The duration of the input electric pulse is 2.5 ns. The spatial distributions are presented for the time moment of 1.5 ns after the maximal value of the input signal.

V. CONCLUSIONS

A study of nonstationary effects of space charge in semiconductor structures, such as nonlinear wave interactions in

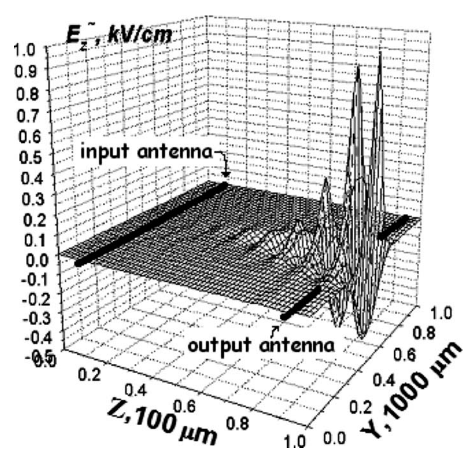

FIG. 6. The spatial distribution of the alternative part of the electric field component $E^{\sim}_z$ of space charge wave at frequency is $\omega=15\times10^{10}$ rad/s.

active media operating in the microwave and millimeter wave range, has been presented in this paper. For this reason, an exhaustive study, at least theoretically, of nonlinear interaction of space charge waves in active media with negative differential conductivity has been carried out, taking into account that the space charge waves operate in thin semiconductor film, possessing negative differential conductivity, and propagate at frequencies that are higher than acoustic and spin waves in solids. Furthermore, the most appropriate nonlocal model in describing the space charge wave propagation in thin films possessing negative differential conductivity is the detailed balance model. It has been demonstrated that the balance models, with averaging over the different energy values, may give incorrect results under simulations of space charge waves in semiconductors possessing negative differential conductivity. A qualitative explanation of this is the under estimation of the jumplike intervalley transitions in the balance models with averaging. However, when thermoconductivity is taken into account, the averaged balance model can lead to physical results. This analysis allows selecting the agreement model to study the propagation and amplification of space charge waves in *n*-GaAs thin films.

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