SPACE CHARGE WAVE DISPERSION IN SILICON WITH ACCOUNT OF HEAT CONDUCTIVITY AND QUANTUM PROPERTIES OF ELECTRON

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An analysis that incorporates quantum corrections and the thermal conductivity term into the classical hydrodynamic model of the propagation of space-charge waves in silicon is presented. From numerical simulations, it is seen that, for frequencies $f < 8$ THz, the classical hydrodynamic model (HD) with the thermal conductivity term and with quantum corrections gives good results, where the thermoconductivity seems to be more essential for these frequencies at room temperature. However for higher frequencies $f > 8$ THz, both quantum corrections and thermoconductivity are important. These results suggest that the accurate simulations of an ultra-small device require the thermal conductivity term to be included in the model.

1. Introduction

When devices are scaled down to ultra-small lengths, the carrier transport becomes different from that in the classical description, because the carrier velocity does not depend on a local electric field, but on the carrier energy, which is a function of spatial and temporal variations of the electric field or, in other words, depends on the nonlocal electric field [1]. Therefore, the classical drift-diffusion (DD) model is no longer satisfactory for the simulation of small devices, since it fails to predict nonstationary effects, such as velocity overshoot and carrier diffusion due to electron temperature gradients. Moreover, the scaling of feature sizes of Silicon Metal Oxide Semiconductor Field Effect Transistors (MOSFETs), compound semiconductor Heterostructure Field Effect Transistors (HFETs), and Heterojunction Bipolar Transistors (HBTs) has pushed the device parameters into the region, where the transistor operation at a few hundred GHz becomes feasible [2].

The microwave technology of monolithic integrated/hybrid circuits moves gradually into the millimeter wave range, up to and above 100 GHz. The development and the manufacturing of microwave or millimeter-wave integrated semiconductor devices depend on the development of computer-aided design tools, based on the accuracy and the adequacy of mathematical models and the rigorous solution of quantum hydrodynamic equations. It was shown in [3] that, when the temperature is not too low, two-dimensional electrons in the channel of a Field Effect Transistor (FET) behave not as a gas (as conventionally expected) but rather as a fluid. Indeed, as one can show, the electron mean free path for collisions with impurities and phonons is much greater than the mean free path for electron-electron collisions. This means that the theoretical description of the electron flow in the FET channel should be based on the equations of hydrodynamics.

A variety of models have been developed for the semiconductor device simulation. However, the classical HD can be extended to include quantum effects by incorporating the quantum corrections, this model being called the quantum hydrodynamical (QHD) one [4]. The QHD model is derived from a moment expansion of the Wigner–Boltzmann equation, using a quantum Maxwellian distribution to close the moments [5, 6]. The QHD conservation laws have the same form as the classical hydrodynamic equations, but the energy density and the stress tensor include additional quantum terms. These quantum corrections allow the particle tunneling through potential barriers and make it possible to build up a potential well.

In this investigation, we use the QHD transport equations expressed in terms of the conservation laws for particles, momentum, and energy, together with the Poisson's equation, to analyze the propagation of volume space-charge waves in silicon. The linear modes of propagation are studied by means of the dispersion equation $D(\omega, k) = 0$ which relates the frequency ω to the longitudinal wave number (or the propagation constant) $k = 2\pi/\lambda$. In general, we consider the cases where ω is real and $k = k' + ik''$ has the real and imaginary parts. The real values of the circular frequency ω correspond to a physical problem of the excitation of waves by an external source [7], like THz irradiation. The case $k'' > 0$ corresponds to the spatial increment (amplification), whereas the case $k'' < 0$ corresponds to the decrement (attenuation, damping) [7, 8]. To obtain the dispersion equation for space-charge waves, it is necessary to use the linear equations of the electron dynamics jointly with the Poisson's equation for the electric potential.

The amplification of space-charge waves is due to the negative differential conductivity, as shown in [9, 10] for the case of GaAs structures in the microwave range. However, the negative differential conductivity does not appear in silicon, so the amplification is not possible but only the propagation and the damping of space-charge waves and plasma wave excitation in submicron field effect transistors, which should allow us to develop a new generation of solid-state tunable terahertz devices that will find numerous applications in industry such as spectroscopy, radar systems, and biotechnology [11].

In this work, we have studied the case where the quantum corrections and the thermal conductivity term are included into the balance equations, which allows us to clarify the propagation of space-charge waves in silicon structures. One can see that, for frequencies $f < 8$ THz, the classical hydrodynamic model added by the thermal conductivity term and quantum corrections gives good results. However, for frequencies $f > 8$ THz, both the thermoconductivity and quantum correction terms give essential inputs, and it is difficult to conclude about which correction term is more important. These results can also be used in the simulation of semiconductor devices of ultra-short lengths.

2. The Quantum Hydrodynamic Model

The QHD model has the same form as the classical hydrodynamic equations only with quantum corrections to the energy density and stress tensor terms. Thus, we employ initially the following set of classical balance equations regarding the carrier density, average velocity, and average energy for electrons added by the Poisson's equation [12]:

$$\frac{\partial n}{\partial t} + \nabla (nv) = 0, \quad (1)$$

$$\frac{\partial v}{\partial t} + (\nabla v)\, v = \frac{qE}{m^*} - \frac{1}{nm^*}\nabla (nk_{\mathrm{B}}T) - \gamma_p (w)\, v, \quad (2)$$

$$\frac{\partial w}{\partial t} + \left(\vec{v}\vec{\nabla}\right) w = q\vec{E}\vec{v} - \frac{1}{n}\nabla (k_{\mathrm{B}}nvT - \kappa\nabla T) -$$

$$-\gamma_w (w)\,(w - w_{00}), \quad (3)$$

$$\varepsilon_0\varepsilon\Delta\varphi = -q(n - n_0), \quad (4)$$

where n is the electron concentration, v is the electron velocity, m^* is the effective electron mass, q is the electron charge, w is the average electron energy; k_{B} is the Boltzmann's constant; and w_{00} is the average electron energy at the temperature of the lattice (when the temperature of the lattice is $T_{00} = 300K$, $w_{00} = 0.026$ eV). The electron temperature (in Kelvins) is $T = (2/3k_{\mathrm{B}})\left(w - m^* v^2/2\right)$, and the electron thermal conductivity can be approximated in a nondegenerated case as in [13] $\kappa = (5/2)\left(nk_{\mathrm{B}}^2 T/m^*\gamma_p (w)\right)$, $\mathbf{E} = -\nabla\varphi$ is the electric field, and γ_p and γ_w are the momentum and energy relaxation rates, respectively.

Then we take into account the quantum corrections in Eqs. (2) and (3) to the stress tensor P_{ij}, the average energy w, and the thermoconductivity taken from [4, 5, 14]. The expressions for the stress tensor and the average energy with quantum corrections can be written as follows:

$$P_{ij} = -nk_{\mathrm{B}}T\delta_{ij} + \frac{\hbar^2}{4m^*} n \frac{\partial^2}{\partial x_i \partial x_j}\log (n)\,;$$

$$w = \frac{1}{2}mv^2 + \frac{3}{2}k_{\mathrm{B}}T - \frac{\hbar^2}{8m^*}\Delta \log (n)\,. \quad (5)$$

These expressions were derived from the equations for the moments of a quantum kinetic equation for the Wigner function [4].

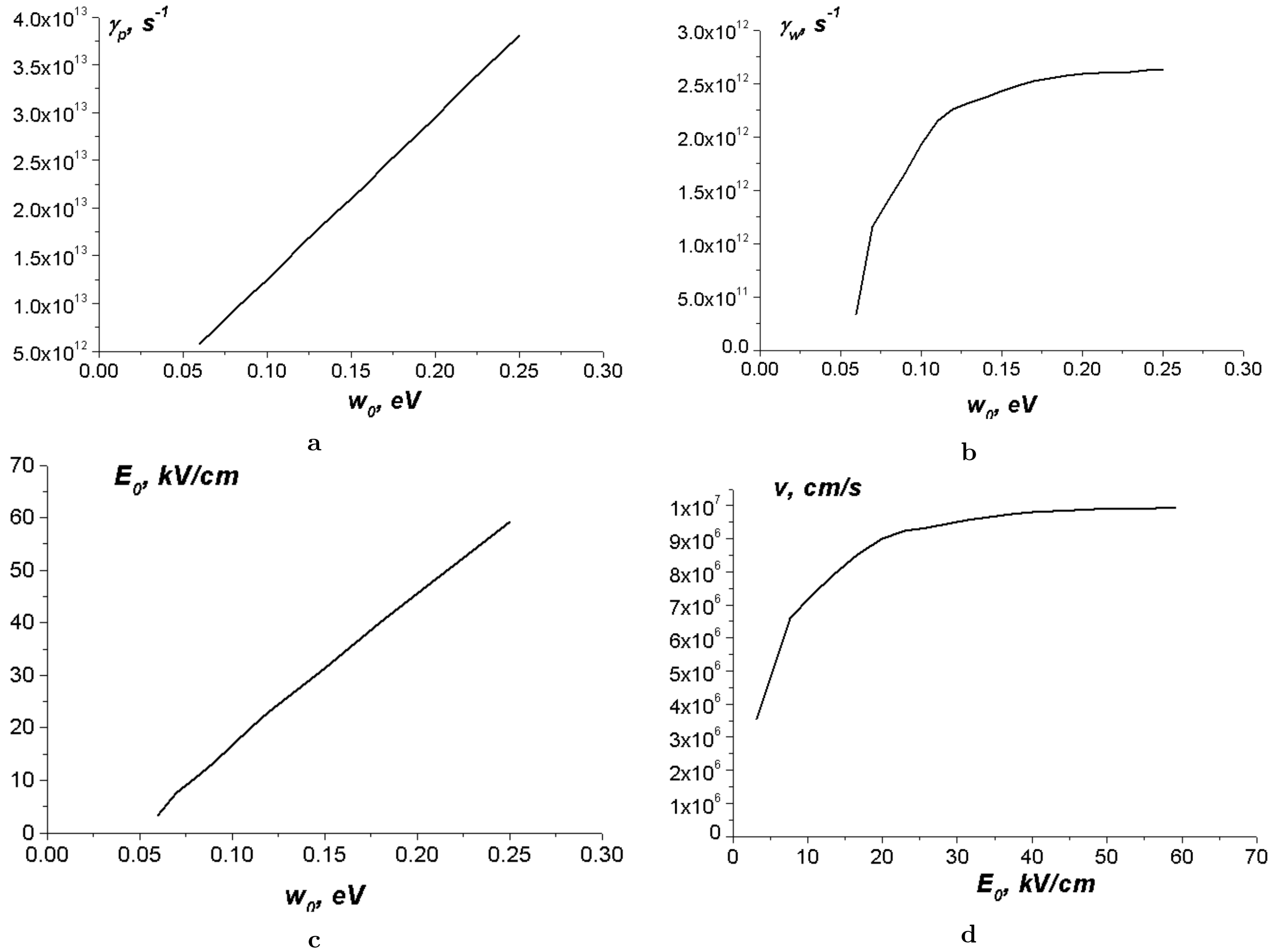


Fig. 1. Data used in simulations for silicon at room temperature of the lattice, $T_{00} = 300$ K. Dependences of the momentum relaxation rate γ_p (a) and the energy relaxation rate $\gamma_w(w)$ (b) on the average electron energy w; the relation between the bias electric field E and w (c); the dependence of the drift electron velocity v on the bias electric field E (d)

In the one-dimensional case, the equations with quantum corrections are given in the following manner. Equation (1) for the carrier density is the same; however, the equations for the average velocity and the average energy have some differences:

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial z} = \frac{qE}{m^*} - \frac{1}{nm^*}\frac{\partial}{\partial z}\times \left[nk_{\mathrm{B}}T - \frac{\hbar^2}{4m^*}n\frac{\partial^2}{\partial z^2}\log(n)\right] - v\gamma_p(w); \tag{6}$$

$$\frac{\partial w}{\partial t} + v\frac{\partial w}{\partial z} = qEv - (w - w_{00})\gamma_w(w) - \frac{1}{n}\frac{\partial}{\partial z}\times \left[v\left(nk_{\mathrm{B}}T - \frac{\hbar^2}{4m^*}n\frac{\partial^2}{\partial z^2}\log(n)\right) - \kappa\frac{\partial T}{\partial z} - \frac{\hbar^2}{8m^*}n\frac{\partial^2 v}{\partial z^2}\right]. \tag{7}$$

In the equation for the average energy w, the quantum correction term $(\sim\partial^2 v/\partial z^2)$ for the thermoconductivity [5, 14] has been added.

We now consider linear space-charge waves $n = n_0 + \tilde{n}$; $\vec{v} = v_0 + \tilde{\vec{v}}$; $w = w_0 + \tilde{w}$; $T = T_0 + \tilde{T}$, where all the small perturbations obey the law $\sim \exp(i(\omega t - kz))$, and use the parameters of silicon from [12]. The dependences of the momentum and energy relaxation rates on the average electron energy are given in Fig. 1,*a*,*b*. Note that the momentum relaxation rate is of order of $(1 \div 4) \times 10^{13}$ s^{-1}, whereas the energy relaxation one is smaller: $(2 \div 3) \times 10^{12}$ s^{-1}; the saturated drift velocity is

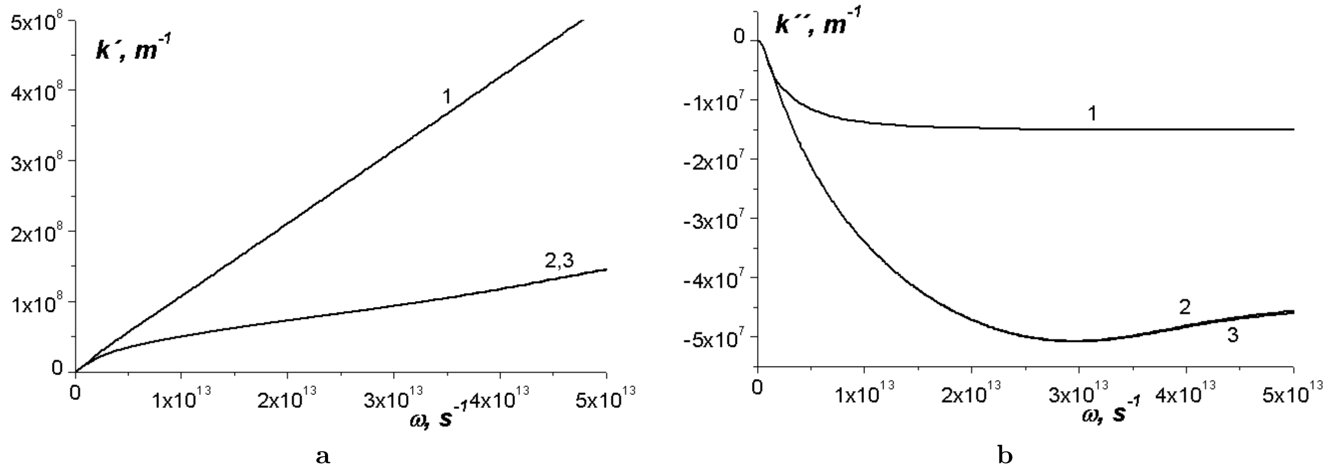


Fig. 2. Dependences of the real (*a*) and imaginary (*b*) parts of the wave number of space-charge waves on the frequency ω; $n_0 = 10^{14}$ cm^{-3}, $E_0 = 31$ kV/cm (the average electron energy is $w_0 = 0.15$ eV). Curve *1* is without both thermoconductivity and quantum corrections, curve *2* is with the thermoconductivity only, and curve *3* is with both the thermoconductivity and quantum corrections

$v_0 = 10^5$ m $\cdot$ s^{-1}, see Fig. 1,*d*. The characteristic spatial scale is $l_n = 10^{-8}$ m $\equiv$ 10 nm.

The linearized quantum hydrodynamic equations and the Poisson's one for perturbations can be presented as:

$$\frac{\partial \tilde{n}}{\partial t} + v_0 \frac{\partial \tilde{n}}{\partial z} + n_0 \frac{\partial \tilde{v}}{\partial z} = 0; \qquad (8)$$

$$\frac{\partial \tilde{v}}{\partial t} + \frac{v_0}{3}\frac{\partial \tilde{v}}{\partial z} + \gamma_p \tilde{v} = \frac{q\tilde{E}}{m^*} - \frac{k_B T_0}{n_0 m^*} \times$$
$$\times \left[1 - \frac{\hbar^2}{6m^* k_B T_0}\frac{\partial^2}{\partial z^2}\right]\frac{\partial \tilde{n}}{\partial z} - \left[\frac{2}{3m^*}\frac{\partial}{\partial z} + v_0 \frac{d\gamma_p}{dw}\right]\tilde{w}; \qquad (9)$$

$$\frac{\partial \tilde{w}}{\partial t} + \frac{5v_0}{3}\frac{\partial \tilde{w}}{\partial z} - \frac{2}{3k_B}\frac{\kappa}{n_0}\frac{\partial^2 \tilde{w}}{\partial z^2} + \gamma_w \tilde{w} = q\left(v_0 \tilde{E} + E_0 \tilde{v}\right) -$$
$$-\left[k_B T_0 - \frac{2}{3}m^* v_0^2 + \frac{2\kappa}{3k_B n_0} m^* v_0 \frac{\partial}{\partial z} - \frac{\hbar^2}{8m^*}\frac{\partial^2}{\partial z^2}\right]\frac{\partial \tilde{v}}{\partial z} -$$
$$-\frac{v_0 k_B T_0}{n_0}\left[1 - \frac{\hbar^2}{6m^* k_B T_0}\frac{\partial^2}{\partial z^2}\right]\frac{\partial \tilde{n}}{\partial z}; \qquad (10)$$

$$\frac{\partial \tilde{E}}{\partial z} = \frac{q\tilde{n}}{\varepsilon_0 \varepsilon}. \qquad (11)$$

3. Simulations and Results

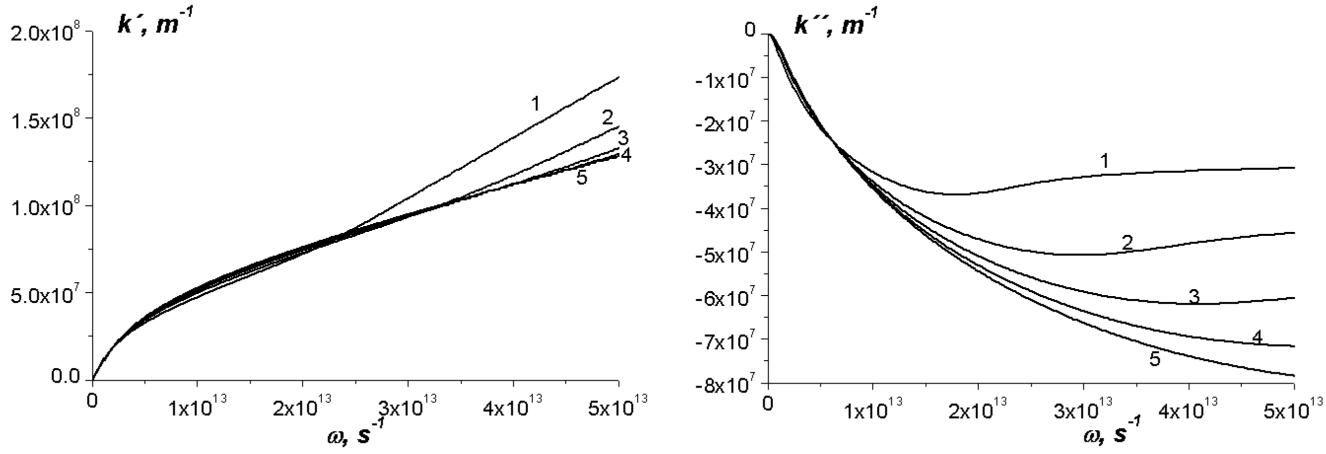
Consider first the simplest case of relatively low frequencies $\omega \ll \gamma_w$, where the drift-diffusion equations are valid. The dispersion equation $k = k(\omega)$ takes the following well-known form [7]:

$$Dk^2 - v_0 k + (\omega + i\omega_M) = 0. \qquad (12)$$

Here, $D \approx k_B T_0 / (m^* \gamma_p)$ is the diffusion coefficient, and $\omega_M = q^2 n_0 / (\varepsilon_0 \varepsilon m^*) \times (dv/dE)$ is the Maxwellian relaxation frequency. The space-charge waves possess relatively low attenuation under the following condition: $\omega_M \ll \omega \ll v_0^2/D$. Because the relaxation frequency ω_M is proportional to the concentration n_0, it is rather better to consider the case of lower concentrations $n_0 \leq 10^{15}$ cm^{-3}. Moreover, it seems natural to utilize the high values of bias electric fields E_0, where the saturation of the electron drift velocity $v(E)$ occurs, see Fig. 1,*d*. But, at high bias electric fields, the electron temperature becomes essentially higher than the lattice one: $T_0 > T_{00} \equiv 300$ K. So, we restrict ourselves below by the values of electron concentration $n_0 = 10^{14} \div 10^{16}$ cm^{-3}, and the bias electric fields are $E_0 = 10 \div 80$ kV/cm. The main goal of our calculations is to specify the possible frequency ranges of relatively low attenuation of space-charge waves at room temperature of the lattice and to clarify an influence of thermoconductivity and quantum corrections on the attenuation.

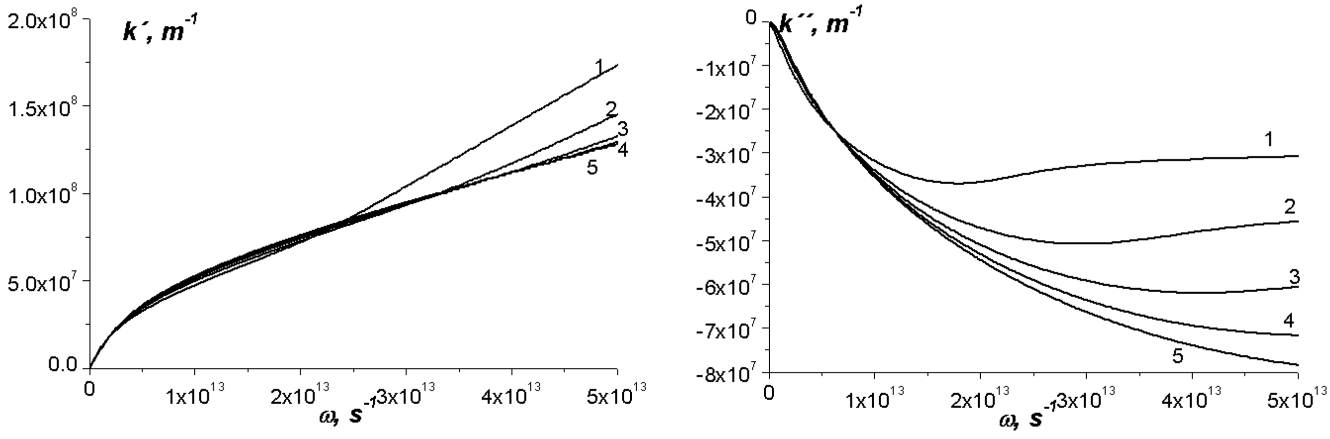
The dispersion relations $k(\omega)$ have been calculated within the framework of the balance equations added by the Poisson's equation (8)–(11). The results of direct numerical simulations of $k'(\omega)$ and $k''(\omega)$ of linear equations are shown in Figs. 2–5 at room temperature of the lattice, $T_{00} = 300$ K.

The influence of thermoconductivity and quantum corrections on the dispersion of space-charge waves is seen from Fig. 2, where the dependences k' (ω) and k'' (ω) are given for $E_0 = 31$ kV/cm ($w_0 = 0.15$ eV). In Fig. 2, the dispersion is presented for three cases: namely, when the classical hydrodynamic equations have been



a **b**

Fig. 3. Dependences of the real (a) and imaginary (b) parts of the wave number of space-charge waves on the frequency ω; the electron concentration is $n_0 = 10^{14}$ cm^{-3}. Both the thermoconductivity and quantum corrections are taken into account. Curve *1* is at $w_0 = 0.1$ eV ($E_0 = 17$ kV/cm), *2* is at $w_0 = 0.15$ eV ($E_0 = 31$ kV/cm), *3* is at $w_0 = 0.20$ eV ($E_0 = 46$ kV/cm), *4* is at $w_0 = 0.25$ eV ($E_0 = 59$ kV/cm), and *5* is at $w_0 = 0.30$ eV ($E_0 = 73$ kV/cm)

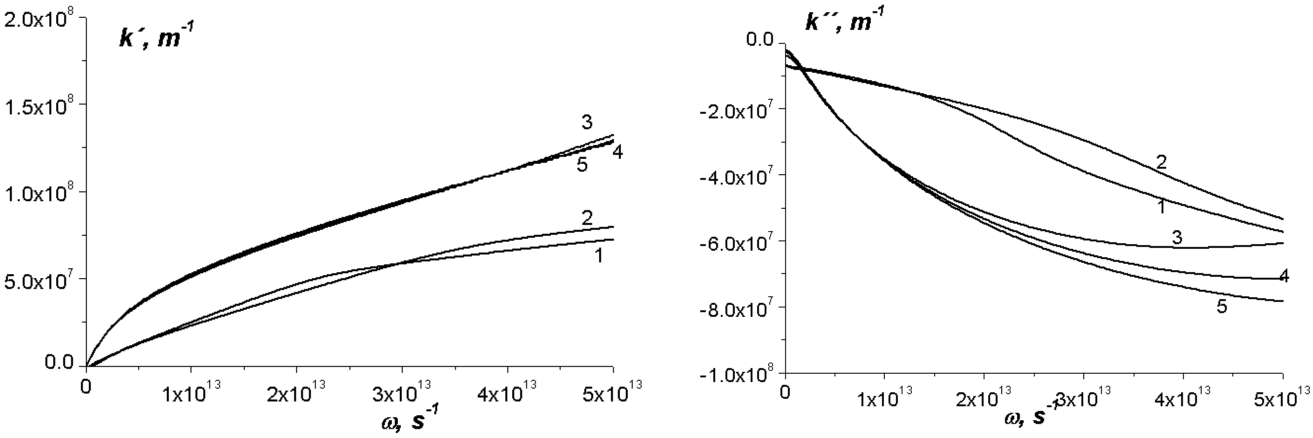


a **b**

Fig. 4. Dependences of the real (a) and imaginary (b) parts of the wave number of space-charge waves on the frequency ω; $n_0 = 10^{15}$ cm^{-3}. Both the thermoconductivity and quantum corrections are taken into account. Curve *1* is at $w_0 = 0.1$ eV, *2* is at $w_0 = 0.15$ eV, *3* is at $w_0 = 0.20$ eV, *4* is at $w_0 = 0.25$ eV, and *5* is at $w_0 = 0.30$ eV

used without both the thermal conductivity term and quantum corrections, with the thermal conductivity only, and with both the thermal conductivity and quantum corrections. One can see that namely the thermal conductivity is the most important in the frequency range 5×10^{12} s$^{-1} \le \omega \le 5\times10^{13}$ s^{-1}. The role of quantum corrections becomes important only at the frequencies $\omega \ge 10^{14}$ s^{-1} (in the infrared range), when the following condition is satisfied: $h^2|k|^2/m^* \ge k_\mathrm{B}T_0$, see Eqs. (9)–(11).

In Figs. 3–5, the dispersion of space-charge waves is given for different values of electron concentration n_0. When the electron concentration is chosen as $n_0 \le 10^{15}$ cm^{-3}, the dispersion of space-charge waves $k(\omega)$ is practically the same for different values of n_0. But at higher values of electron concentration $n_0 \approx 10^{16}$ cm^{-3}, both the real part $k'(\omega)$ and the imaginary part $k''(\omega)$ of the wave number are changed drastically. To excite a space-charge wave with smaller attenuation, it seems better to use the smaller values of electron concentration



a b

Fig. 5. Dependences of the real (a) and imaginary (b) parts of the wave number of space-charge waves on the frequency ω; $n_0 = 10^{16}$ cm^{-3}. Both the thermoconductivity and quantum corrections are taken into account. Curve *1* is at $w_0 = 0.1$ eV, *2* is at $w_0 = 0.15$ eV, *3* is at $w_0 = 0.20$ eV, *4* is at $w_0 = 0.25$ eV, and *5* is at $w_0 = 0.30$ eV

$n_0 \sim 10^{15}$ cm^{-3}. Moreover, in different frequency ranges $\omega \leq 10^{13}$ s^{-1} and $\omega \geq 10^{13}$ s^{-1}, the minimum attenuation of space-charge waves is realized for different bias electric fields. Namely, at smaller frequencies, the attenuation is smaller at high bias electric fields E_0>30 kV/cm, whereas, at higher frequencies due to an influence of the thermoconductivity, the lower bias electric fields $E_0 < 20$ kV/cm are preferable.

The attenuation of space-charge waves at the frequencies $\omega \sim 2 \times 10^{13}$ s^{-1} is very high, if the lattice temperature is $T_{00} = 300$ K. Therefore, to decrease the attenuation, it is necessary to cool silicon devices.

This work is of interest for theoretical studies of new hydrodynamic phenomena in a two-dimensional electron fluid. These phenomena taking place in the channel of a ballistic FET may be used for the generation and detection of the terahertz radiation. Such transistors can be used also as oscillators, mixers, frequency multipliers, and detectors [11].

4. Conclusions

We have presented and discussed the dependences of the real $k'(\omega)$ and imaginary $k''(\omega)$ parts of the complex longitudinal wave number on frequency, which are obtained from balance equations with regard for the thermal conductivity term and quantum corrections. For frequencies $f \equiv \omega/2\pi \leq 8$ THz, the thermal conductivity term is more essential than the quantum corrections. For frequencies $f > 10$ THz, both the thermal conductivity term and quantum corrections are important at room temperature of the lattice.

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ДИСПЕРСІЯ ХВИЛЬ ПРОСТОРОВОГО ЗАРЯДУ В КРЕМНІЇ З ВРАХУВАННЯМ ТЕПЛОПРОВІДНОСТІ ТА КВАНТОВИХ ВЛАСТИВОСТЕЙ ЕЛЕКТРОНІВ

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Р е з ю м е

Проаналізовано поправки на теплопровідність електронного газу та на його квантові властивості при поширенні хвиль просторового заряду в кремнії в рамках гідродинамічної моделі за допомогою чисельних розрахунків. Виявилося, що у діапазоні частот, менших за 8ТГц, при кімнатних температурах поправки на теплопровідність є більш суттєвими ніж квантові. На частотах, вищих за 8ТГц, ці поправки стають одного порядку. Отримані результати вказуть на необхідність врахування поправок на теплопровідність при більш точному моделюванні роботи ультрамалих приладів, що використовують хвилі просторового заряду.