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High-frequency properties of systems with drifting electrons and polar optical phonons

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Abstract. An analysis of interaction between drifting electrons and optical phonons in semiconductors is presented. Three physical systems are studied: three-dimensional electron gas (3DEG) in bulk material; two-dimensional electron gas (2DEG) in a quantum well, and two-dimensional electron gas in a quantum well under a metal electrode. The Euler and Poisson equations are used for studying the electron subsystem. Interaction between electrons and polar optical phonons are taken into consideration using a frequency dependence of the dielectric permittivity. As a result, the dispersion equations that describe self-consistent collective oscillations of plasmons and optical phonons are deduced. We found that interaction between electrons and optical phonons leads to instability of the electron subsystem. The considered physical systems are capable to be used as a generator or amplifier of the electromagnetic radiation in the 10 THz frequency range. The effect of instability is suppressed if damping of optical phonons and plasma oscillations is essentially strong.

Keywords: drifting electrons, polar optical phonons, dispersion equation, instability.

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1. Introduction

High-frequency properties of electron gas induced by plasma and optical phonon oscillations in different semiconductor structures were studied in theoretical [1-9] and experimental [10-12] works.

When electrons are accelerated by an electric field in such a manner that their drift velocity exceeds the sound velocity in semiconductor, a large number of acoustic phonons can be emitted coherently. This so-called "Cherenkov acoustoelectrical effect" was predicted and demonstrated in the 1960s in semiconductors [1, 2, 10, 11]. A similar effect for optical phonons was also predicted in bulk materials and experimentally proven in [10] and [11]. Typical frequencies of optical oscillations of the crystal lattice for polar semiconductors are of the order of 10 THz. Thus, that makes such systems interesting for high-frequency applications.

2. Theory

For our purposes, it is sufficient to analyze the high-frequency properties of systems with drifting electrons and polar optical phonons using the simple hydrodynamical model.

Let $n(x,y,t)$, $\vec{v}(x,y,t)$ and $\varphi(x,y,z,t)$ be the volume concentration, velocity of electrons and electrostatic potential, respectively. Then, we can write Euler and continuity equations [3] as follows:

$$\frac{\partial \vec{v}}{\partial t}+\left(\vec{v}\vec{\nabla}\right)\vec{v}+\frac{\vec{v}-\vec{v}_0}{\tau}=-\frac{e}{m^*}\vec{\nabla}\varphi , \quad (1)$$

$$\frac{\partial n}{\partial t}+\mathrm{div}\left(n\vec{v}\right)=0 , \quad (2)$$

where e, m^* are the charge and effective mass of the electron, respectively; $\vec{v}_0$ denotes the stationary drift velocity of electrons. The term $\frac{\vec{v}-\vec{v}_0}{\tau}$ describes scattering of the electrons by crystal defects, τ denotes the relaxation time.

The Poisson equation [4] can be written as

$$\Delta\varphi=\frac{4\pi e}{\kappa}\left(n-n_{3D}\right), \quad (3)$$

where κ and n_{3D} is the dielectric permittivity and stationary bulk density of electrons.

Presence of optical phonons in polar semiconductors leads to dispersion of the dielectric permittivity $\kappa(\omega)$. The dielectric permittivity as a function of frequency can be found using the following method. A relation between dielectric permittivity κ and polarizability α can be written as:

$$\kappa = (1 + 4\pi\alpha). \qquad (4)$$

There are two contributions in the polarizability α: the atomic polarizability as well as the polarizability bound with the dipole momentum, arising due to lattice distortion [13]. Let $\vec{u}^+$ and $\vec{u}^-$ be displacements of two oppositely charged ion sublattices. The respective dipole momentum is:

$$e\vec{W} = e\left(\vec{u}^+ - \vec{u}^-\right). \qquad (5)$$

With the model of harmonic oscillator, the equation for the vector $\vec{W}$ is

$$\ddot{\vec{W}} + \gamma_g \dot{\vec{W}} + \omega_{to}^2 \vec{W} = \frac{e}{m}\vec{E}, \qquad (6)$$

where γ_g is responsible for damping of the optical vibrations, ω_{to} denotes frequency of transverse optical vibrations of the lattice.

Using (4), (5), and (6), we get

$$\kappa(\omega) = \kappa_\infty \frac{\omega_{lo}^2 - \omega^2 - i\gamma_g\omega}{\omega_{to}^2 - \omega^2 - i\gamma_g\omega}, \qquad (7)$$

where $\omega_{lo} = \omega_{to}\sqrt{\frac{\kappa_0}{\kappa_\infty}}$ is the frequency of longitudinal optical vibrations of the crystal lattice; κ_∞ and κ_0 denote the optical and static dielectric constants, respectively. Note that dispersion of optical phonons is ignored in this paper.

As $\omega \to \infty$, we obtain Liddane-Sachs-Teller relation [13]:

$$\frac{\kappa_0}{\kappa_\infty} = \left(\frac{\omega_{lo}}{\omega_{to}}\right)^2. \qquad (8)$$

The interval of frequencies $\omega = [\omega_{to}, \omega_{lo}]$ is called in [13] as *a residual radiation zone* (Reststrahlung).

Using (1), (2), (3), and taking into account (7), we receive a system of the partial differential equations.

We study the referred system of the partial differential equations using the methods of the theory of instability [16, 18]. Namely, we consider an unlimited homogeneous dielectric medium and an electron gas characterized by the certain set of magnitudes U_0 (in this article, this is the equilibrium concentration and drift velocity). At a certain moment $U(\vec{r},t) = U_0 + U'(\vec{r},t)$, where the magnitudes with primes characterize deviations from the respective steady-state values. Assuming sinusoidal variations for all perturbed quantities $U' \propto e^{i\vec{k}\vec{r} - i\omega t}$, where $\vec{k}$ is the wave vector, $\vec{r}$ is the radius-vector; ω and t denote the frequency and time respectively. Thus, we suppose that the perturbation is the wave packet with a limit size, and plane waves are its separate Fourier components. Due propagation, the package "spreads", and its amplitude (in unstable system with $\mathrm{Im}(\omega) > 0$) grows up. At the same time, as it is inherent each wave packet, it will move in space [18]. The main problem of the theory of instability is to study exploration of the package behavior in some fixed region.

According to the theory of instability [16], it is necessary and sufficient be aware of connection between the frequency and wave vector to characterize behavior of the wave packet. Thus, all problem is reduced to determination and investigation of *the dispersion relations*. If the dispersion equation suppose some complex solutions, then this physical system is capable to *amplify* oscillations [16]. That is the properties that make such systems interesting for high-frequency applications.

In the next section, we shall study interaction between drifting electrons and optical phonons in three different physical systems. The main differences among them will be given in the next sections. Using methods of the theory of instability, we shall prove that these physical systems are capable to generate electromagnetic radiation in the 10 THz frequency range.

3. An analysis of the dispersion equations

In this section, we have represented the results without taking into account an electron scattering on the crystal defects (i.e. $\tau \to \infty$). An analysis of scattering contribution to *the increment of instability* (the imaginary part of frequency) will be given in Section 4.

3.1. Interactions between three-dimensional electron gas and optical phonons

Let us assume that 3DEG is in bulk polar semiconductor, and has the unperturbed carrier density n_{3D} and drift velocity v_0. There is also the electrostatic potential $\varphi(x,y,z,t)$ defined everywhere inside the structure.

After substitution of perturbations in the system of partial differential equations, the problem is reduced to solution of a homogeneous system of algebraic equations. Setting the determinant of these equations to zero yields the dispersion relation

$$(\Omega - K)^2 = \Omega_{pl}^2 \frac{\gamma^2 - \Omega^2 - i\Gamma\Omega}{1 - \Omega^2 - i\Gamma\Omega}, \qquad (9)$$

where it is designated: $\Omega = \frac{\omega}{\omega_{lo}}$, $K = \frac{k\nu_0}{\omega_{lo}}$, $\gamma = \frac{\omega_{to}}{\omega_{lo}}$, $\Omega_{pl} = \frac{\omega_{pl}}{\omega_{lo}}$, $\omega_{pl}^2 = \frac{4\pi e^2 n_{3D}}{\kappa_\infty m^*}$. The value ω_{pl} is called as *the plasma frequency*.

The equation (9) is quadratic to wave vector *K*, so it is simple to find two radicals:

$$K_{1,2} = \Omega \pm \Omega_{pl}\sqrt{\frac{\gamma^2 - \Omega^2 - i\Gamma\Omega}{1 - \Omega^2 - i\Gamma\Omega}}\,. \qquad (10)$$

It is obvious that in the certain interval of frequencies the imaginary part of the wave vector becomes nonzero. If $\Gamma \to 0$, then this interval of frequencies coincides with the residual radiation zone.

The dispersion equation (9) is solved numerically, and we find the frequency as a function of the wave vector. The corresponding plots are presented in Fig. 1. It is seen that the function $\Omega(K)$ has a positive imaginary part, which leads to instability. The hatched line displays the Cherenkov criterion ($\Omega < K$ in our labels). According to that criterion, systems, of which wave vectors and frequencies are under the hatched line, are capable to amplify oscillations.

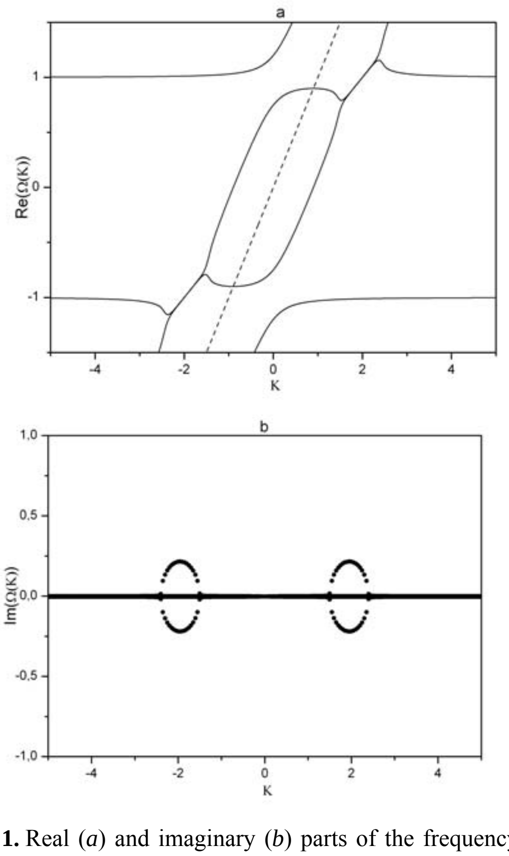

Fig. 1. Real (*a*) and imaginary (*b*) parts of the frequency as a function of the wave vector for 3DEG (at fixed parameters $\Gamma = 0.01$, $\gamma = 0.9$, $\tau \to \infty$ and $\Omega_{pl} = 1$).

Thus, according to common criterion of instability and amplification of oscillations [16], it is possible to state that the effect of amplification/generation of optical oscillations is presented in the considered physical system.

This amplification of optical oscillations by drifting 3DEG has been considered in papers [1] and [2]. Authors used another approaches to solve this problem. They specified a possibility of optical phonons amplification by drift of charge carriers in three-dimensional polar semiconductors.

3.2. Interaction between two-dimensional electron gas and optical phonons

The 2DEG lies in the plane $z = 0$, is infinitely extended parallel to the x axis in both directions, and has an unperturbed two-dimensional carrier density (carriers per unit area) n_0 and drift velocity ν_0. There is also an electrostatic potential $\varphi(x,z,t)$ defined everywhere inside the structure, whereas the density and velocity are confined to the plane $z = 0$ and are functions only of x and t.

Two-dimensional electron gas is studied similarly to 3DEG. There is $(n - n_0)\delta(z)$ instead of $(n - n_{3D})$ in the Poisson equation (3), where $\delta(z)$ is the Dirac delta-function. That is the main mathematical difference among 3D and 2D situations.

Substituting $\nu(x,t)$, $n(x,t)$, $\varphi(x,z,t)$ for

$$\begin{cases} \nu(x,t) = \nu_0 + \nu_1 e^{ikx - i\omega t}, \\ n(x,t) = n_0 + n_1 e^{ikx - i\omega t}, \\ \varphi(x,z,t) = \varphi_1(z)\, e^{ikx - i\omega t} \end{cases} \qquad (11)$$

in the system of partial differential equations, we get

$$\begin{cases} (\omega - k\nu_0)\nu_1 + \frac{e}{m^*} k\varphi\big|_{z=0} = 0, \\ (\omega - k\nu_0) n_1 - kn_0\nu_1 = 0, \\ \frac{d^2\varphi(z)}{dz^2} - k^2\varphi(z) = \frac{4\pi e n_1}{\kappa(\omega)}\,\delta(z). \end{cases} \qquad (12)$$

It is necessary to introduce two boundary conditions to solve the set of equations. The first of them is the requirement of continuity of the potential at the point $z = 0$. The second one describes the field jump at the point $z = 0$. Besides, the potential must decrease as $z \to \infty$. Hence, we can find a potential at the point $z = 0$:

$$\varphi(z)\big|_0 = \frac{2\pi e n_1}{\kappa(\omega)\Phi(k)k}\,. \qquad (13)$$

By definition, put

$$\Phi(k) = \begin{cases} 1, & \mathrm{Re}(k) \ge 0, \\ -1, & \mathrm{Re}(k) < 0, \end{cases} \qquad \Phi(k)\Phi(k) = 1\,. \qquad (14)$$

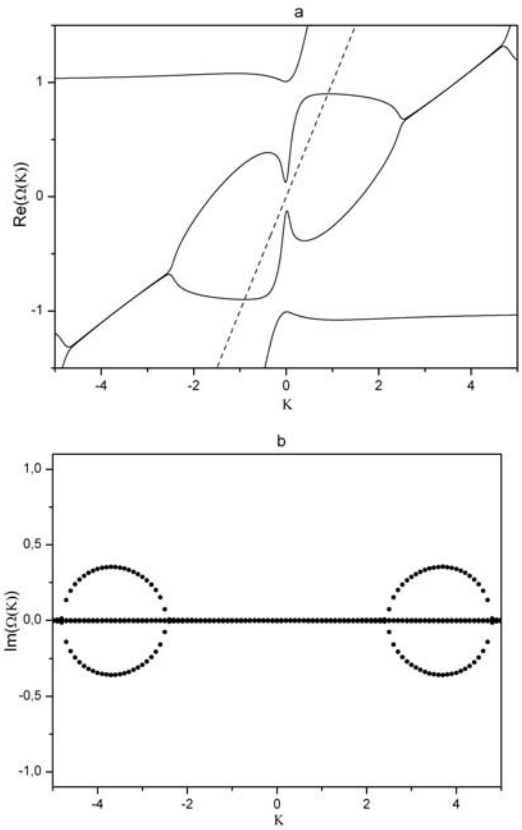

Fig. 2. Real (*a*) and imaginary (*b*) parts of the frequency as a function of the wave vector for 2DEG (at fixed parameters $\Gamma = 0.01$, $\gamma = 0.9$, $\tau\to\infty$ and $\nu = 1$).

Then, the potential is substituted in the first of equations (12). Setting the determinant of the homogeneous system of algebraic equations (12) to zero yields the following dispersion relation:

$$(\Omega - K)^2 = 2\nu \frac{\gamma^2 - \Omega^2 - i\Gamma\Omega}{1 - \Omega^2 - i\Gamma\Omega} \Phi(K) K \, , \qquad (15)$$

where all the magnitudes designated by the same notations as in equation (9), ν denotes the term

$$\frac{\pi e^2 n_0}{\kappa_\infty m^* \nu_0 \omega_{lo}} .$$

The equation (15) is quadratic to the wave vector *K*. Taking (14) into account, it is simple to find four analytical solutions for *K*:

at $\mathrm{Re}(K) \ge 0$

$$K_{1,2} = \Omega + \nu \frac{\gamma^2 - \Omega^2 - i\Gamma\Omega}{1 - \Omega^2 - i\Gamma\Omega} \left(1 \pm \sqrt{1 + \frac{2\Omega}{\nu} \frac{1 - \Omega^2 - i\Gamma\Omega}{\gamma^2 - \Omega^2 - i\Gamma\Omega}} \right) \qquad (16)$$

at $\mathrm{Re}(K) < 0$

$$K_{1,2} = \Omega - \nu \frac{\gamma^2 - \Omega^2 - i\Gamma\Omega}{1 - \Omega^2 - i\Gamma\Omega} \left(1 \pm \sqrt{1 - \frac{2\Omega}{\nu} \frac{1 - \Omega^2 - i\Gamma\Omega}{\gamma^2 - \Omega^2 - i\Gamma\Omega}} \right). \qquad (17)$$

It is possible to show that in the certain interval of frequencies the imaginary part of the wave vector is not equal to zero. Solutions of the dispersion equation are represented in Fig. 2. It is obvious that the function $\Omega(K)$ has the positive imaginary part (instability). The hatched line maps the Cherenkov effect.

3.3. Interaction between two-dimensional electron gas and optical phonons under the metal electrode

Let us assume that 2DEG lies in the plane $z = 0$, is infinitely extended parallel to the *x* axes in both directions, and has the unperturbed two-dimensional carrier density n_0 and drift velocity ν_0. The electrostatic potential $\varphi(x, z, t)$ is defined everywhere inside the structure, whereas the density and velocity are confined to the plane $z = 0$ and are functions only of *x* and *t*. The symbol *h* denotes the distance between the electrode and 2DEG.

High-frequency properties of two-dimensional electron gas under the metal electrode are studied similar to the case with 2DEG (without any electrode). The difference consists in boundary conditions. Now, it is necessary to consider the presence of the metal electrode. The first boundary condition is an equality to zero of the potential at the point $z = h$, which is cased by the equipotential surface of the metal. The second of them is the requirement of continuity of the potential at the point $z = 0$. The third condition is presence of the field jump at the point $z = 0$. In addition, the potential must decrease as $z \to -\infty$. Thus, we can find a potential at the point $z = 0$:

$$\varphi\Big|_{z=0} = \frac{2\pi e}{\kappa(\omega)\Phi(k)k} n_1 \left(1 - e^{-2\Phi(k)kh}\right). \qquad (18)$$

Then, the potential is substituted into the first of equations (12). Setting the determinant of the homogeneous system of algebraic equations (12) to zero yields the following dispersion equation:

$$(\Omega - K)^2 = 4\nu \frac{\gamma^2 - \Omega^2 - i\Gamma\Omega}{1 - \Omega^2 - i\Gamma\Omega} \left(1 - e^{-\Phi(K)KS}\right) \Phi(K) K \, , \qquad (19)$$

where $S = \dfrac{2h\omega_{lo}}{\nu_0}$.

It is possible to recreate the dispersion equation (15) as $h \to \infty$ (as $|KS| >> 1$), because $\left(1 - e^{-\Phi(K)KS}\right) \cong 1$. This can be understood as follows. If the metal electrode is sufficiently far from the transport channel, then the 2DEG influence is not appreciable.

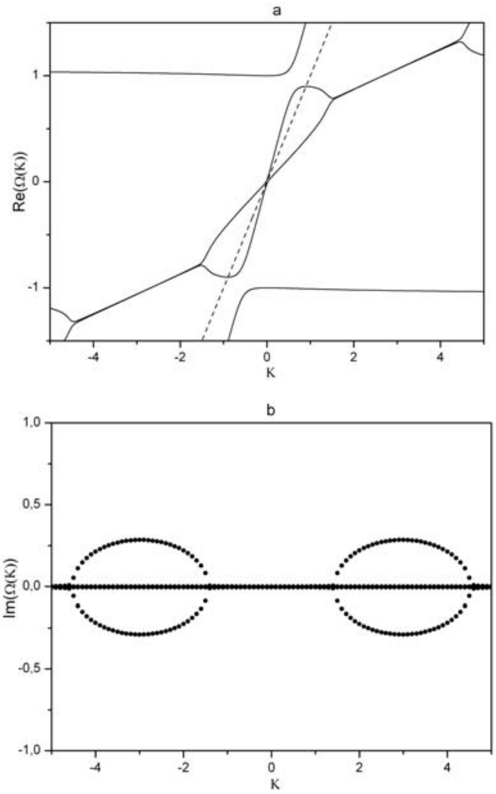

Fig. 3. Real (*a*) and imaginary (*b*) parts of the frequency as a function of the wave vector for 2DEG under the metal electrode (at fixed parameters $\Gamma = 0.01$, $\gamma = 0.9$, $\tau\to\infty$, $S = 0.2$ and $\nu = 1$).

As $|KS| << 1$, we get

$$(\Omega - K)^2 = 4\nu S \frac{\gamma^2 - \Omega^2 - i\Gamma\Omega}{1 - \Omega^2 - i\Gamma\Omega} K^2 . \qquad (20)$$

The dispersion equations (19) and (20) contain complex solutions (the numerical solutions of the equation (20) are represented in Fig. 3), therefore this device is capable to be used as a generator or amplifier of electromagnetic radiation in the 10 THz frequency range. Changing the distance between 2DEG and the electrode, it is possible to manipulate these dispersion curves.

4. A dissipative processes and an increment of instability

An analysis of scattering contribution to *the increment of instability* (an imaginary part of the frequency) has been made for all the cases considered in this paper. It has been shown that dissipative processes influence on dispersion curves and are analogous for all the considered cases. Therefore, it is sufficient to see any of three physical systems. The second of them (2DEG without a metal electrode) is presented in this section.

Tacking scattering on crystal defects into account, we obtain the dispersion equation:

$$(\Omega - K)^2 + iT(\Omega - K) = 2\nu \frac{\gamma^2 - \Omega^2 - i\Gamma\Omega}{1 - \Omega^2 - i\Gamma\Omega} \Phi(K) K , \qquad (21)$$

where $T = \dfrac{1}{\tau\,\omega_{lo}}$. If we put $T = 0$, then the dispersion relation becomes the same as (15).

The numerical solutions of the equation (21) are illustrated in Fig. 4. As we can see in Fig. 4, dissipative processes lead to a shift of the imaginary part of the frequency and/or decreases the increment of instability. For the comparison of cases (a) and (b) it is seen: if $\Gamma = T$, then the imaginary part of the frequency has a shift, but curves do not split.

Thus, changing the parameters γ, ν, Γ, and T reduces to variation of the increment of instability $\mathrm{Im}(\Omega(K))$. In particular, at certain fixed values of these parameters, it is possible to realize the situation shown in Fig. 5a, i.e. maximum of the $\mathrm{Im}(\Omega(K))$ is equal to zero. If $\mathrm{Im}(\Omega(K)) \le 0$, then the effects of amplification and generation of optical vibrations are absent. Therefore, it is necessary to analyze this situation.

At some values of parameters γ, ν, Γ, and T, at the certain point K_0, the peak of the imaginary part of the frequency tends to zero value (as shown in Fig. 5a). If we know K_0 and fix parameters γ and ν, then it is possible to get three curves shown in Fig. 5b. These curves are built at the fixed parameter $\gamma = 0.9$, and have the following indexation. The curve 1 is built at the fixed parameter $\nu = 0.5$; curve 2 is built at fixed $\nu = 1$; curve 3 is built at the fixed $\nu = 1.5$ (the magnitude ν is continuous, so we can build the perpetual amount of these curves). Each of these curves is a geometrical place of points, and these points correspond to critical values of the parameters Γ and T. In addition, each of them is the boundary between the region of the perturbation damping and region corresponding to amplification/generation of optical phonons.

If γ and ν are fixed, then it is necessary to examine only one of displayed curves. If magnitudes Γ and T belong to the critical curve or lie above it, then corresponding perturbation has been damp. Suppose fixed parameters Γ and T are under the curve; then effects of amplification and generation of optical vibrations take place. It is clear that any pair of fixed values Γ and T create the certain point at the plane presented in Fig. 5b. The longer the distance between this point and the critical curve, the stronger contribution of damping effects (in the damping region), and greater increment of instability (in the amplification/generation region). In particular, if $\Gamma = T = 0$ (this indicates that the dissipative processes are absent in the system), then an increment of instability will be the greatest one. On the other hand, the stronger the dissipative processes, the faster perturbation will be damped.

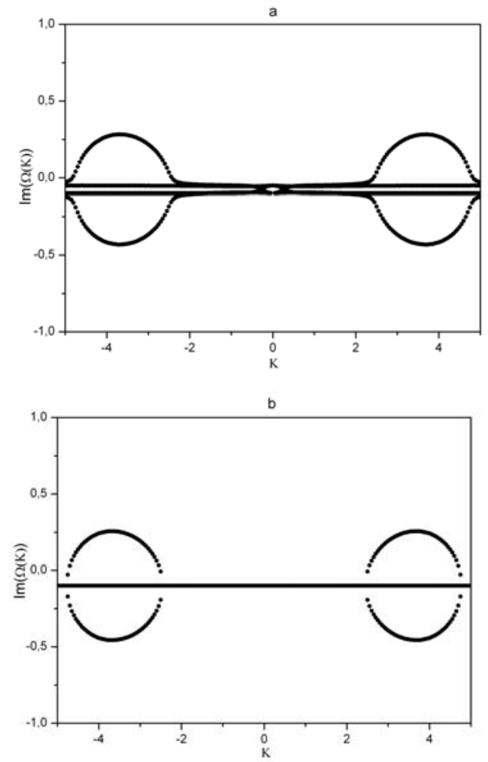

Fig. 4. Increment of instability as a function of the wave vector for 2DEG (at fixed parameters Γ = 0.1, *T* = 0.2 (*a*) and Γ = 0.2, *T* = 0.2 (*b*)).

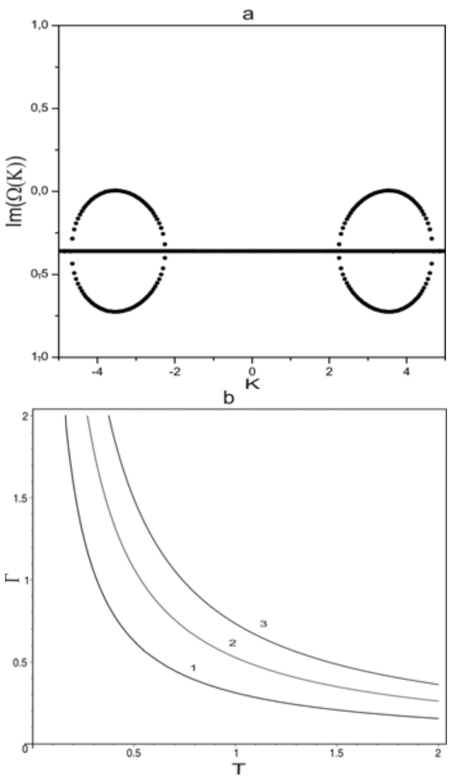

Fig. 5. Increment of instability as a function of the wave vector for 2DEG (at fixed parameters Γ = 0.73, *T* = 0.73 (*a*)). The measure between the amplification/generation of the optical vibrations region and damping of the perturbations region (*b*).

Using Fig. 5b, it is possible to make the following analysis. Even if electron scattering on crystal imperfections are inappreciable $T \to 0$, but damping of optical phonons is essentially strong ($\Gamma >> 1$), then the effects of amplification and generation will be absent. Even if we could neglect the optical phonons damping $\Gamma \to 0$, but there are many imperfections in the crystal, then $\mathrm{Im}(\Omega(K)) < 0$, and this leads to damping of perturbation.

Let values of parameters Γ and *T* create the point at curve 2 in Fig. 5b.

If we increase the density of electrons (increase the parameter ν), then $\mathrm{Im}(\Omega(K)) > 0$, and this leads to instability.

So, it is possible to make conclusions about the possibility of amplification/generation of optical oscillations in the considered physical system by using Fig. 5b.

5. Conclusion

In this paper, we have deduced and studied the dispersion equations that describe self-consistent collective oscillations of plasmons and optical phonons.

Collective interaction between charge carriers and optical vibrations in the crystal lattice leads to reorganization of dispersion curves in residual radiation zone and also depends on dimensions of the system.

Our analysis of the dispersion curves for 3DEG and optical phonons is presented. A convective instability and amplification of optical oscillations by drifting electrons take place in this physical system.

Examination of the dispersion law for 2DEG and optical phonons is performed. Instability and amplification of the optical phonons by drifting electrons take place in this system.

Investigation of the dispersion equation for 2DEG under the metal electrode is presented. An instability and amplifications of optical vibrations of the crystal lattice by drifting electrons take place in this physical system. Changing the distance between 2DEG and electrode gives the possibility to manipulate dispersion curves.

The dissipative processes lead to diminution of the instability increment in all the considered cases. The effect of instability is suppressed if damping of optical phonons and plasma oscillations is essentially strong.

Thus, all the considered physical systems are capable to be used as a generator or amplifier of electromagnetic radiation in the 10 THz frequency range.

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